Activities & Scientific Reports



2025

cecam
Centre Européen de Calcul Atomique et Moléculaire

SINCE 1969

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INTRODUCTION

In 2025, CECAM once again brought its community together around current leading questions of computational science. The Flagship program comprised 76 events hosted at the Headquarters (HQ) and across the network of Nodes, representing 82% of all submitted proposals, indicating a competitive and engaged community (Fig. 1).

Scientifically, the program combined state-of-the art and new topics; while core areas like computational materials science, computational life sciences, and quantum/classical simulations still dominated, machine learning was increasingly integrated across all disciplines.
New priorities also emerged, particularly in quantum computing (e.g., joint workshop with IBM and EPFL) and high-performance computing (HPC), where focus on code optimization and architecture adaptation is an increasing concern of the community.

The Flaghship program is a shared achievement of the HQ and the Nodes. The CECAM HQ at EPFL hosted 23 events, 21 workshops and 2 schools, accounting for 30% of the completed program (25% of total submissions). The 21 Nodes accommodated 53 events, comprising 32 workshops and 21 schools (*Fig. 1*), bringing CECAM close to local research communities and giving the network a leading role in training young researchers.

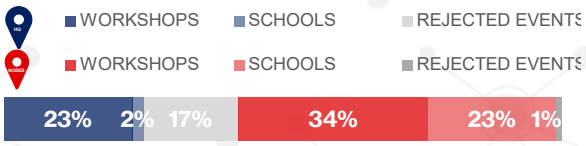


Figure 1: CECAM Flagship program 2025. Acceptance rate for Workshops and Schools in the HQ and the Nodes.

At the heart of CECAM's mission is the conviction that science advances when people meet in a conducive environment. On-site events represent 74% of CECAM's total activities at the HQ and the Nodes. Hybrid options extend our reach worldwide, but it is the in-person format that sparks spontaneous discussion and turns encounters into lasting collaborations (*Fig. 2*).

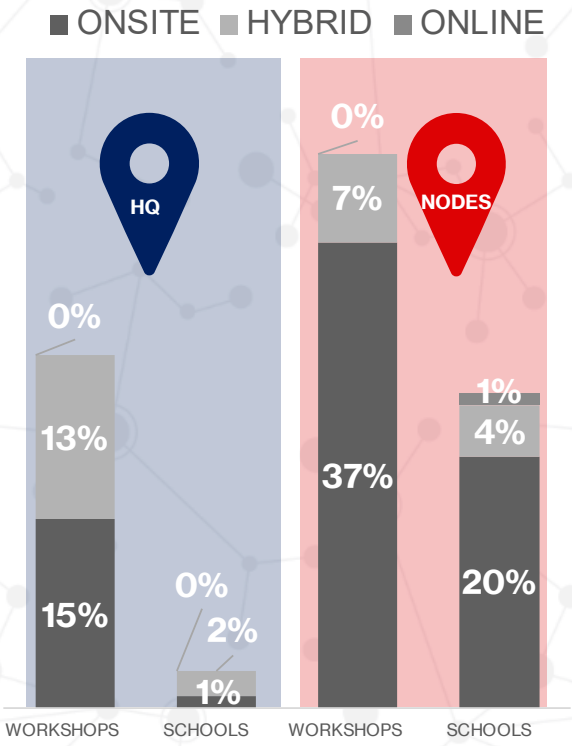


Figure 2: CECAM Flagship program 2025. On-site, Hybrid and Online part of Workshop and Schools in the HQ and the Nodes.

Participants feedback confirms that meeting in person significantly enriches scientific exchange, eases networking, and makes it easier to plan future collaborations.

Attendance figures reinforce this message: on-site participation reached 78% across all events, 64% at HQ events and 88% at Node events (*Fig. 3*). The particularly strong in-person presence at the Nodes is indicative of the more local character of their audiences.

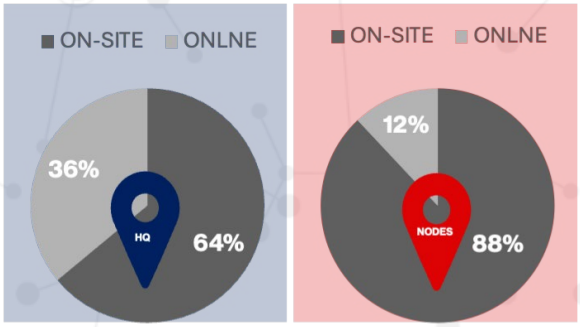


Figure 3: CECAM Flagship program 2025. On-site and Online participation to events in the HQ and the Nodes respectively.

At the same time, virtual attendance remains a valued complement, lowering the program's environmental impact and opening CECAM's events to those who could not otherwise attend. This inclusive role is visible in the data: about 7% of CECAM's online participants are from emerging communities. The breakdown for HQ and Nodes is detailed below (*Tab. 1*).

	HQ	NODES	ON SITE	ONLINE
DEVELOPED COUNTRIES	25%	46%	10%	4%
EMERGING COMMUNITIES	1%	6%	4%	3%

Table 1: CECAM Flagship program 2025. Developed countries and Emerging communities' participation to On-site and Online events in the HQ and the Nodes.

CECAM is, as always, strongly community driven. The 2025 events were shaped by 383 scientists across 31 countries, 120 organizers for HQ events and 263 for Node events, who together welcomed 3,958 participants: 41% at the HQ and 59% at the Nodes.

An open community is also a balanced one. The gender ratio is comparable between HQ and Node events, for both organizers and attendees. Female participation at CECAM remains stable below 30%, a consistent baseline over time (*Fig. 4*) from which further progress can be built. In addition to current actions, CECAM is finalizing its Diversity and Inclusivity Plan to mitigate remaining hindering factors that prevent full and equal participation of female and other minorities to its program.

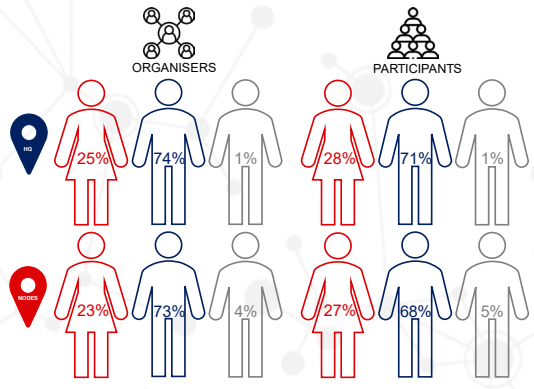


Figure 4: CECAM Flagship program 2025. Gender distribution among Organizers and Participants at HQ and Node events.

Beyond the Flagship program, in 2025 the HQ continued to propose to the community conversations on cultural and strategic topics.

The *Mary Ann Mansigh conversation series* comprised two meetings, both looking at how science connects with the wider world.

The first, "*Science and diplomacy*", highlighted how science diplomacy strengthens international relations and fosters stability through scientific exchange, computational research and joint infrastructure management. Such collaborative efforts promote global security and sustainable development, even in conflict-prone areas.

The second, "*Telling scientific stories – from science journalism to comics and visual storytelling*", explored how researchers can broaden their impact beyond academic settings through news media, science-themed comics and other communication tools, with a focus on simplifying complex data, overcoming communication challenges and fostering public trust in science.

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The *Classics in Molecular and Materials Modelling* series, which revisits the foundations of our field, featured a lecture on "*Quantum Monte Carlo methods in the continuum*".

The lecture traced the seven-decade evolution of QMC methods and their role in calculating precise microscopic properties in condensed matter physics, before turning to the present: how QMC now provides accurate data to train machine learning potentials, enabling the modeling of large-scale phase diagrams, with a specific focus on new findings regarding dense hydrogen.

As part of its expanding outreach strategy, CECAM also supported four MDDB webinars in 2025. The Molecular Dynamics Data Bank (MDDB) is a European-scale biosimulation repository that unifies and organizes data from Molecular Dynamics simulations, building on decades of cutting-edge computing power. This collaborative project brings together leading European institutions to transform data handling and accelerate open science.

The webinar series explored the importance of data sharing alongside its technical and methodological challenges, questions that concern the whole community.

These events are available on the CECAM Lhumos space.

www.lhumos.org

Taken together, the 2025 activities reaffirm CECAM's role as a focal point for the global computational materials and molecular modeling community: a place where scientists meet, ideas are tested and collaborations take shape. Through its Headquarters and Nodes, CECAM continues to bridge disciplines and borders, train new generations of researchers, and drive the next wave of scientific progress.

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Molsim-2025



Location: CECAM-NL, The Netherlands

Webpage : Event webpage

Dates: Jan 6, 2025 - Jan 17, 2025

1. What were the major topics presented in the School?

The MolSim-2025 school took place over a period of two weeks in January 2025. It offered a program focusing on basic and advanced molecular simulation methods. The program has an integrated and balanced structure of lectures (10 full morning plenary sessions) and hands-on exercises (9 full afternoon sessions, in two groups).
The school is organized on a yearly basis, and targets PhD candidates and postdoctoral researchers who want to enhance their understanding and skills of employing molecular simulation to study topics in physics, chemistry or biology. The setting - learning and working together for a more extended period - provides the participants ample time to interact with their peers (also socially), allowing them to build and/or enhance their scientific network.
The structure of the school's content was as follows:
Basic theory and methods: statistical thermodynamics, Monte Carlo, molecular dynamics
Advanced topics (theory and methods): free energy, enhanced sampling, rare events, machine learning
Topical items: biological systems, (nanoporous) materials, soft matter, coarse graining
Group activities: poster session, common daily meals/breaks, outing and school's dinner (weekend)

2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

Given the type of the event, providing a detailed report on items (questions/remarks/...) that were brought up would be outside of the scope of this report.
Participants are made aware (from the start) that "live interaction" is an important aspect of the lecture and lab sessions. The participant group was in this respect very active while in session. "Out of session" moments (breaks/lunch time) were typically fully used (to continue) discussions with the lecturer.
The lab-course session (carrying out calculations on participants laptops using prepared problems with minor coding / proper parameter setting) is by nature very interactive. It is carried out in a sectioned (3-5) setting, consisting of a "plenary introduction / individual work on a specific problem (in pairs) / plenary guide-to-answers". A (rather natural) aspect is that fully completing a problem is not always reached, as not all participants are on equal level. The provided guide-to-answers allows for post-school completion of most of the problems.

On the practical side, having the participants' laptops well-configured is essential. Regarding this, the participants are provided detailed instructions a few weeks prior to the school's start. Remaining issues are resolved during the first lab course session.
In this edition of the school we introduced a newly developed labcourse environment, providing Python notebooks and dedicated visualation software in a single "molsim"-package, available for all major computing platforms (mac, linux, windows). Also the content was adapted to optimally match the current lectures content, and provide some connection with present day research in the field of molecular simulation. The newly designed computing environment was accompanied by (almost from scratch) rewritten lab-course manual.
As the "molsim"-package is free and transferable it allows the participants to continue working, or refer back to what was done during the school, at a later stage.
Questions and remarks brought forward during the lecture/labcourse sessions were on a level and intensity typical for postgraduate classes, ranging from the basic to the (very) advanced level. The range of the level indicates that variation in knowledge/understanding/skills among the group is substantial. The school is well aware of this and the content of lectures and lab-course is built such that it serves the whole group, as much as possible.

3. What was the take-home message for the participants?

- use acquired understanding, knowledge and skills in the current (and future) research
- spend some time to further understand the lecture topics
- look at the non-completed/non-covered problems in lab-course manual
- keep interactions and contacts alive
- notify potential future participants of a next edition of the MolSim school

4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

The hard-copy and digital (compchem.nl/molsim) trace of the school:
- lecture slides (digital)
- lab course manual (paper & digital)
- lab course computing environment (digital package)
- lab course guide to solutions (digital)

5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

Participants
Here we aim for an evenly distributed diversity (match of research interest with school's focus / country of residence / research group / gender / underrepresented groups / nationality). This is reasonably well achieved.
Gender balance (F|M) applicants (109) /participants (75) was 0.32|0.68 / 0.44|0.56. Note that almost all of the eligible female applicants were admitted.

Teaching
Although aimed for, the composition of the team is not truly evenly diverse, though some broadness in the distribution.
lecturers: 4 countries / mixed seniority / 2 females.
labcourse team: countries/reasonably mixed gender.

6. Participant list

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International workshop on computational physics and materials science: Total Energy and Force Methods



Location: CECAM-IT-SISSA, Italy

Webpage : Event webpage

Dates: Jan 8, 2025 - Jan 10, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop explored several key themes, including the development of novel density functionals and extensions to standard DFT. Researchers presented new approaches that can accurately model complex electronic excitations while maintaining computational efficiency, even for molecular dynamics simulations.

Another major area of focus was machine learning in materials modeling. Presenters demonstrated how AI can be used to develop more accurate interatomic potentials, neural-network quantum states, and other models that can capture intricate electronic effects. By combining physics-based models with data-driven techniques, researchers can explore larger configuration spaces and accelerate materials discovery.

The workshop also addressed strongly correlated systems and excited-state phenomena, including diagrammatic DMFT extensions, dynamical Hubbard functionals, and nonadiabatic dynamics. These methods account for both local and non-local interactions, enabling studies of magnetism and ultrafast processes that were previously out of reach with simpler mean-field approaches.

Large-scale and time-dependent techniques were another focus area, including finite-element DFT for larger systems and the exact factorization of the electron-nuclear wavefunction for ultrafast dynamics. New theories allow modeling carrier, phonon, and exciton behavior beyond traditional Boltzmann equations.

Sessions on electron-phonon coupling, materials design, and quantum computing platforms covered both foundational advances and practical applications. Researchers presented innovative and accurate ways to push the accuracy and scope of first-principles simulations, including anisotropic Migdal-Eliashberg theory for superconductivity and spin defects in quantum materials.

The adoption of AI-driven emulators, alongside progress in electronic stopping and optical activity, signals a shift toward multi-scale, interdisciplinary research. Overall, these developments enhance the accuracy, computational efficiency, and range of phenomena that can be reliably modeled. The synergy of quantum-mechanical rigor, ML acceleration, and new theoretical methods mark a significant leap forward, ensuring that first-principles simulations continue to offer transformative insights across physics, chemistry, and materials science.

2. What were the primary outcomes of this workshop, including limitations and open questions?

The workshop showcased significant advancements in computational methods for electronic structure, spanning a wide range of systems and phenomena, including correlated materials, particle-matter interactions, and time-dependent processes. Despite this progress, key challenges were also highlighted. A notable outcome was the demonstration that advanced Density Functional Theory (DFT) functionals can accurately predict properties such as optical excitations in increasingly complex systems.
However, it became clear that no single method can effectively address every system or property, and researchers must often tailor their approaches by combining different levels of theory to obtain robust results. This underscores the limitations of existing techniques, which, although powerful, require careful consideration.
Another major focus of the workshop was the growing importance of machine learning (ML) in materials science, with applications ranging from ML-driven force fields to neural-network quantum states for many-body problems. These developments highlight the potential of data-driven frameworks to accelerate materials discovery and reduce computational costs. Nevertheless, participants emphasized the need for rigorous validation, particularly when extrapolating beyond known training data. Ensuring that models accurately predict unseen phenomena remains a significant challenge, requiring deeper theoretical insights and close comparisons with physics-based simulations and experiments.
The workshop also highlighted the effectiveness of well-established or emerging ab initio methods in providing accurate in-silico characterization and reliable predictions for novel materials, such as semiconductors, and properties like optics. Furthermore, multiple techniques are now capable of addressing more complex systems, strongly correlated materials, and time-dependent phenomena with growing accuracy and efficiency, substantially broadening the scope of what can be simulated from first principles.
Interestingly, the near-term impact of quantum hardware on electronic structure simulations appears to be limited, and classical high-performance computing is likely to remain the primary workhorse in the field for some time. Overall, the workshop underscored the significant progress made by the electronic structure community in developing new methodologies and applying them to real-world materials, thereby enhancing the accuracy and efficiency of computational approaches while expanding both the complexity of systems modeled and the range of phenomena studied.
To overcome remaining limitations and drive further innovations in fundamental science and technology, continued investment in scientific software is essential, along with comprehensive benchmarking, validation, and verification. By doing so, researchers can ensure that computational methods continue to advance and provide reliable predictions, ultimately accelerating materials discovery and breakthroughs in various fields.

3. What was the take-home message for the participants?

Advanced physics-based and data-driven methods have significantly enhanced electronic structure calculations, extending ab initio simulations. Their expanding impact on science, technology, and societal needs (e.g., sustainability) demands rigorous validation – especially for ML – and better applicability and efficiency of emerging approaches.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

The workshop's outcomes have significant potential for real-world impact. By advancing ab initio methods and machine learning approaches, researchers can better understand, discover, and design new materials that can lead to breakthroughs in sustainable energy solutions, such as more efficient solar cells and batteries, as well as improved catalysts for chemical processes. These advancements can also accelerate industrial development by enabling the prediction and optimization of new compounds before they are synthesized and tested.
The workshop showcased how ML, time-dependent, and many-body formalisms can tackle pressing challenges in areas like photonics, superconductivity, radiation damage, and quantum information technologies. The resulting insights can lead to improvements in next-generation devices, including high-performance transistors, sensors, and radiation shields, which can drive growth in critical industries.
The workshop's relevance to industry was evident from the participation of representatives from a diverse range of companies and R&D labs, including Microsoft. This broad interest underscores the potential for the workshop's research to have far-reaching impacts beyond academia.
Ultimately, the workshop's focus on pushing the boundaries of theoretical and methodological innovation, enhancing computational efficiency, and improving predictive power reflects a concerted effort to translate cutting-edge research into meaningful benefits for society. By prioritizing sustainability, energy, and emerging technologies, the workshop aims to drive progress in areas that can have a significant impact on our daily lives.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

While the workshop has not yet yielded tangible outcomes in the form of publications, our experience with past workshops suggests that this is only a matter of time. Historically, these events have consistently led to a significant number of high-impact publications, and we anticipate that this workshop will be no exception.
In addition to forthcoming publications, the workshop has already sparked new collaborations among participants, which are expected to lead to exciting research projects and proposals in the near future. The exchange of ideas and expertise during the workshop has fostered a sense of community and cooperation, laying the groundwork for joint submissions to funding agencies and other collaborative endeavors.
Furthermore, the workshop's focus on advancing ab initio methods and machine learning approaches has also led to plans for developing new software tools and codes. Researchers are already discussing ways to implement and share their newly developed methodologies, which will not only accelerate progress in their respective fields but also facilitate broader adoption of these innovative techniques.
In summary, while the tangible outcomes of the workshop may not be immediately apparent, we are confident that the event has set the stage for a wide range of productive collaborations, publications, and software developments in the months and years to come. The workshop's emphasis on pushing the boundaries of theoretical and methodological innovation, combined with its strong industry participation and focus on societal impact, ensures that its outcomes will have far-reaching consequences for both academia and industry.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

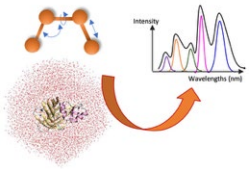
The workshop was designed with inclusivity in mind, recognizing how diversity fosters vibrant idea exchange. We prioritized sponsorship for early-career researchers, enabling them to learn from established experts and share fresh perspectives. By actively inviting participants and speakers from 47 nations – such as Ghana, Nigeria, Ethiopia, Bangladesh, and Cuba – we achieved significant geographical diversity. We also recorded presentations to extend our reach. Regarding gender representation, we aimed for balance, resulting in approximately one-third female speakers and two-thirds male speakers, with overall attendance split 79% men and 21% women. Though not perfect, these figures show progress and set a precedent for greater inclusivity in the future. We acknowledge there is more to do on accessibility, having not provided specific accommodations for participants with disabilities. Nonetheless, we hope future events build on our efforts to ensure a welcoming environment for all.

7. Organiser list

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Advanced force fields in multiscale approaches to computational spectroscopy

Location : CECAM-FR-MOSER, France



Webpage : Event webpage

Dates: Jan 13, 2025 - Jan 15, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The major topics discussed at the event revolved around the challenges of modeling spectra, particularly infrared (IR) vibrational spectroscopy, including 2DIR, vibrational circular dichroism (VCD) spectroscopy, and sum frequency generation (SFG) spectroscopy. Additionally, discussions covered UV-visible spectroscopy for electronic transitions, including pump-probe spectroscopy, in the context of complex systems. The challenge lies not only in determining band positions but also in accurately modeling band shapes.

To achieve this, it is crucial to account for environmental factors and interactions with solvents, macromolecules, interfaces, or surfaces that influence the studied molecule. Classical molecular dynamics simulations with force fields are essential for system sampling. Presentations explored the methodology behind force field generation, addressing challenges, difficulties, proposed solutions, and the integration of machine learning and automation.

The workshop highlighted common challenges in spectrum modeling across different scales (electronic and vibrational). While existing solutions, including automation and machine learning tools, are already available, chemists remain essential for validating the physical and chemical relevance of models and parameters.

2. What were the primary outcomes of this workshop, including limitations and open questions?

The first outcome was the meeting of the three communities: modelers of IR spectra, UV-visible spectra and machine learning developers. It shows how these three communities have common challenges. The workshop gave the opportunity to an open discussion in smaller groups with the PhD-postdocs with the invited lecturers about the challenge of our community.

It helped to raise the questions that have to be resolved in the near future:

Sampling the system: how to make sure that we have enough conformations for having the correct dynamic behavior of the system? How to choose the relevant coordinates to sample?

The use of machine learning potential: how to keep the physical/chemical meaning, how to choose the good descriptors to represent the molecules? How to trust the training data of machine learning?

Transferring of the knowledge: how to train the next generation? How to help choosing between the available methods? How to make the data and models more available? How to give information on the limitations of the methods?
Pushing the frontiers: How to simulate larger systems, with less computer time and less human time?

3. What was the take-home message for the participants?

The community of developers and users of force fields for the simulation of spectra (IR, UV-visible) exists. The machine learning is a nice tool to use but there is still need of human knowledge and intelligence to be able to overcome the difficulties of dealing with such complex challenges.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

Spectroscopy (IR as well as UV-visible) is a powerful tool to characterize chemical processes, but in-depth interpretation of experimental spectra generally requires comparison with atomic-scale simulations. The improvement of spectroscopic modeling methods can therefore potentially find applications in various areas. In particular, we have discussed ways to secure funding from pharmaceutical companies to support our community. It has been concluded that we should improve our communication with the industry, even if our developments are still at an early stage. Simulations can help save time – and therefore money.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

No publication directly from the workshop. We hope that there will be new collaborations. Many younger participants have asked for a summer school on the subject. Software packages like Tinker HP, JOYCE, PROTACS... are already in development, with some of the leading developers among the participants of the workshop, who presented the capabilities of the software, for the other communities and the younger participants.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

We have paid attention to the gender balance.
The organization community was composed of 3 women and one man (for a community that is much larger masculine).
The invited researcher were 11 men and 5 women (68% men and 31% women). The participants were 60% men and 40% women.
We gave the opportunity of 3 PhD students/postdoc to present their work with an oral presentation and 12 with a poster presentation. Participants were coming 25 from France

(the organization country), 20 from the rest of Europe (Switzerland, Sweden, Spain, Belgium, Italy, Germany, Czech Republic, +UK), and 2 from USA, 2 from India, 2 from Qatar, 1 from Taiwan.
The workshop has supported the attendance of PhD students by offering them lodging or payment of travel expenses to facilitate their access to the workshop.

7. Participant list

Organisers
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Duboué Dijon, Elise
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Computational methods for enzyme engineering

Location: Politecnico di Milano, Italy

Webpage : Event webpage

Dates: Jan 27, 2025 - Jan 31, 2025

1. What were the major topics presented in the School?

The workshop, titled "Computational Methods for Enzyme Engineering," took place from January 27th to 31st, 2025, at Politecnico di Milano in Lecco, Italy. This interactive workshop provided participants with essential theoretical knowledge in various areas of enzyme engineering, complemented by hands-on experience with several software tools. The workshop covered a comprehensive range of topics integral to computational enzyme engineering. The curriculum included in-depth sessions on molecular modeling techniques, such as homology modeling and molecular dynamics simulations, which are crucial for predicting and analyzing enzyme behavior at the molecular level.
A significant focus was placed on computational design strategies. These strategies are essential for tailoring enzyme properties to specific industrial applications. The workshop also delved into the application of bioinformatics tools for enzyme mining and the identification of novel enzymatic functions, highlighting the importance of data-driven approaches in modern enzyme engineering.
Practical sessions provided participants with hands-on experience in using state-of-the-art software tools for enzyme engineering and modelling. These sessions were designed to reinforce theoretical knowledge and enhance practical skills, ensuring that attendees could apply computational methods effectively in their research.

2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

Throughout the workshop, several limitations and open questions in the field of computational enzyme engineering were identified. One prominent challenge discussed was the accuracy of current machine learning models in predicting enzyme behavior. While molecular modeling techniques have advanced significantly, there remains a gap between in silico predictions and experimental outcomes, underscoring the need for improved algorithms and validation methods.
Another limitation highlighted was the computational cost associated with high-fidelity simulations. Detailed molecular dynamics simulations, while informative, require substantial computational resources, which can be a barrier for widespread adoption, especially in resource-limited settings. This raises questions about the accessibility of these tools and the need for developing more efficient computational methods.
The integration of computational and experimental approaches also emerged as a topic of discussion. Participants noted the challenges in effectively combining in silico predictions with laboratory experiments to achieve desired enzyme modifications. This includes issues related to the scalability of computational predictions to real-world applications and the translation of theoretical designs into functional enzymes.

Open questions were raised regarding the exploration of enzyme functions beyond natural capabilities. Specifically, how can computational methods be leveraged to design enzymes with novel functions that do not exist in nature? This question touches on the broader challenge of expanding the catalytic repertoire of enzymes through computational design, which remains an active area of research.

3. What was the take-home message for the participants?

Participants left the workshop with a reinforced understanding of the critical role computational methods play in enzyme engineering. They recognized the importance of integrating theoretical knowledge with practical skills to effectively design and optimize enzymes for various applications. The workshop emphasized the need for continuous learning and adaptation to emerging tools and techniques in this rapidly evolving field.

4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

The workshop provided several tangible resources to support participants' ongoing learning:

- Comprehensive lecture notes detailing theoretical concepts and practical applications.
- A curated list of recommended readings.
- An extensive list of online resources for further study in computational enzyme engineering.

5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The organizers implemented several measures to ensure inclusivity across various dimensions:

- **Gender Diversity.** The registration was gender-blind on a first-come, first -served basis. The participation was well balanced with 55% male participants and 45% female participants.
- **Geographical Representation:** The workshop was advertised on several channels and social media and as a result attracted participants from 17 different countries.
- **Career Stage:** The event was open to individuals at various career stages, from Master's students and early-career researchers to established professionals, encouraging knowledge exchange across experience levels. The majority of participants were PhD students (42%) and postdocs (22%).
- **Accessibility:** The venue was selected for its accessibility features to accommodate participants with disabilities.

6. Organiser list

Organisers
Gautieri, Alfonso
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Parisini, Emilio
Latvian Institute of Organic Synthesis, Latvia
Pavlidis, Ioannis
University of Crete, Greece
Rebros, Martin
Slovak University of Technology, Slovakia

Greening AI with Software Engineering



Location: CECAM-HQ EPFL, Lausanne, Switzerland

Webpage : Event webpage

Dates: Feb 3, 2025 - Feb 7, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop brought together 29 researchers and practitioners from software engineering (SE), AI/ML, systems and education to examine how SE can reduce the environmental footprint of AI-enabled systems. Through keynotes, flash talks and rotating co-creation sessions, participants converged on five focus areas.

(1) Energy assessment and standardisation: measurement tools, granularities and reporting practices are fragmented. Participants discussed multi-granular methodologies, from system-wide reporting to fine-grained measurement, and a meta-methodology or public catalogue of assessment methods to help practitioners choose the right approach for their context.

(2) Evaluation and benchmarking: extending established suites (e.g., MLPerf, Hugging Face leaderboards) with standardised energy and carbon metrics, evaluated alongside accuracy and latency, amortising training costs over inference, and normalising metrics across heterogeneous hardware

(3) Architecture and lifecycle: moving beyond single-model optimisation to system-level design, treating AI models as architectural components, with green tactics, runtime self-adaptation, observability and traceability of energy-relevant decisions across MLOps pipelines.

(4) Empirical methods and reproducibility: inconsistent study designs and metrics prevent evidence from accumulating; participants proposed a taxonomy of direct, proxy and composite metrics with community-driven curation of measurement practices.

(5) Education and awareness: embedding sustainability into SE and AI curricula, including mandatory courses, and addressing prerequisites, tooling and cognitive load. The workshop advanced the state of the art by consolidating a fragmented field into a shared vocabulary and structured research agenda, and by positioning SE, with its system-level, lifecycle and empirical traditions, as a key contributor to Green AI beyond model-level efficiency.

2. What were the primary outcomes of this workshop, including limitations and open questions?

The primary outcome is a research agenda for environmentally sustainable AI rooted in SE, co-written by organisers and participants and published in ACM SIGSOFT Software Engineering Notes. Beyond the five focus areas, the discussions revealed three cross-cutting themes: (i) standardisation of measurement, benchmarking and reporting, without which results across research, industry and policy remain incomparable; (ii) metrics, since sustainability cannot be captured by a single number and trade-offs between energy, accuracy, latency and explainability need well-defined, context-sensitive yet comparable metrics; and (iii) holistic and longitudinal thinking, assessing systems across their full lifecycle and over time rather than optimising components in isolation.

Concrete directions include multi-granular, interoperable assessment methodologies; energy-aware extensions to benchmarks; lifecycle-aware metrics such as amortised training cost per inference; architectural tactics and runtime adaptation for green AI systems; a metric taxonomy with community oversight; and teaching approaches for sustainability in SE and AI.

Limitations and open questions: the agenda is conceptual, not a finished blueprint. Open questions include how to normalise energy metrics across hardware when FLOPs are a poor proxy; how to explain and reproduce the energy behaviour of non-deterministic ML models; how to keep methodologies valid as AI evolves; who is accountable for sustainability across the MLOps pipeline (infrastructure providers, architects, AI developers or software engineers); how to balance standardisation with openness to new metrics; how to account for rebound effects such as the Jevons paradox; and how to build stable teaching material in a fast-moving, largely experimental field. Social-science and policy perspectives, part of the original ambition, were only partly covered and remain a gap for future editions.

3. What was the take-home message for the participants?

Sustainable AI is not only a model-efficiency problem; it is a system-wide software engineering concern. Progress depends on shared, standardised ways to measure and report energy and carbon, on metrics that expose trade-offs rather than hide them, and on reasoning across the whole lifecycle and over time. Software engineering is well placed to lead this, as a coordinated, interdisciplinary community effort.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

Yes. AI is being deployed at unprecedented scale, and its energy use, carbon emissions and demand on data-centre infrastructure are growing fast. Much of this impact is decided not only by model researchers but by the software engineers who select, integrate, deploy and operate AI-enabled systems every day. By giving these practitioners methods, metrics and design practices to measure and reduce energy consumption, the workshop outcomes can directly lower the environmental footprint of digital services used by society at large.

Standardised, comparable energy and carbon reporting also supports transparency for citizens, organisations and regulators. It can inform compliance with emerging

requirements such as the EU AI Act and CSRD sustainability reporting, and help public and private organisations make informed procurement decisions, e.g., choosing a model that is good enough rather than the largest one. Energy-efficient AI also lowers operational costs, making AI more accessible to SMEs, public institutions and regions with limited computing resources.

The education outcomes aim to prepare the next generation of engineers to treat sustainability as a core quality attribute, spreading awareness beyond the research community. Finally, the emphasis on holistic thinking and rebound effects (Jevons paradox) guards against naive efficiency claims and supports a more honest public debate about the real environmental cost of AI.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

We know that many participants have collaborated beyond this workshop but we cannot objectively say the collaboration started with the workshop. Our most objective data point is the publication submitted a few months after the event that brought most participants together in the same thread beyond the workshop:

- "Greening AI-enabled Systems with Software Engineering: A Research Agenda for Environmentally Sustainable AI Practices", co-authored by the 5 organisers and 20 participants from 11 countries, ACM SIGSOFT Software Engineering Notes (preprint: arXiv:2506.01774).

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The organising team was balanced in gender (2 women, 3 men) and spanned institutions in Denmark, the Netherlands, Spain and the UAE. Invitations deliberately mixed career stages: participants ranged from students and PhD candidates to postdocs, early-career and senior professors, alongside applied-research and industry practitioners. Participants came from institutions in 11 countries across Europe, the Middle East and Asia, and roughly a third of the report's co-authors are women. Besides the planned program, any participant could schedule an unplanned lightning talk during the week, giving everyone, especially junior researchers, a chance to present their work and stand out. The co-creation format (individual sticky-note input, rotating small groups, writing teams) gave every participant an equal voice, and all were invited to co-author the resulting report.

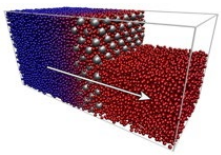
7. Participant list

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Anwar, Hina - University of Tartu, Estonia
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Flowing matter in porous media



Location: Freie Universität Berlin, Germany

Webpage : Event webpage

Dates: Feb 24, 2025 - Feb 27, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The main topics covered during the event were fluid flows in single nano- and meso-pores, as well as in more complex, structured and disordered environments. Flows for a wide range of fluids were discussed: from simple molecular fluids and their mixtures, through complex fluids such as passive and active colloids, to biological fluids. Each topic can contribute to advancing the state of the art in different ways. The topics "Nanofluidic Flows", "Unsteady Flows in Microfluidics", "Tortuous Flows in Random Media" and "Flows in Energetic Materials" can contribute to the advancement of the state of the art through new technologies and materials, such as, for example, new synthetic and multi-scale porous materials for filtration, seawater desalination or as electrode materials in supercapacitor applications, through engineering the phononic spectra of materials to improve flow performance in industrially relevant nanofluidic channels and membranes, for the sustainable extraction of fossil fuels from shales, or for various nanofluidic and ionotronic applications. On the other hand the topics "Microscopic Theory of Confined Liquids", "Density Functional Theory in a State of Flux", "Multi-phase Flows and Mixtures", "Active Colloidal Flows", and "Active Flows under Confinement" contribute to advancing the state of the art through theoretical, experimental and computational advancements , such as development of mode coupling theory for colloidal fluids in slits and random environments or of modelling flows of active fluids in porous media, in micro-channel networks and in patterned environments that improve our understanding of these systems and allow for more accurate predictions. The topic "Self-assembly under Flow " contributes to advancing the state of the art through new applications that could be potentially useful in medical and biochemical applications.

2. What were the primary outcomes of this workshop, including limitations and open questions?

The workshop allowed participants to deepen their knowledge of fluid flows in porous materials at various scales – from the macroscale to the nanoscale.
The pore surface (atomic roughness, grafting heterogeneities, surface charge) was shown to control liquid friction, slip, and intrusion/extrusion, while confinement and disorder can lead to localisation, depinning, and clogging. Flow instabilities can be harnessed for mixing and self-assembly. On the methodological side, non-equilibrium molecular dynamics (NEMD) simulations driven at the boundaries by pressure or concentration gradients have progressed rapidly and are available for research. However, simulations of dense liquids in realistic, also irregular pores remain costly and can depend on the driving protocol.

There is notable progress in classical density functional theory employing machine-learned density functionals, which also extends to non-equilibrium fluids. However, the application to more complex geometries is computationally demanding and prompts for further development on both the mathematical and algorithmic sides. Mode-coupling theory was shown to now cover confined fluids and random energy landscapes, and a statistical mechanics of two-phase flow is emerging. Its extension to flowing states under confinement is still in its beginning. Overall, a consistent up-scaling of nanoscale slip and friction to continuum models remains open.

3. What was the take-home message for the participants?

The field is expanding to include new types of fluid matter such as active and biological fluids. Moreover, new fascinating phenomena can be expected, such as hierarchical ordering in 3D structures, or electrolubrication may appear as a result of flow in confined geometry. The field has enormous potential for application, but more work needs to be done to develop theory and computer simulations to better understand the complex phenomena associated with flows in various types of materials.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

Our workshops can bring societal benefits by sharing knowledge among scientists working in a very broad and diverse field of fluid flow and porous media, as well as by training PhD students and young PhD students, who will go on to work in industry and research. The majority of talks demonstrated research topics in an engaging way, so they could inspire participants to pursue further learning and a deeper interest in the field of flows in porous media. Some of the topics discussed at the workshop piqued the participants' interest due to their potential for further development. These included, for example, machine learning approaches to describing spatially inhomogeneous multibody systems in equilibrium and with flow, and active flows.
We were pleased to learn in retrospect that the Nobel Prize in Chemistry 2025 has highlighted the timeliness of some of the aspects covered in the workshop (e.g., species separation via metal-organic frameworks).

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

An invitation to F. Höfling and A. Özgür Yazaydin for a review article in Communications Physics with working title “Flowing matter in Nano-Porous Materials”, covering some aspects of the workshop.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

To promote geographical diversity of participants we have encouraged remote participation via GatherTown for discussions and online posters and Zoom for broadcasting lectures. This allowed the active participation of young scientists from countries such as Egypt, Ethiopia, Malaysia, Morocco, India, and Iran, for whom obtaining a visa to Germany is a long and cumbersome procedure. The rooms in which the workshop took place were selected to be barrier-free for potential disabled participants. The organizing committee was selected so that women and men were equally represented, which was intended to encourage women in particular to participate in the workshop.
The workshop announcement included a call to apply for an Emerging Topic Lecture. It was awarded to Eleonora Secchi (ETH Zürich).

7. Participant list

Organisers
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CCP9/CECAM Graduate School

Location: CECAM-UK-DARESBURY, United Kingdom

Webpage : Event webpage

Dates: Feb 24, 2025 - Feb 28, 2025

1. What were the major topics presented in the School?

The "CCP9/CECAM Graduate School" took place at Daresbury Laboratory 24-28 February 2025 and included a selection of lectures, tutorials and hands-on sessions intended to teach advanced electronic structure theory and the use of codes on HPC. The school was intended to teach beginning PhD or postdocs in the field how to effectively use different electronic structure codes for different problems and application areas. Best practice in HPC, workflows, etc, was combined with theory lectures and exercises using state-of-the-art methods implemented in the CASTEP, CRYSTAL and QUESTAAL codes and one day each was dedicated to the respective codes. Each code project brought a group of demonstrators to assist with tutorials and hands-on sessions which followed the introductory talks and formal method lectures.

Topics covered:

- Fundamentals of electrons in solids: band theory
- Models for electron correlation
- Density Functional Theory (DFT); its successes and limitations
- Many-body Perturbation Theory (*GW* and related approximations)
- Optical and dielectric properties of materials
- Structural relaxation and dynamics
- Calculation of phonon modes
- How to efficiently use hybrid functionals for improved accuracy
- Treatment of surfaces
- Treatment of magnetism
- Use of Atomic Simulation Environment and best practices for HPC

For more information: See the workshop page.

2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

The students arrived with a good understanding of the basic methods of density functional theory but without the detailed experience or understanding to appreciate, for example, the connections between screened-exchange (hybrid functionals), +U and GW; ideas of multi-determinant wave functions were largely new. The school addressed these conceptual and experiential gaps directly and provided a forum where participants were able to freely ask questions on different topics without feeling intimidated. The structure of presenting different codes and topics in succession supported this because all participants were new to some parts and felt comfortable asking questions to bridge their backgrounds with the presented material.

A large spectrum of ability and experience in HPC use was evident in the participant group; some participants got more out of practical work on the command line, while others excelled at this and were able to move ahead more directly to concentrate on physics questions. The generally sociable atmosphere helped participants teach each other by exchanging tips and tricks that they each brought to the meeting; accordingly, also the tutors and demonstrators learnt a lot from the younger generation's style in computing (highly integrated IDEs, python best practices, etc).
Each of the three main codes had only limited time to demonstrate and explain their capabilities; to compensate for this and to allow discussion of topics that we couldn't arrange in the formal program, and to allow us to respond to variation in the skill level of the participants, we assigned the final day of the meeting to an ad-hoc, self organised session. After a week together, the group was able to discourse very effectively together and everyone took the microphone in turn to express what they would like to discuss and what might help them for their work in the future; gathering the main items together we were able to form subgroups that tackled each topic in detail. Because we had the developers and tutors for each of the codes present on site, we enjoyed a huge wealth of experience that we could apply to all of the topics raised: important larger items included how to use Wannier90 (we gave an impromptu lecture and tutorial), how to calculate magnetic exchange interactions and an extra session on advanced ASE usage.

3. What was the take-home message for the participants?

- foundations of density functional theory and band theory
- understanding of +U, hybrid functionals and GW as beyond DFT methods
- understanding all-electron and plane-wave basis sets and their pros and cons
- hands-on experience in HPC use and understanding of its environmental impact (including how to evaluate this)
- understanding which codes to use for molecular-dynamics, spectroscopy or magnetism
- network building for younger researchers

4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

Lecture notes and detailed course materials for all the codes and tutorials are shared with all participants.

5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

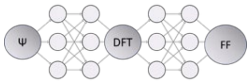
Organised accommodation and transport were provided to ensure that cost would not present any barrier to attendance. Starting and finishing at midday ensured that nobody would need to travel outside of business hours and we proactively engaged participants registered with the meeting to ensure that we might be aware of special individual requirements.

6. Organiser list

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Density Functional Theory and Artificial Intelligence learning from each other

Location: CECAM-HQ-EPFL, Switzerland



Webpage : Event webpage

Dates: Mar 3, 2025 - Mar 6, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

Major Topics Discussed and Their Contributions to Advancing the State of the Art.
A core theme was the challenge of applying machine learning (ML) to quantum chemistry when the underlying reference methods (typically DFT) themselves contain inaccuracies. Unsolved problems in exchange-correlation (XC) functional approximations limit the reliability of ML models trained on DFT data and this is a challenge that should be resolved.
The importance of capturing chemical diversity when training ML models was highlighted. Training only on narrow chemical subspaces leads to models that fail in generalization. Effective training must incorporate representative chemical variation – in both molecular types and electronic environments – to ensure robustness and transferability.
A central question was how much physical knowledge (e.g., exact conditions, asymptotics, symmetries) needs to be embedded in Machine-Learned Potential (MLP) architectures. Some argued for heavily constrained models to ensure physically meaningful outputs, while others demonstrated that even relaxation of some of these constraints at the foundational level can recover accurate physics.
A key point of reflection was the extent to which ML can assist in developing better XC functionals. While promising results exist, ML-assisted XC development has stagnated. Lessons from traditional XC development – like using constraints and their relative importance as well as the use of new functional features can directly guide and improve ML-based functional design.
The workshop also featured active debate on the relative merits of neural networks (NNs) and kernel methods.
The workshop brought together "old school" DFT developers and ML researchers, facilitating essential knowledge exchange. This common language is crucial for hybrid approaches like ML orbital-free DFT and ML-enhanced functional development.
ML-assisted functional development had seen stagnation. The workshop catalyzed renewed interest, identified bottlenecks, and is expected to inspire new publications addressing both fundamental and practical limitations.

2. What were the primary outcomes of this workshop, including limitations and open questions?

The workshop highlighted that the interface between machine learning (ML) and quantum chemistry is rapidly evolving. Discussions showed clear progress but also critical limitations.
ML has advanced in learning electronic densities, but the workshop showed that density distortions – especially from van der Waals interactions – are not well captured and remain an open problem.
The workshop emphasized that ML is promising for orbital-free DFT, especially in approximating kinetic energy functionals, yet practical applications are still missing.
It was also noted that reference data is uneven. For single-reference systems, CCSD(T)-level datasets are growing fast. But for transition metals, especially multireference cases, reliable data is scarce – less than 100 small systems – severely limiting ML development in this space.
Discussions showed that ML-based exchange-correlation (XC) functionals have not yet surpassed traditional ones in reliability. Generalization remains a major challenge, and physical constraints are often missing. Participants stressed that insights from traditional XC development are still essential.
Machine-learned potentials (MLPs) have progressed significantly, often reaching DFT-level accuracy. However, the workshop pointed out that DFT itself is now the bottleneck, with poor training data limiting MLP performance – captured by the phrase: "ML is an excellent student, but DFT can be a lousy teacher."
Overall, the workshop identified key directions for future work: improved data, better treatment of density distortions, and integrating physics into ML models.

3. What was the take-home message for the participants?

The take-home message was that machine-learned density functional theory is not yet reliable, physical constraints remain crucial for improving machine-learned exchange-correlation models, machine-learned potentials are advancing rapidly but limited by poor training from standard methods, and there is a major lack of high-quality data for strongly correlated systems.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

The outcomes of the workshop, particularly the emphasis on bottlenecks in the current machine learning–quantum chemistry interface, led to a clear identification of key problems – such as lack of data for strongly correlated systems and limitations of existing functionals. This contributes to solving foundational issues, which in turn can benefit society by improving simulations for materials and drug design, enabling faster and more cost-effective development of batteries, catalysts, and pharmaceuticals.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The workshop led to multiple new collaborations, particularly between traditional quantum chemistry and density functional theory developers and machine learning researchers. A

new workshop submission was discussed and is planned for two years from now, aiming to track progress and deepen integration across these communities.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The workshop promoted inclusivity by selecting speakers and participants across a range of career stages, geographical regions, and research backgrounds. Participation was open globally, and the online attendance option enabled broader engagement.

7. Participant list

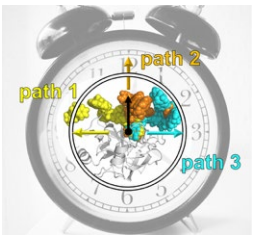
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Predicting and understanding drug-target binding kinetics via molecular simulations



Location: CECAM-HQ-EPFL, Switzerland

Webpage : Event webpage

Dates: Mar 10, 2025 - Mar 12, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The participants discussed the current state-of-the-art in the prediction, as well as the measurement, of protein-ligand binding and unbinding rates. From the side of theory, we focused on the capabilities and the shortcomings of both relative and absolute rate prediction methods. We considered the current error range in theoretical predictions in relation to experimental accuracy, what a possible overlap of the interests of academia and industry may be, how to best benchmark predictions, and how to best integrate the different simulation approaches into existing software toolboxes.
These discussions helped to first and foremost focus and align the diverse research efforts within the molecular modeling and simulation community: so far, each group has tended to use their own prediction method, mostly using their own test systems, with little overlap between investigations, which has now become more apparent, and hopefully leads to refocusing the field. Furthermore, the exchange with experimentalists made clear that even experimentally obtained reference data may be subject to large uncertainties from systematic errors in experimental techniques, as well as random errors based on sample quality, machine setup, etc. Lastly, the exchange between academics and applied researchers from industry revealed a general interest on the side of industry for binding kinetic rate predictions, but a need for more tangible results and proof-of-principles for the usefulness of rate prediction, as well as user-friendly tools, in industry-driven drug design campaigns.

2. What were the primary outcomes of this workshop, including limitations and open questions?

The participants recognized the need for a sustained exchange on the discussed topics and the formation of an international, well-connected community focusing on prediction of binding kinetics. All participants explicitly expressed their desire for a continuation of the workshop on a biannual basis.
Furthermore, we anticipate generating data for and organizing a blind challenge for rate prediction along the lines of the SAMPL challenges. For doing so, we will need to generate data in experimental labs in academia on a defined timeline. This data will need to be for several different protein targets with substance libraries based on different chemical scaffolds, ideally being measured with various experimental techniques. We recognize that this data basis will have to be generated from the side of academia, as the protection

of IP in industry will likely be at odds with the generation and public availability of this data set.
On the side of theory, we recognized a significant mismatch between the capabilities of absolute rate prediction and experimental measurements. Theoretical predictions are therefore currently often too imprecise to be of particular use in virtual screening campaigns, though methods to estimate relative values can be useful in lead optimization scenarios. A better understanding of the source of errors in computations therefore needs to be carried out. At the same time, the present experimentalists noted the necessity to use different measurement techniques to derive unbinding rates to remove systematic bias.
Applied scientists from industry raised the need for the use of more complex systems to benchmark computational methods, moving beyond trypsin-benzamidine to larger proteins (GPCRs, kinases) and larger drug-like molecules.

3. What was the take-home message for the participants?

The participants recognized that we need to focus the research field and coordinate and network research efforts, as well as to push for proving the potential of optimizing ligand kinetics in industrial drug design campaigns. Along with shortcomings, the workshop highlighted recent substantial advances, making clear that it is now a good time to advance both computational and experimental studies of protein binding kinetics.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

If drug design based on tailoring protein-ligand binding kinetics becomes routinely feasible, it would pave the way for the generation of drugs with fewer side effects, making the drug discovery process more efficient and resulting in fewer terminations of drug discovery campaigns at late clinical stages. This may therefore lead to more varied choices in pharmaceuticals with lower prices due to the smaller initial investment necessary in the drug discovery pipeline.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

We currently plan to summarize our discussions in the form of a Perspective article. Furthermore, we are in the early stages of drafting a proposal for a grant for a combined academic-industrial PhD training network program. In addition, we aim to hold a follow-up workshop on the same topic in two-year's time.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

We focused on balancing gender ratio (40 participants, 26 men, 14 women), geographic location (1 from South America, 7 from North America, 32 from Europe, including Germany, Italy, Denmark, Poland, Hungary, Belgium, Switzerland and United Kingdom), as well as the career stages of the speakers and participants, which we think we succeeded in. We focused on generating an environment in which all participants felt free to speak their minds and opinions freely without the fear of being ridiculed or reprimanded. The overall atmosphere of the meeting was very positive and collaborative. Especially noteworthy is that in the final discussion, reports on the progress within different discussion subgroups in half of the cases were given by PhD students or postdocs. Thanks to the CECAM sponsorship, we could bring one PhD student from Chile (Felipe Bravo Moraga) to participate in the workshop.

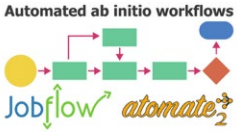
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Automated *ab initio* workflows with Jobflow and Atomate2



Location: CECAM-HQ-EPFL, Switzerland

Webpage : Event webpage

Dates: Mar 17, 2025 - Mar 20, 2025

1. What were the major topics presented in the School?

The school provided a comprehensive introduction to automating computational materials science workflows using Jobflow and Atomate2.

The school introduced high-throughput simulations and their management challenges. Jobflow, a powerful Python API for building workflows, was highlighted as crucial for managing large numbers of calculations. Advanced features of Jobflow were also presented, including chaining workflows by forwarding structure and previous directory (prev_dir) from one job to another. Furthermore, the school covered techniques for managing dependencies between Jobs within a Flow using OutputReference. The JobStore as the primary database was introduced, along with its integration with multiple DFT codes.

The school also delved into the architecture and job execution process of Jobflow-Remote, which enables remote execution on High-Performance Computing systems.

A significant portion of the school was dedicated to Atomate2, a library for building automated workflows with a strong initial focus on the VASP code. The building blocks of VASP workflows were introduced, including Jobs for single calculations (like relaxation or static energy calculations) and Flows for chaining together multiple Jobs to achieve more complex tasks.

The concepts of RelaxMaker and StaticMaker for creating these basic jobs were explained, along with BaseVaspMaker, which handles the fundamental steps of a VASP job: writing input files, running VASP, and reading output files. The school covered how to customise input sets using VaspInputGenerator and its various options.

Error handling was also a crucial topic, with Custodian introduced as a tool for automatically detecting and fixing common VASP errors. The VASP output parsing was explained through the Task Document, which contains key information from the calculation, including inputs, outputs, and intermediate calculation steps. Beyond VASP workflows, FHI-aims and especially ABINIT workflows were covered as well.

The school detailed how to navigate the Task Document to access specific data. Methods for querying the Task Document using the JobStore and MongoDB query syntax were taught, enabling users to efficiently retrieve data based on various criteria. Data management through metadata and tags was also covered as a way to organise and track calculations beyond what is available in input/output files.

The school also delved into specific application areas enabled by automated workflows:

- LOBSTER for Bonding Analysis
- Machine Learning Interatomic Potentials (MLIPs) like M3GNet and MACE
- Phonon Calculations (via Phonopy)
- Point Defects formation energies (including finite-size corrections)

2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

The lectures and hands-on sessions highlighted several limitations, open questions, and potential pitfalls in using Atomate2 and Jobflow for high-throughput simulations. One of the main concerns was usability - certain functions or databases can be complex enough to pose a barrier to entry or source of errors. Additionally, traditional methods have inherent limitations, such as requiring guesswork/eyeballing for finite-size corrections for defects, while machine learning interatomic potentials (MLIPs) may not accurately describe bond breaking or larger forces.
Another challenge is interoperability - different computational chemistry tools do not seamlessly integrate with each other, necessitating separate environments. For example, the Python package for GFN-xTB does not work well with any MLIP package, posing a practical limitation. Furthermore, data management can be an issue in Jobflow, where Pydantic models cannot be stored in additional stores, restricting data organisation and management.
Ongoing development and known issues also emerged during the sessions - custom pseudopotentials are difficult to use with ABINIT, while the experimental GUI for Jobflow-Remote is still evolving. Overall, these limitations highlight the need for users to be aware of potential pitfalls, carefully validate results, and understand the nuances of the tools in order to effectively utilize Atomate2 and Jobflow for high-throughput simulations.

3. What was the take-home message for the participants?

The key takeaway was that automation of calculations is essential for materials discovery. To design custom workflows, it is crucial to understand Jobflow and Atomate2. Effective job management involves defining, connecting, and executing Jobs and Flows. Data handling includes managing output in a database, accessing data, standardizing output, and tracking calculations. The course also stressed the importance of community engagement and critically evaluating results.

4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

There are several tangible outcomes associated with the school.
A GitHub repository was set up with notebooks for the hands-on sessions: https://github.com/Matgenix/atomate2_cecam_school
The presentations are all available as PDF files on the CECAM website. They include a lot of practical information about the different tools, including links to various tutorials already available online.
The lecture notes include code examples demonstrating the use of Jobflow and Atomate2. These examples can serve as practical resources.
Finally, all the lectures were recorded and will be uploaded on YouTube.

5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The team of organizers originated from various countries (Germany, the United Kingdom, and Belgium), consisting of one woman and two men, with two younger researchers and one older one. Though the selection process for our tutors focused on competence, we achieved a geographical diversity among them (the United States, India, Italy, and Belgium).
In selecting our tutees, we sought to create a diverse group of individuals. We made a conscious effort to favor participants from developing countries. Additionally, we paid close attention to ensuring that female participation was well-represented.
Unfortunately, not everyone who had expressed interest and enthusiasm for participating managed to join us. Disappointingly, many registered people (~5) were unable to attend due to unforeseen circumstances such as visa issues or health conditions. There were 20-30 remote attendees during the lectures, enabling a larger diversity of attendees.

6. Participant list

Organisers
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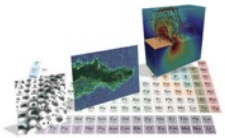
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Fulfilling the Multiscale Promise in Materials: Getting Information out of the Atomistic Scale

Location: CECAM-HQ-EPFL, Switzerland



Webpage : Event webpage

Dates: Mar 31, 2025 - Apr 3, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop centered on key challenges and advancements in extracting atomic-scale information to inform macroscopic materials models. Discussions covered scale-bridging difficulties, successes in linking atomistic and continuum models, infrastructure needs, and interdisciplinary collaboration.

A major topic was the difficulty of quantitatively accurate machine learning interatomic potentials (MLIPs) that balance precision and computational efficiency. Time-scale and length-scale limitations hinder the ability of atomistic models to predict macroscopic properties. Validating simulation results with experimental data remains a challenge, particularly for properties that are easy to compute but difficult to measure.

There appeared to be a consensus that multi-scale modeling requires problem-specific methods and workflows, and that there cannot be a one-size-fits-all solution. The specific hurdles are therefore highly problem-specific. Examples were shown both where classical interatomic potentials are sufficient for predictive accuracy and where they can give qualitatively incorrect behaviour in contrast to MLIP models.

2. What were the primary outcomes of this workshop, including limitations and open questions?

Despite challenges, notable successes include:

- Mechanical property predictions (e.g., yield strength related to solution/precipitate strengthening) linked to atomistic insights, and including effective dislocation behaviour necessary to predict macroscopic yield stress.
- Thermodynamic modeling, connecting electronic and atomistic scale, for example to calculate phase diagrams.
- Lubrication and friction modeling, where atomistic results are passed to continuum lubrication models (e.g. Reynolds equations) to predict friction.

Participants emphasized the fragmentation of existing modeling tools and the lack of standardized infrastructure for data and code sharing. Key concerns included:

- Unmaintained codes developed for specific studies but no longer supported.
- Poor interoperability between different simulation tools.
- Limited benchmarking and validation efforts across scales.
- Sustainability, for example the high CPU and GPU costs of training and using MLIPs.

Proposed solutions include creating a permanent team for code maintenance (e.g. as exists for some ab initio codes), and establishing benchmarking initiatives to validate results.
The need for multiscale training programs was highlighted to equip researchers with cross-disciplinary expertise in terms of technical skills (e.g. software engineering, data science) but also disciplinary skills (e.g. interatomic interactions, dislocations, or continuum theories). Participants also called for long-term visitor programs, interdisciplinary collaborations, and alternative engagement formats like hackathons to improve knowledge exchange.

3. What was the take-home message for the participants?

The take-home message was that while multiscale modeling has seen successes – e.g. in yield strength predictions, solute strengthening, and phase diagrams – significant challenges remain. These include the need for better interatomic potentials, computational efficiency, scale-bridging methods, and interdisciplinary collaboration. Participants emphasized the importance of infrastructure, standardized benchmarks, and long-term support for simulation tools to realize the multiscale promise.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

Yes, the outcomes of the workshop hold significant potential for societal benefits. Multiscale materials modeling can accelerate the discovery and design of new materials with enhanced properties, impacting industries such as aerospace, energy, healthcare, and manufacturing. By improving the predictive capabilities of simulations, researchers can reduce the need for costly and time-consuming experiments, leading to faster innovation cycles and more sustainable material development.
For example, successes in predicting yield strength, solute strengthening, and phase behaviour can directly contribute to the development of stronger, lighter, and more durable materials for infrastructure and transportation. Advances in friction modeling and defect behaviour could lead to improved wear-resistant coatings and lubricants, enhancing the efficiency of mechanical systems and reducing energy consumption as well as contributing to the replacement of harmful materials (e.g. PFAS in lubricants). An approach based on atomistic simulation and high-throughput screening was proposed for the recovery of expensive elements (e.g. tantalum) from industrial waste slags.
Additionally, the workshop highlighted the need for better data sharing, code integration, and interdisciplinary collaboration. Establishing shared infrastructure and standardized methodologies could lead to broader accessibility of computational tools, benefiting both academia and industry. Training initiatives and long-term support for software development would ensure that future generations of scientists can continue to refine and apply these models effectively.
Ultimately, by addressing current challenges – such as scale-bridging, computational limitations, and experimental validation – multiscale modeling can contribute to breakthroughs in materials science that improve sustainability, energy efficiency, and technological advancements, benefiting society as a whole.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The workshop facilitated several tangible outcomes, although specific deliverables such as publications or funded proposals may take time to materialize. Key takeaways include:

- **New Collaborations:** The discussions fostered interdisciplinary connections, particularly between researchers working on different scales (atomistic, mesoscopic, and macroscopic), as well as between academia and industry. Some participants expressed interest in coordinated efforts to bridge methodologies and standardize approaches.
- **Plans for Future Proposals & Research Initiatives:** Several participants emphasized the need for a unified research effort tackling a specific multiscale challenge. Ideas such as benchmarking studies, software development initiatives, and structured interdisciplinary collaborations could lead to future funding proposals.
- **Software & Infrastructure Developments:** The need for maintaining and integrating atomistic simulation codes was a recurring theme. Suggestions for a multiscale modeling platform, shared databases, and improved interoperability between codes indicate potential directions for future software development projects.
- **Training & Knowledge Dissemination:** Calls for long-term visitor programs, interdisciplinary training initiatives, and structured workshops suggest that follow-up activities may include new educational efforts to enhance expertise in multiscale modeling.

While no immediate publications or software releases were reported, the workshop established a strong foundation for future developments in multiscale materials modeling. The organisers are hoping to develop this report into a perspectives article.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

Gender & Geographical Diversity: We included speakers and participants from a range of backgrounds, ensuring representation across genders, regions and institutions. Of our 26 speakers, 6 were female (23%), comparing favourably with similar events.
Career Stage Balance: The workshop included early-career researchers, postdocs, and senior scientists, fostering mentorship and knowledge exchange. Contributed talks were allocated preferentially to early-career researchers.
Hybrid Participation: Given the high interest in the workshop, hybrid participation was added. Engagement was good, with ~15 people joining online and asking some questions.
Interdisciplinary Representation: Bridging physics, chemistry, materials science, and computational fields helped ensure inclusivity in scientific perspectives.

7. Participant list

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Machine learning for Advanced Material and Molecular Modelling



Location: CECAM-UK-DARESBURY, United Kingdom

Webpage : Event webpage

Dates: Mar 31, 2025 - Apr 4, 2025

1. What were the major topics presented in the School?

Basics of machine learning:

- Data preparation and analysis
- Generating chemical representations and features
- Dimensionality Reduction
- Clustering
- Kernel-based model fitting
- Hyperparameter Optimization
- Uncertainty Quantification

Supervised Learning

Here, we will look at models based on linear regression and Kernel Ridge Regression as they form a good starting point.

Unsupervised Learning

- Principal component analysis (PCA)
- PCA for dimensionality reduction
- PCA for compression
- k-means clustering
- DBSCAN
- Task – Exploring the ChEMBL small molecule database

Representations

Fundamentals of neural networks

Graph neural networks

Machine learned interatomic potentials

- **Understanding the data: diverse configs, reference labels**
- **Understanding MACE parameters: architecture and training**
- **Fitting and testing MACE models**
- **Ultimate goal: stable and accurate Molecular Dynamics**

Generative Machine Learning

2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

There was lost of discussion on how transferrable or generalisable machine learned interatomic potentials are. Lots of discussion about how to best train new models and how we can know if the model is really predicting in an area that it can confidently work in. There was similar discussion about generative models and how we can do uncertainty

quantification for generative models. We did have a lot of discussion about methods that can be used for uncertainty quantification, such as ensembles, and Gaussian processes. We discussed the pros and cons of these different approaches.

There was also lively discussion about if ML can really discover new viable materials. This included discussions about how once can really quantify the novelty of a new chemical or material. It also involved detailed discussion about what kind of metrics can be used to assess the synthesisability or otherwise of a new system. We discussed measures such as the energy with respect to the competing phases and the uses and limitations of these approaches.

3. What was the take-home message for the participants?

Machine learning is really useful in many areas of chemical and materials modelling - but one should always make sure that we understand the methods that we are using, to avoid making bad decisions.

4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

We wrote up the teaching material in an online e-book of the course material: https://workshop.camml.ac.uk/intro.html.

5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

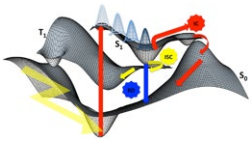
We tried to ensure that all advertising was accessible and tried to advertise as widely as possible, including outside of the major channels. We ensured that all assessment criteria were balanced. We made sure that all judgement panels were as diverse as possible, to try to protect against unconscious biases. We were conscious of the very un-diverse makeup of our teaching team (all white men) and tried to balance this with the plenary speakers we invited. Next year we hope to do better, we are trying to build a more diverse conference teaching team.

6. Organiser list

Organisers
Butler, Keith
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Quantum and Mixed Quantum Classical Dynamics in Photochemistry



Location: CECAM-ES, Spain

Webpage : Event webpage

Dates: Mar 31, 2025 - Apr 4, 2025

1. What were the major topics presented in the School?

The school presented an overview of the state-of-the-art in computational photochemistry. This ranges from basic photophysics and photochemistry concepts like absorption/emission processes to non-radiative decays and photochemical transformations, the underpinning electronic structure describing the electron correlation problem and its varying role across multiple potential energy landscapes, and how these estimates are then used both statically and dynamically to model photo-reactions and infer mechanisms to rationalise both steady-state and time-resolved experimental observables.
Particularly, an introduction to photochemistry and spectroscopy set the stage, making connections between the observables measured experimentally and the computable magnitudes that are often used in the literature to elucidate/support them. This was followed by a review of electronic structure methods used in the field, making special reference to multiconfigurational CASSCF approaches and their perturbation theory (CASPT2) extensions, and also on TD-DFT, extracting their strengths and weaknesses, and attempting to instruct on their correct use to model a given photochemical problem. The different magnitudes obtained with electronic structure packages (particularly ground and excited state minima, Hessians and transition dipole moments) were then used with analytic harmonic models under the Born-Oppenheimer approximation to produce realistic spectra matching the experimental observable and its vibrational lineshape. Subsequent lectures further introduced advanced dynamical treatments, including non-adiabatic couplings that trigger population transfer among excited electronic states. In this sense, both mixed quantum-classical treatments, focussing mostly on surface hopping, and fully quantum dynamical methods were covered. These methods were then shown to pave the way to monitor photochemical phenomena in real time.

2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

The school provides an overview of a highly active area of research, from the basis to state-of-the-art methodologies, highlighting their limitations and associated open scientific questions. Among these, we discuss the intricacies of selecting appropriate electronic structure methods for describing excited-state potential energy surfaces, and elaborate on various nuclear quantum effects, exploring appropriate strategies to apply cost-effective mixed quantum-classical approaches depending on the specific problem.

Several of these challenges are addressed explicitly in the hands-on sessions, equipping students with the tools needed to confront such open questions and apply them to their own research.
On the practical side, some limitations were associated with the computing resources available for the workshops, which meant some simulations took a long time to complete and could not be integrated within the activities as well as originally intended. This issue will be addressed by providing students with intermediate results, which streamline the sessions while preserving the experience of a complete computational study. In the longer term, we work on tailoring the labs by carefully selecting the computational settings to ensure fast yet pedagogically valuable simulations. In this sense, we acknowledge support from the IT team at CECAM-ES, who provided adequate resources to carry out the sessions this year. Additionally, the last workshop addressed a different molecule, as it was unclear how to effectively apply the fully quantum dynamical treatments covered in the lectures to the system adopted for the other workshops. We plan to both revise the theoretical lectures and eventually integrate such methodologies in a fully unified computer lab.
Another shortcoming intrinsic to the course lies in balancing its duration with the breadth of content: this school brings together a wide range of sub-disciplines to be covered on only one week, exposing participants to a significant amount of new content. There is no easy way around this. We do not envision extending the length as it has other associated challenges, including scheduling and the increased cost on participants, which would affect most those with financial difficulties and thus negatively impact the participants' diversity. We are however actively working to partly mitigate this issue by strengthening the coordination between lectures towards a unified view across them: this includes avoiding unnecessary repetition, use consistent nomenclature and foster connections between them. Moreover, the design of the hands-on sessions, centered on a common molecular system, tries to help students assimilate the content by clearly illustrating the applicability/limitations of the different strategies covered in the lectures by applying them on top of a shared setting.

3. What was the take-home message for the participants?

The main take-home message was to carefully select the model that best fits your problem at hand. The course showcases different methodologies available in open-source software and suggests ways in which they can be applied to solve given photochemical problems, thus showing how to extend well-defined cases to different scenarios applicable to the student's own research. This was stressed at the end in a Round Table that summarised/merged the different lectures.

4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

 The course made all lecture notes (i.e. slides) available to all attending students for future reference: the lectures are interconnected and avoid repetition as much as possible, each lecture building upon the previous and setting the stage for the next in a clearly defined manner. A longer-term goal of ours is to curate this information and publish it as a short review, enclosing all important topics related to computational

photochemistry (photophysics & photochemistry, electronic structure in the excited state, mapping of potential energy surfaces, electron & nuclear dynamics (both semi-classical and fully quantum mechanical, ...) in one single piece, something that is not yet available to our knowledge: this would help train the next generation in a more general way, providing a fair and plural take on computational photochemistry while avoid scientific bias (i.e. using a given "preferred" model just due to familiarity) as much as possible.

 The workshops were redesigned in this edition to all tackle different aspects of acrolein and its photophysics: from one-photon spectroscopy to the low-lying dark state to the dynamics of the excited system over multiple electronic states. A virtual machine was created which included all required software, as well as the different inputs and other files to be used throughout the workshops. The software used was mostly open-source (OpenMolcas, FCClasses3, Turbomole & Newton-X), and our plan is to reach a fully open-source setting, or at least resort to licenses free for academics. This virtual machine is expected to be therefore shareable and a resource for training globally beyond the immediate scope of the school. We are currently curating this machine and its content (including also the exercise manuals with problem introduction and specific questions to solve) and uploading it to Zenodo to facilitate its free worldwide access: in this way, this workshop might be ported to any other location on the planet, thus significantly increasing its impact.

5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The workshop was advertised via X/Bluesky using the #compchem hashtag, and further by personally contacting a wide range of experts worldwide in the field, ensuring it found its target audience. This strategy was successful, as we had to leave out 10+ applicants due to exceeding the capacity of the allocated venue.
The school was attended by 14/34 women, amounting to ~40% and far from the 50% we'd hope for, but above the field's current average, which is encouraging. Most attendees were MSc (15) or PhD (15) students. To lower costs and the associated carbon footprint, most speakers were based in Spain. The school attracted a wide pool including people from Africa and Australia, with the main core being Europeans (17 Spanish, 1 Polish, 6 Italians, 3 French, 3 British and 1 Danish), and a significant number of Spanish-based participants being originally from Latin-American countries.

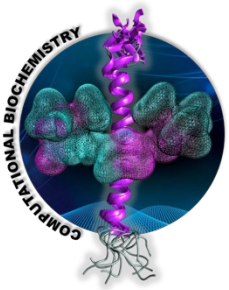
6. Participant list

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Computational Biochemistry. Efficient Tools to fight Diseases



Location: CECAM-ES, Spain

Webpage : Event webpage

Dates: Apr 7, 2025 - Apr 11, 2025

1. What were the major topics presented in the School?

The major topics were presented in the following 4 blocks:
Block 1: Biomolecules and their properties, structural databases of biomolecules, biomolecules modeling, molecular mechanics force fields, potential energy surfaces, solvent, periodic boundary conditions, molecular simulations. Molecular visualization.
Block 2: Timescale problem, enhanced sampling methods, collective variables, umbrella sampling simulations, metadynamics simulations, accelerated molecular dynamics, replica exchange molecular dynamics. Estimation of kinetics from molecular simulations.
Block 3: Biochemical reactivity, continuum solvation models, cluster models, QM/MM models, subtractive and additive schemes, electrostatic and polarizable embedding. Reaction free energy profiles in biochemical systems, Transition state theory in biochemical reactivity.
Block 4: Binding free energies, alchemical transformations, MM-PBSA & MM-GBSA methods, protein-ligand interaction, docking and QSAR.

2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

Several open scientific questions emerged during the lectures and follow-up discussions, underscoring the dynamic and evolving nature of computational biochemistry. These included how to better integrate machine learning with classical simulation techniques, how to enhance the modeling of long-timescale conformational changes in biomolecular systems, and how to effectively capture rare events in enzymatic reactions. Participants also showed strong interest in understanding the current limitations of force fields and QM/MM methods, particularly in the context of metalloproteins and reactive intermediates. These discussions fostered stimulating exchanges and emphasized the importance of continuous methodological development and rigorous benchmarking.
On the practical side, a few technical challenges were noted during the hands-on sessions. One issue was the slow performance of molecular visualization tools (such as VMD and PyMOL) when run remotely on the school's virtual machines, especially during protein-in-solution analysis. This likely stemmed from bandwidth limitations when multiple students connected simultaneously. Improving classroom wireless capacity could help resolve this in future editions.
Additionally, some variability in the performance of the virtual machines was observed. According to discussions with the ZCAM IT team – who were consistently professional and highly responsive, even providing support during bank holidays and weekends – this

issue may stem from the fact that the virtual machines were not always allocated the same underlying physical hardware (e.g., CPUs, RAM). Ensuring consistent hardware resources throughout the duration of the course would help deliver more stable performance and enable more reliable estimates of the computational time required for the students' practical exercises.

3. What was the take-home message for the participants?

A key takeaway for students is the understanding that each method serves as a specific tool suited to particular types of problems. By the end of the course, participants will have assembled a foundational "toolbox" that will enable them to begin exploring and analyzing complex biomolecular systems.

4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

Lecture Materials: Slide presentations from all theoretical sessions are publicly available as PDFs on the official CECAM school webpage. They offer a comprehensive overview of the covered topics and serve as a valuable reference for both participants and the broader scientific community.
Tutorials and Practical Exercises: All hands-on tutorials – including instructions, input files, and sample outputs – were shared with students. These self-contained materials allow participants to repeat the exercises independently or adapt them for their own research or teaching.
Open-Source Software: Except for Gaussian, all practical sessions used open-source tools such as GROMACS, PyMOL, and VMD. This ensures participants can continue exploring these methods without licensing barriers. Where possible, links to repositories and installation guides were provided.
Reproducibility and Continued Learning: Students were given access to all scripts, datasets, and example files used during the school. This supports reproducibility and encourages further exploration of the problems addressed in the sessions.
Documentation and Self-Guided Learning: Tutorials were designed to be self-explanatory, with background information, step-by-step instructions, and guidance on interpreting results, making them ideal for independent study.
Community Building and Collaboration: By sharing resources and fostering hands-on engagement, the school helped strengthen a growing community of early-career researchers in computational biochemistry and laid the foundation for future collaboration.

5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

To promote inclusivity, we implemented broad outreach strategies across multiple platforms to engage a diverse audience. All applicants were accepted, creating an open and welcoming environment. The speaker lineup was thoughtfully balanced in terms of

career stage, featuring both early-career and senior researchers. The course took place in a fully accessible venue, and materials were shared in advance to support participants with varying needs. Additionally, we fostered meaningful interaction and mentoring opportunities across experience levels to enhance learning and engagement for all attendees.

6. Participant list

Organisers
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Sujal, Sujal - Universidad Del País Vasco, Spain
Tohidi Nafe, Zahra - HUN-REN Research Center for Natural Sciences, Hungary
Valenzuela Antón, Alejandro - Universidad Autónoma de Madrid, Spain
Yang, Yiyi - UAM, Spain

10th School and Workshop on Time-Dependent Density-Functional Theory: Prospects and Applications

Location: CECAM-ES, Spain



Webpage : Event webpage

Dates: Apr 7, 2025 - Apr 18, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop built upon a six-day school that introduced Time-Dependent Density-Functional Theory (TDDFT) alongside neighboring methods such as many-body perturbation theory (MBPT). Key school topics included:
- Time-resolved spectroscopies in solids, liquids, and molecules using TDDFT;
- Spin dynamics and exciton physics in materials;
- Non-adiabatic molecular dynamics coupled to TDDFT;
- Exchange-correlation functional development, addressing non-adiabaticity and charge-transfer challenges;
- Coupling to electromagnetic fields (classical Maxwell and quantized QEDFT approaches);
- Connections to advanced MBPT schemes such as the Bethe–Salpeter equation.

The ensuing three-day workshop featured 22 talks spanning foundational theory (e.g., lattice DFT, ensemble DFT), novel functional approximations (range-separated hybrids, mGGAs), light-matter applications beyond linear response (nonlinear light propagation, cavity QED), and real-world challenges (biomolecular and 2D-material excitations). By revisiting original speakers from the first edition, the event traced two decades of progress, situating new developments – such as Maxwell–TDDFT coupling and QEDFT – within a historical framework. Moreover, hands-on sessions during the school part with the Octopus and BerkeleyGW codes empowered participants to apply cutting-edge algorithms directly to spectral calculations, thereby lowering the barrier between theoretical advances and practical simulations.

2. What were the primary outcomes of this workshop, including limitations and open questions?

Outcomes:
- Skill development: Tutorials and practical exercises enabled 35 students to perform TDDFT, GW, and Bethe–Salpeter calculations on real systems.
- Community building: Poster sessions (including a best-poster prize) and extended coffee/lunch breaks fostered cross-institutional collaborations.
- Theoretical insights: Discussions highlighted promising directions – ensemble DFT for periodic systems, stable long-range-corrected functionals, and photon-mediated many-body interactions.

Limitations:

- Schedule density: Feedback indicated the program was tight; participants requested an additional free day for reflection and networking.
- Dietary variety: Vegetarian options lacked diversity, limiting inclusivity for certain dietary needs.

Open questions:

- How to systematically improve non-adiabatic exchange-correlation functionals for charge-transfer excitations?
- What are the computational trade-offs in QEDFT implementations for large biophysical systems?
- Can Maxwell–TDDFT coupling be extended to real-time multiscale modeling of devices under extreme fields?

3. What was the take-home message for the participants?

Focused, hands-on training combined with historical perspective has catalyzed both theoretical innovation and practical expertise, underscoring that collaborative, community-driven events remain essential to push the frontiers of TDDFT and its extensions.
This event has demonstrated that TDDFT in its different incarnations and extensions is a very active field of research, with ongoing developments from its most fundamental aspects to its applications to real-life problems.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

Yes. Advances in TDDFT and its integration with electromagnetic and many-body methods directly inform the design of next-generation materials and devices.
By translating theoretical breakthroughs into accessible software workflows and forging a global network of collaborators, the workshop provides expertise for potential innovations that can address pressing challenges in energy, healthcare, and information technologies.
In particular, equipping early-career researchers with open-source code expertise (Octopus, BerkeleyGW) enhances computational literacy across institutions.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

There is no official outcome of the workshop. However, many informal discussions took place, and we expect, as for prior editions, that these discussions will translate into the coming months to new collaborations and research projects.

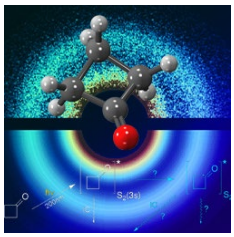
6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

Gender balance: Out of 72 total participants, 9 were women, and efforts are underway to increase female representation in future editions.
Geographical diversity: Attendees hailed from 17 countries across Europe, North America, and Asia, with targeted invitations to underrepresented regions.
Career stages: The program blended lectures by senior researchers with poster prize talk by an early-career scientist, and awarded a poster prize to elevate young voices.
Accessible scheduling: Inclusion of a full free day, extended coffee/lunch breaks, and online availability of lecture materials helped accommodate varying needs and time zones.
Dietary considerations: Vegetarian options were provided (with feedback collected for improvement), and remote attendance materials were offered to participants unable to travel.

7. Organiser list

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Building a roadmap for future developments in computational photochemistry based on a prediction challenge



Location: CECAM-HQ-EPFL, Switzerland

Webpage : Event webpage

Dates: Apr 8, 2025 - Apr 10, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

This workshop was organized around the prediction challenge on the photochemistry of cyclobutanone, initiated during a CECAM workshop in 2023. This challenged the community of computational photochemists to predict the photochemistry of cyclobutanone (excited at 200nm) and the experimental signals that would be measured in a time-resolved mega electronvolt ultrafast electron diffraction (MeV-UED) experiment. Each contributor would have to write an article based on their predictions, and submit it to the Journal of Chemical Physics (as part of a special issue) *before* the experiment took place in January 2024 at SLAC (Stanford Linear Accelerator). 15 contributions were published in the Journal of Chemical Physics and 2 experimental papers on MeV-UED experiments, and the goal of this workshop was to discuss the results of the challenge. Nearly all contributors to the challenge were present (only one could not make it due to US restrictions on travel), and we also invited two experimentalists who took part in the MeV-UED experiment. We also invited other members of the communities who had not participated to the challenge to provide a broader perspective on the outcome of this challenge.

The sessions were organized around 4 topics: initial conditions, electronic structure, nonadiabatic dynamics, and calculation of observables. Each session was composed of a 1h30 part, where each contributor presented their results for a maximum of 5 minutes, and a 1h30 discussion session. Additional presentations from the experimental team and the invited speakers from the community were proposed.

As detailed below, this workshop allowed us to disentangle the 15 contributions to the challenge and understand what worked and what did not work when it comes to the four 'ingredients' of an excited-state dynamics simulation. These discussions will allow us to calibrate our strategies for simulating the photochemistry of an unknown molecule, and to highlight which parts of our simulations need most attention. This workshop also allowed us to agree on what can be said about the different methods employed based solely on the results of the challenge, and what would require additional calculations in the future.

2. What were the primary outcomes of this workshop, including limitations and open questions?

The central outcome of this workshop is a general agreement between the different groups that contributed to the 15 articles of the challenge on what worked and what did not work in our excited-state dynamics of cyclobutanone. The discussions were intense yet highly constructive, stimulating numerous ideas on what could be tested in the future and which protocols (employed in some contributions) led to more robust predictions. They revealed, in particular, the critical need for the community of nonadiabatic dynamics to create a bridge with the electronic-structure community and stimulate the development of more robust approaches to describe the electronic component of the problem. Another element was the description of the photoexcitation process, which is usually done in a rather simplistic way, which may have penalized the accuracy of some predictions.
Based on the factual analysis during the workshop of the results of the challenge and discussions, we are currently writing a perspective article that will be included in the special issue of the Journal of Chemical Physics. This perspective article will summarize, for each category, the outcome of the challenge and the consensus reached by the participants during the workshop in terms of what worked and what did not. The perspective will also be used as a medium to inform the broader community about the protocols employed as part of the challenge (initial conditions or electronic-structure benchmark) that appeared to have led to better predictions. The perspective will also highlight the various ideas for future work that emerged from the workshop, aiming to better understand our results. The perspective will also provide an analysis of what elements of the challenge (organization, timeline) could have been improved to enhance the participation.

3. What was the take-home message for the participants?

The main take-home message was that, despite the various methods used to describe nonadiabatic dynamics, the primary factor determining the quality of the predictions was the electronic structure. This information is well-known within the community, but this challenge (and workshop) provided a unique opportunity to highlight it and raise awareness of this important outcome among the electronic-structure community. The other outcome was the importance of describing initial conditions adequately and the challenge in describing experimental observables.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

The outcome of this workshop is mostly fundamental. Yet, the prediction challenge made it clear to the experimental community, which performs multi-million experiments at advanced light sources, that computational photochemistry is mature enough to provide information ahead of the experiment, thereby maximizing the chance of success during beamtime.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The primary tangible outcome of the workshop will be a perspective article, which will be published in the Journal of Chemical Physics. The planned submission date is the end of the summer (2025). Another outcome of the workshop is the idea to organize a discussion meeting that will bring together members of the nonadiabatic and electronic-structure communities.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

Our workshop had a broad diversity in terms of gender, geographical origin, and career stage. All participants contributed to the numerous discussions during the workshop, further highlighting the overall good and friendly atmosphere during the workshop. A session was organized to discuss the diversity of the prediction challenge, and recommendations for future iterations of the challenge were suggested (connected to its time constraint).

7. Participant list

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Modeling & simulation of fluid-structure interactions across scales

Location: CECAM-IT-SISSA-SNS, Slovenia

Webpage : Event webpage

Dates: Apr 8, 2025 - Apr 11, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

Modeling and simulation of complex systems span a wide range of disciplines, from biology and chemistry to engineering and beyond. Understanding these systems requires a multiscale approach that integrates processes from molecular interactions to macroscopic behavior. This is crucial for tackling challenges in diverse fields such as bioliquids, energy storage devices, and helicopter dynamics. In bioliquids, multiscale modeling plays a pivotal role in unraveling the complexities of biological processes. Multiscale models not only enhance our fundamental understanding of biological systems but also have practical applications in drug design and personalized medicine. Similarly, the design and optimization of batteries demand a multiscale perspective to address issues ranging from electrode materials to system-level performance. Atomistic simulations provide insights into the behavior of ions and electrons within electrode materials, guiding the development of novel chemistries with enhanced energy storage capabilities. Meanwhile, continuum models facilitate the prediction of battery performance under various operating conditions, aiding in the design of safer and more efficient energy storage devices. In the field of helicopter dynamics, multiscale modeling enables engineers to simulate the interaction between aerodynamics, structural mechanics, and control systems. By integrating these disparate disciplines, engineers can optimize helicopter design for improved performance, maneuverability, and safety. Despite significant advancements, multiscale modeling of complex systems still faces challenges. Bridging the gap between different scales, accurately representing system dynamics, and incorporating uncertainty remain areas of active research. Furthermore, the increasing complexity of modern systems demands innovative computational techniques and interdisciplinary collaboration. In conclusion, the state of the art in multiscale modeling and simulation of complex systems encompasses a diverse range of applications, from bioliquids and batteries to helicopters. By integrating knowledge across multiple scales, researchers strive to unravel the mysteries of nature, optimize technological innovations, and address pressing societal challenges.
The scientific program addressed several key areas in this field, including cutting-edge hydrodynamics methods, multiscale approaches for coupling different models and methods across length scales, the use of artificial intelligence techniques to improve couplings, boundary conditions, and constitutive equations, as well as large-scale simulations of hydrodynamic applications. Additional attention was paid to high-performance computing enabling technologies (e.g., GPUs), software packages (e.g., MetaWalls, Tinkerhp, ESPResSo, and lammps), and workflows (e.g., eessi, StreamFlow, and capio).

2. What were the primary outcomes of this workshop, including limitations and open questions?

The participants enjoyed the variety and quality of the lectures. Although the workshop covered a wide range of topics, participants with different scientific backgrounds and interests did not find the lectures (too) challenging. However, many would prefer shorter, more pedagogical lectures that focus on some of the general challenges in the field and allow participants familiar with different modeling techniques to learn from each other. Most of the participants appreciated the discussion sessions where opinions and current challenges, as well as solutions in the field of supercomputing were debated. Overall, participants enjoyed the talks and appreciated the ample time for networking, and in the end rated the workshop as excellent. To document scientific contributions, a book of Abstracts was compiled and published on the cobiss platform. The collection is available online at https://plus.cobiss.net/cobiss/si/en/bib/231451395#full. Participants were also provided with a BibTeX citation template to reference their work, and the publication was shared via the workshop mailing list.

3. What was the take-home message for the participants?

The event provided an important opportunity to understand the needs of the community working on multiscale fluid-structure interaction modeling. Informal discussions during social events and poster sessions allowed participants and organizers to exchange ideas about ongoing projects and explore new research directions. The recordings of presentations are available on both the MultiXscale website and the Lhumos portal, ensuring continued access to the event's content.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

This flagship workshop successfully fostered scientific exchange, skill-building, and new collaborations within the CECAM community and beyond. We thank all participants for their active involvement and look forward to future opportunities to build on the momentum created during this event.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

New collaborations have been established between members of MultiXscale CoE and some of the remaining participants on the topics related to biomolecular systems and sustainable energy.
These collaborations are concerned with scientific collaboration as well as software developments.
New proposal submissions were also discussed and are planned.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

Most of the on-site participants came from prominent European research institutes, representing a diverse range of backgrounds. Of the total of the attendees, 41 identified as male and 14 as female. The vast majority came from academia (51), with smaller numbers from industry (2) and other institutions (2). Geographically, the workshop brought together researchers from 10 countries, including Slovenia, Italy, Germany, France, Spain, the United Kingdom, Switzerland, the United States, and Iran. Most of the participants were based in Europe, with single representatives from Asia and North America. The highest national representation came from Slovenia (26 participants), followed by France (7), Germany and Italy (6 each), Spain (5), the United Kingdom (2) and one participant each from Switzerland, the United States, and Iran.

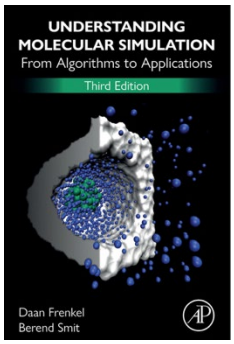
7. Participant list

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Grigori, Laura - EPFL & PSI, Switzerland
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Vannozzi, Carolina - None, Italy
Vasin, Semen - INSA Lyon, France
Zhou, Zihan - Technical University of Munich, Germany

Understanding Molecular Simulation



Location: CECAM-CN, China

Webpage : Event webpage

Dates: Apr 25, 2025 - May 3, 2025

1. What were the major topics presented in the School?

This week-long school offers a program focusing on numerical techniques for studying properties of many-particle systems. It targets PhD and postdoctoral researchers who want to learn these techniques to study topics in physics, chemistry or biology. The course may also be followed by advanced MSc students. It offers a recap of the statistical mechanics relevant for molecular simulation and addresses basic and advanced simulation techniques including Monte Carlo, molecular dynamics, free energy calculations, rare events, modelling systems with many-body and long-range interactions, and coarse graining procedures – without discussing particular software packages. Additionally, two special topics will be organized on machine learning and on modelling of the fluid flow. The school consists of an integrated program of lectures and hands-on exercises mostly based on the book “Understanding Molecular Simulation" by Frenkel and Smit. Exercise handouts and copies of the lecture slides will be provided. A poster session will be an opportunity for participants to present their research in an informal setting.

2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

No particular limitations or open questions have been identified. If anything, it was challenging to achieve that the students were active and asking questions (mostly due to cultural differences), but eventually this was achieved and the hands-on session proved to be lively and useful.

3. What was the take-home message for the participants?

Despite the rise of AI, it is still extremely useful to understand the basics of molecular simulation and to code simple programs yourself. This can prevent mistakes produced by just using AI...

4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

Lecture slides and hands-on exercises are hosted on the Bohrium platform (https://bohrium.dp.tech/) developed by one of the sponsors of the school.

5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The few speakers were selected on the basis of their expertise. We accepted all participants (in total 150) and charged no registration fee. The gender balance turns out to be good with about 40% of female students. As the school was organized in Beijing, naturally the majority of students were Chinese, but there were around 20 international students attending as well.

6. Participant list

Organisers
Dobnikar, Jure
Institute of Physics, Chinese Academy of Sciences, China
Frenkel, Daan
U Cambridge, United Kingdom
Pagonabarraga, Ignacio
University of Barcelona, Spain

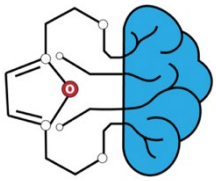
Alibakhshi, Amin - SISSA, Italy, Italy
Bai, Shiyi - The Hong Kong University of Science and Technology, China
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Bensassi, Abdelghani - Mohammed V University, Morocco
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Chen, Ziqiang - Xiamen University, China
Chen, Jiahang - University of Chinese Academy of Sciences, China
Chen, Bolin - UCAS, China
Chen, Jiadong - Peking University, China
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AIChemist



Location: CECAM-HQ-EPFL, Switzerland

Webpage : Event webpage

Dates: Apr 28, 2025 - May 2, 2025

1. What were the major topics presented in the School?

The AiChemist CECAM Flagship School brought together a diverse group of researchers and students to explore the intersection of artificial intelligence (AI), machine learning (ML), and chemical sciences. A central theme of the school was the **prediction and optimization of chemical reactions** using machine learning. Lectures covered a wide range of topics, from retrosynthesis and reaction condition optimization to the use of large-scale reaction databases and generative models. Tools such as AiZynthFinder and web-based modeling and visualisation applications were introduced, enabling participants to explore multistep synthesis pathways interactively. Another major focus was on **machine learning potentials (MLPs)** and their application in molecular simulations. Several talks highlighted how MLPs can be trained on quantum mechanical data to simulate complex chemical systems with high accuracy and efficiency. These methods were applied to study reaction mechanisms, solvation effects, and excited-state dynamics. **Large language models (LLMs)** and **transformers** were another highlight, with presentations demonstrating their use in encoding chemical knowledge, predicting molecular properties, and even controlling robotic synthesis platforms. The integration of LLMs with cheminformatics tools showcased the potential of AI to automate and accelerate the drug discovery pipeline. Several lectures also touched on improving **model interpretability and explainable AI (XAI),** a critical area for ensuring the interpretability and trustworthiness of AI models in chemistry. Hands-on sessions complemented the lectures, offering practical experience with retrosynthesis tools, transformer models, and multi-task learning for compound profiling using QSAR.
The poster session showcased a diverse, innovative range of research at the intersection of AI and chemistry. Key themes included advancements in **retrosynthetic planning**, as well as the **integration of quantum mechanical data with ML for reaction feasibility prediction** and charge assignment. Several contributions focused on **XAI**, and others explored topics in drug discovery such as **personalized cardiotoxicity prediction** using pharmacovigilance data and **privacy risks** in neural network publication. **Environmental applications** were also featured, including the in-silico design of enzymes for PFAS degradation and the development of nano-QSAR models for nanoparticle toxicity prediction.

2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

In the field of MLPs: Universal MLPs for accurately predicting reactivities are starting to gain traction but still require more work. Many effective methods for accounting for long-

range interactions have been developed, but accounting for changes in oxidation state with MLPs is still very challenging and expensive.
In the field of ML for biomolecular simulations: Traditional molecular dynamics simulations are limited by timescale bottlenecks, and while ML can accelerate sampling, capturing rare events and long-timescale dynamics remains difficult. Bridging resolution gaps without losing essential information is still a challenge.
In the field of computer-aided synthesis planning: Reaction datasets are often incomplete, biased, and lack negative examples, limiting model training and generalization. Models often struggle to adapt across different chemical domains, requiring improved transfer learning and domain adaptation techniques. The field still lacks standardized benchmarks and reliable metrics to fairly assess and compare synthesis planning tools.
In the field of protein-ligand complex prediction: Accurately modelling both rigid and flexible docking scenarios, including side-chain movements and induced fit effects, remains a major computational challenge. Bridging the gap between computational predictions and experimentally validated structures is still difficult, especially for novel or poorly characterized targets.
In the field of LLMs for chemistry: Uncertainty quantification is still a challenge, but recent advances such as integration of LLMs with Gaussian Processes provide grounds for optimism. Nevertheless, these approaches are computationally expensive, interpretability of learned representations is limited, and testing in real-world industrial pipelines is yet to be done. LLMs must be adapted to extract meaningful insights from noisy, incomplete, or informal data sources to mitigate tacit knowledge loss. There is a need for multimodal models that can combine language with visual and structural data for richer scientific understanding.

3. What was the take-home message for the participants?

ML/AI is transforming synthesis, reactivity, and molecular design, while redefining tools and methods available to chemists. Participants explored retrosynthesis, MLPs, LLMs, and GNNs, gaining insights into interpretability, data quality, and domain knowledge for building trustworthy AI models, and real-world use cases. Chemistry's future lies in blending data-driven innovation with expert insight, to tackle complex challenges with greater precision, efficiency, and creativity.

4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

- Video recordings of almost all lectures will be made available on Lhumos, and will also be made available on AiChemist/YouTube website. 8 out of 24 speakers consented to recording.
- The hands-on tutorial by Kevin Jablonka is available on GitHub for all participants (online and offline) and a recording of the hands-on session too.
- For the hands-on by Gilles Marcou, materials were sent via email to all participants, and a recording of the hands-on session will be available on Lhumos.

5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The organisers met regularly to plan the program and organise invitations to speakers and attendees. From the start, we aimed to have a 50/50 split of male and female speakers and a good balance of more senior researchers/professors, recently established group leaders and early career researchers (PhD students and postdocs), without compromising on the quality of the program and the level of expertise of the speakers. We also made sure to feature a handful of lecturers from speakers working in industry, so that participants had some exposure to the practical use of AI in chemical/pharmaceutical industries. The same strategy was adopted for selection of attendees, ensuring a mix of different academic backgrounds (chemistry, biology, nanotechnology, computer science, materials science) and cultural backgrounds (European, Asian, South American, American, African) to maximise opportunities for interdisciplinary, intersectoral and cultural exchange.

6. Participant list

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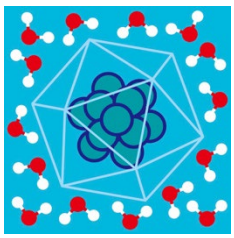
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Crystallization and Self-Assembly: from Soft Matter to Pharmaceuticals to Biomineralisation



Location: Roscoff CNRS Conference Centre, France

Webpage : Event webpage

Dates: May 5, 2025 - May 7, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

Crystallisation and self-assembly are everyday phenomena with great industrial and environmental importance. The underlying process of a drop in free energy leading to ordering is exhibited by a very wide range of systems and length scales. This includes systems where the self-assembling building blocks are atoms, (bio)molecules, proteins, colloids, and even granular particles. The aim of this workshop was to bring together a broad group of experimental, theoretical, and computational research with an interest in different self-assembly processes.

Broadly, the discussion at the workshop could be divided into four major topics:

- **Controlling and understanding phase behavior.** A large share of our understanding of self-assembly derives from having clear knowledge of the phase behavior of a given system. Topics discussed here include novel simulation methods for probing phase behavior, techniques for experimentally tuning the interactions between particles to tune relative phase stability, and the bottom-up design of particles with selective interactions (often DNA-based) optimized to specifically form desired structures.
- **The physics of nucleation and polymorph selection.** Several talks were dedicated to the fundamentals of classical nucleation theory, and the possibility of non-classical nucleation pathways.
- **Non-equilibrium self-assembly.** A number of presentations addressed the key role that kinetic effects play in many self-assembly processes, both in systems that are inherently out of equilibrium (active, living, or driven matter) and in equilibrium systems that can get kinetically trapped in non-equilibrium states.
- **Bridging communities.** An explicit intention of the workshop was to build links between communities, for example those working on fundamental systems (colloids, simple models of water) and those in more applied fields (biomineralization, MOFs, nanoparticles). An example of such bridging was the talk of Molinero, who used basic models to address a relatively complex clathrate system.

For all four of these topics, the systems discussed again covered a wide range of systems. A key takeaway from this meeting is that similar methodologies and open questions arise at all length scales that are relevant for self-assembly processes. By bringing people from different communities (colloidal, biomineralization, active matter, DNA-based design) together and exchanging expertise, this workshop has aided in the spread of methodologies and insights across a wide range of fields.

2. What were the primary outcomes of this workshop, including limitations and open questions?

Primary outcomes:

- **Exchange of insights into different systems.** Perhaps the most important aspect of the workshop was the inclusion of experts in self-assembly processes taking place in highly different systems. Numerous presenters shared their findings and insights related to intriguing self-assembly phenomena in systems spanning length scales ranging from the atomic to the colloidal scale, based on both experiments and simulations. To this end, the workshop included e.g. several sessions on colloid and nanoparticle self-assembly, two sessions on biomineralization, and a session on water crystallization. Other topics included pharmaceuticals and metal-oxide frameworks.
- **Exchange of computational and theoretical methodology.** From a computational perspective, enhancing our understanding of self-assembly methods requires reliable theoretical and simulation approaches to probe phase behavior and nucleation processes. Advances in this area that were discussed include the design of new simulation methods for efficiently simulating systems with long-range interactions (Krauth), methods for probing polydisperse phase transitions (Castagnède), and seeding-based approaches to studying nucleation (Li). Additionally, there was stimulating discussion on the interpretation and potential limitations of classical nucleation theory, and the capillarity approximation often used therein (Russo, Vega).
- **Exchange of design strategies.** A key open question in the field of self-assembly is how to design model systems that reliably self-assemble into a given target structure. A number of useful methodologies were discussed that assist in this quest. This includes design strategies based on e.g. satisfiability criteria (Sciortino), and topological defect engineering (Lenz), as well as the development of software to assist in designs for DNA origami (Schabanel).

The discussion session at the end of the workshop identified several challenges and opportunities:

- DNA-based engineering of nano structures has made impressive advances. It would be interesting to explore whether similar strategies could be employed in the engineering of proteins (for e.g. pharmaceutical use) or for controlling their crystallization. A significant amount of trial and error is still used in this field, and hence improving control over their behavior by drawing inspiration from other fields could be highly beneficial.
- Major advances have been made in understanding biomineralization processes, but the relevance of multiple crystal structures whose selection is strongly influenced by many factors present in living systems makes this phenomenon complex from a fundamental perspective. Aspects like the competition between nucleation and aggregation, the possibility of guided (by e.g. proteins) crystallization, and the presence of non-equilibrium effects make these systems challenging for theory. New insights would be welcome here.

3. What was the take-home message for the participants?

The key take-home message was that study of self-assembly at different scales and in many different systems faces similar challenges and open questions, and can benefit from sharing methods and design strategies.

A central aim was to bring together researchers from different fields. One observation, from those in more applied fields, was the degree to which nucleation and assembly are highly active and challenging areas of research even for well-understood model systems.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

Nucleation and self-assembly are key processes that take place essentially everywhere: they are vital for life, for many technological and industrial processes, and in determining the weather, to name a few examples. While a significant part of this workshop was aimed at the fundamentals of self-assembly, as these are universal across different fields, there were numerous discussions that explored these fundamentals in the context of systems with real-world importance.
A clear example of this are the biomineralization sessions, in which the overall goal of much of the research is to better understand vital processes in living organisms, in particular understanding deposition of calcium carbonate in corals and bones. The former is threatened, while the latter opens application in bone tissue engineering. The talk by Wolf addressed development in our understanding of calcium carbonate crystallisation while Nassif addressed tissue engineering. Another key application for crystallisation of calcium carbonate is limescale and its suppression. Mechanisms by which limescale can be controlled were discussed by De Yoreo.
Among the greatest uncertainties in climate change modelling is the rate of water droplet nucleation in the atmosphere. The water session in particular included a presentation of the role of interfaces in water nucleation by Tanaka.
Additionally, an overarching goal in the study of colloidal self-assembly is the design of new functional materials, whose microscopic structures give rise to materials with a pre-designed response to e.g. plasmonic, photonic, or mechanical stimuli. A key example here is the plasmonic nanoparticle systems discussed by Truskett.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The workshop gave rise to many fruitful discussions between participants, which are likely to spark new collaborations and research avenues. While not all of these are directly known to us as the organizers, we are aware of new collaborations between the groups of John Russo (Rome) and Laura Filion (Utrecht) on nucleation of patchy particles, and the groups of Julien Lam (Lille) and Frank Smallenburg (Orsay) on machine learning of colloidal interactions. Additionally, Yiyeoun Kim (Leeds) and Stefan Wolf (Erlanglen-Nuremberg) are planning a network around bio-inspired crystallisation for industry applications.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The workshop included around 75 participants in total. This was enabled by securing additional funding from the Agence Nationale de Recherche and the GDR Soft Physics

for Hard Materials (France). For the selection of invited and contributed speakers, gender balance, geographical origin, career stage, and diversity in terms of scientific fields were all considered. The workshop was advertised via the (world-wide) soft matter mailing lists, as well as more local channels.
The workshop included participants from 15 different countries (France, China, Germany, India, Israel, Italy, Japan, Netherlands, Norway, Slovenia, Spain, Sweden, Switzerland, United Kingdom, and United States). The participants were a mix of researchers at different career stages, with invited talks mixed between early-career and senior researchers, while contributed talks and poster presentations were available mostly for younger researchers (including PhD students). Of the speakers, 27% were female.

7. Participant list

Organisers
Cugliandolo, Leticia
Sorbonne Université, France
Leocmach, Mathieu
CNRS, France
Royall, C. Patrick
ESPCI Paris, France
Smallenburg, Frank
CNRS, Université Paris-Saclay, France

Abécassis, Benjamin - École Normale Supérieure de Lyon, France
Aizen, Ruth - Tel Aviv University, Israel
Albéric, Marie - CNRS Sorbonne Université, France
Andarzi, Sahar - Sorbonne University, France
Arif, Mariam - University of Edinburgh, United Kingdom
Ayre, Oliver - University of Leeds, United Kingdom
Azaïs, Thierry - Sorbonne Université, France
Bonn, Daniel - Institute of Physics, University of Amsterdam, Netherlands
Brar, Yashpal Singh - Scuola Superiore Sant'anna, Italy
Carn, Florent - Université Paris Cité, France
Castagnede, Antoine - Laboratoire de Physique des Solides, France
Chakrabarti, Dwaipayan - University of Birmingham, United Kingdom
Charbonneau, Patrick - Duke University, United States
Chen, Pengxu - University of Edinburgh, United Kingdom
Cottin-Bizonne, Cecile - University Lyon 1, France
De Yoreo, James - Pacific Northwest National Laboratory, United States
Diharce, Jeremy - Sorbonne Université, France
Dijkstra, Marjolein - Utrecht University, Netherlands
Durelle, Maxime - University of Leeds, United Kingdom
Engel, Michael - Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany
Filion, Laura - Debye Institute for Nanomaterials Science, Utrecht University, Netherlands
Fraden, Seth - Brandeis University, United States
Gauffre, Fabienne - Rennes Institute of Chemical Sciences, France
Gonnella, Giuseppe - University of Bari Aldo Moro, Italy
Grelet, Eric - CNRS & University of Bordeaux, France

Grisanti, Luca - Consiglio Nazionale Delle Ricerche, Italy
Hedderick, Konrad - Université de Genève, Switzerland
Herboth, Radost Milena - Stockholm University, Sweden
Issoufou Alfari, Leila - Université Claude Bernard Lyon 1, France
K, Nagalingam - NITT, India
Kim, Yi-Yeoun - University of Leeds, United Kingdom
Koehler, Lara - MPI for the Physics of Complex Systems, Germany
Krauth, Werner - Ecole Normale Supérieure de Paris, France
Kürten, Lars - ESPCI Paris, France
Lam, Julien - CNRS, France
Lenz, Martin - U. Paris-Saclay, ESPCI & CNRS, France
Li, Lunna - University College London, United Kingdom
Marin-Aguilar, Susana - Sapienza University of Rome, Italy
Mendez, Emilio - Sorbonne Universite, France
Molinero, Valeria - University of Utah, United States
Mondal, Sangita - Sorbonne Université, France
Mondal, Soumya - IIT DELHI, India
Nassif, Nadine - CNRS, France
Nawani, Akanksha - Sorbonne University, France
Neha, Neha - Indian Institute of Technology Delhi, India
Paloni, Matteo - University College London, United Kingdom
Peraza Ku, Silvia Argelia - Institute des Sciences Chimiques de Rennes, France
Poletayev, Andrey - University of Oxford, United Kingdom
Roach, Lucien - École Normale Supérieure de Lyon, France
Russo, John - Sapienza University Of Rome, Italy
Sacanna, Stefano - New York University, United States
Salvalaglio, Matteo - University College London, United Kingdom
Sastry, Srikanth - Jawaharlal Nehru Centre for Advanced Scientific Research, India
Schabanel, Nicolas - ENS Lyon, France
Schreiber, Frank - Universität Tübingen, Inst. für Angewandte Physik, Germany
Sciortino, Francesco - Sapienza, University of Rome., Italy
Sear, Richard - University of Surrey, United Kingdom
Semino, Rocio - PHENIX, Sorbonne Université, France
Sidler, Elizaveta - NTNU, Norway
Speck, Thomas - University of Stuttgart, Germany
Tanaka, Hajime - University of Tokyo, Japan
Trokhymchuk, Andrij - University of Ljubljana, Slovenia
Truskett, Thomas - University of Texas at Austin, United States
Turci, Francesco - University of Bristol, United Kingdom
Valeriani, Chantal - Universidad Complutense de Madrid, Spain
Van Mastrigt, Ryan - ESPCI Paris, France
Vega, Carlos - Universidad Complutense de Madrid, Spain
Wang, Chaohong - Utrecht University, Netherlands
Wang, Junwei - Eastern Institute of Technology, Ningbo, China
Wilding, Nigel - University of Bristol, United Kingdom
Wolf, Stephan - Friedrich-Alexander University Erlangen-Nürnberg, Germany
Zelenskiy, Andrey - CNRS, France

Machine Learning for Materials Discovery (ML4MD)



Location: CECAM-FI, Finland

Webpage : Event webpage

Dates: May 5, 2025 - May 8, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The major theme of the event was machine learning (ML) for materials discovery. The subthemes were generative AI, active learning, and machine learning potentials for periodic, polymer, and inorganic materials. The speakers highlighted the current state-of-the art in exploration of the chemical / materials space as a key driver of novel discovery as well as cautionary tales on the overreliance of benchmarks. Invited speakers came from both academic and industrial backgrounds, which provided a good overview for diverse flavours of ML methods. The industry speakers discussed how ML methods are being utilized in real-world applications and how we can continue to push the boundaries of materials discovery via industry-academia crosstalk. During the workshop we hosted two panel discussions where audience members were able to ask either specific questions regarding ML-guided discovery of certain materials, or more broadly on the state of the field and where effort should be invested. Both panels highlighted the need for domain-specific expertise as a bottleneck in many machine learning-based discoveries and the need for continued multidisciplinary education. Overall, we showcased to the community the latest developments in ML, how to utilize them, and what pitfalls to watch out for.

2. What were the primary outcomes of this workshop, including limitations and open questions?

The workshop brought together researchers from computational chemistry, physics, and machine learning to explore the latest advancements and persistent challenges in AI-driven materials innovation. The discussions highlighted both the transformative potential of machine learning (ML) in accelerating materials discovery and the key hurdles that must be addressed to translate these methods into real-world applications. One of the central themes of the workshop was the development of novel machine learning approaches tailored for materials science. Graph neural networks (GNNs) and transformer-based architectures emerged as powerful tools for predicting material properties. Additionally, there was significant emphasis on improving model interpretability through reasonable benchmarking and/or uncertainty quantification. Several contributors showcased how active learning could enable inverse materials design coupled with ML-enabled high-throughput DFT calculations.
The panel discussions highlighted the need for open communication during industry-academia collaborations and the need for domain-specific expertise to continue to push forward novel ML that is specific to the field of materials. Several open questions emerged from the discussions, pointing toward future research directions. One unresolved issue

was the method to incorporate the domain knowledge into ML: whether through hybrid physics-ML approaches or symbolic regression techniques. Another pressing topic was the role of data requirements: how much data, and what kind of data, should we request for publication.

3. What was the take-home message for the participants?

The take-home message we aimed for was the depth of progress we have made in materials discovery with machine learning: from hybrid DFT-ML aided calculations to automation of laboratories, polymer discovery and use of large language models for predicting the materials. However, we highlighted that there is still so much more room for development.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

The workshop not only advanced the technical frontier of ML in materials science but also highlighted numerous pathways through which these innovations could yield tangible societal benefits. By accelerating the discovery and optimization of next-generation materials, the research presented at this workshop holds promise for addressing critical global challenges: sustainable energy, healthcare, biomaterials.
One of the most compelling societal implications lies in the transition to clean energy. Machine learning's ability to rapidly screen and design materials could revolutionize renewable energy technologies, such as high-efficiency solar cells, advanced battery systems, and catalysts for green hydrogen production. Similarly, the numerous posters on materials for carbon capture underscored how ML could help identify porous polymers or metal-organic frameworks (MOFs) with unprecedented efficiency in sequestering CO_2, offering a technological lifeline in the fight against climate change.
Faster discovery of materials for medical devices will shorten development cycles and reduce costs, making critical treatments more accessible worldwide. The societal impact also extends to industrial innovation and economic resilience. By reducing the time and cost associated with traditional trial-and-error experimentation, ML-driven materials discovery will help industries develop better materials at a fraction of the cost. Furthermore, the democratization of materials informatics, exemplified by our workshop, will allow for the seamless transition of siloed education models to an integrated one where early career researchers are able to explore the tangible benefits of ML from day one.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

While concrete outcomes such as publications or new collaborations are still developing, the workshop laid strong foundations for future impact. ML4MD 2025 brought together researchers and industry experts, facilitating knowledge exchange during talks, coffee breaks, and poster sessions. These interactions often lead to joint proposals and collaborative projects. We anticipate the submission of workshop-inspired publications,

as feedback received during the workshop can help participants develop their posters and talks into full manuscripts.
The event highlighted future funding opportunities through pan-European supercomputing resources like LUMI, which can result in more research utilizing these infrastructures.
Post-workshop feedback indicates strengthened scientific networks, valuable peer input, and professional development, key ingredients for impactful research and long-term collaboration.

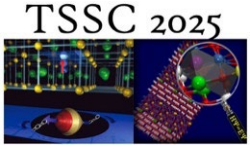
6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

We actively encouraged women and early career researchers to participate, and waived the registration fee to support broader access to the event. During speaker selection, we considered both the diversity of research ideas and the background of our speakers. As a result, 21% of the in-person attendees and 20% of our speakers were women. We hosted the event in a hybrid form, enabling the attendees to participate through a Zoom webinar. We structured the event program in a way which ensured that each day covered a wide range of topics. We planned the event such that travel to and from the conference could be done during the work week. Finally, we made sure to start the conference no earlier than 9 am and to have regular breaks to accommodate those with health conditions that prevent them from attending early in the morning or for sustained periods of time. The sessions were recorded so that those who missed a talk could watch at their own convenience.

7. Organiser list

Organisers
Dzeroski, Saso
Jozef Stefan Institute, Slovenia
Galica, Tomasz
University of Turku, Finland
Henkel, Pascal
Aalto University, Finland
King-Smith, Emma
University of Edinburgh, United Kingdom
Rinke, Patrick
Technical University Munich, Germany
Todorovic, Milica
University of Turku, Finland

Theoretical Solid-State Chemistry: theory, modelling, and simulation



Location: CECAM-ES, Spain

Webpage : Event webpage

Dates: May 5, 2025 - May 9, 2025

1. What were the major topics presented in the School?

- Electronic Structure. Cluster and periodic models. Kohn-Sham equations and DFT methods.
- Thermodynamic Properties. Static models. Equation of state of solids. Phase transitions.
- Macroscopic Maxwell equations. Hamiltonians for light-matter interaction. Time-dependent evolution of a periodic system under electric fields. Absorption and reflectivity.
- Multiscale methods. Scaling in the construction of the Hamiltonian. Linear scaling techniques. Metals, insulators, and the Fermi energy. QM/MM and force-fields. Excitons and polarons.
- Structure of solids' surfaces: relaxation, rumpling, and reconstruction of surfaces. Surface energies. Surface defects. Reactivity at surfaces.
- Phonons and dispersion curves. Free energy. Quasi-harmonic approximation. Thermal properties. Anharmonicity and thermal transport.
- Topologies of scalar fields in crystals. Electron density, electron localization function and reduced density gradient chemical functions.
- Effective Magnetic Hamiltonian theory. Spin waves for ferromagnets. Antiferromagnetic lattices. Electron transport. Magnetic anisotropy, double exchange, and spin wave theory.

2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

The different specialists of each area paid particular attention to the approximations used in the simulations so that the students can understand critically the advantages and limitations of each technique. The level of the school is too basic to enter into open questions in the atomistic modelling of solids. Anyway, known limitations of current state-of-the-art density functional methods are mentioned. With respect to surfaces, the limitation of models regarding experimental coverages of adsorbates and the open problem of predicting surface reconstructions in real catalytic conditions (temperature and reactant pressure) have been discussed. The need to go beyond the harmonic or quasi-harmonic approximation to properly describe heat transport have also been addressed. During the practical sessions a relatively large part of the students (around 1/3) asked the presenters questions about their particular projects related to Master's and PhD theses. In some cases, these questions involved relatively advanced problems

like gap calculation in large systems or the best way to deal with correlation in metals containing 3d elements.

3. What was the take-home message for the participants?

The school provides the students with a wide toolkit with which to approach many facets of Solid-State Chemistry with applications in important current topics of the area.

4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

Lecture notes for theoretical sessions and hands-on tutorials for the practical sessions are deposited in the CECAM web page for the school. In addition to these, input files for the practical sessions are also provided to ensure that all exercises can be completed within the tight schedule of the course.

5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

We hosted a total of 24 students this year, coming from Finland (2), France (4), Italy (1), Poland (1), Spain (13), Switzerland (2), and India (1). One third of the speakers are female as well as about 20% of the students.
We are open to geographical provenance of the participants, but its geographical location results in a majority of students coming from European countries.

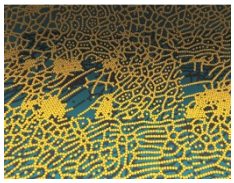
6. Participant list

Organisers
Garcia Fernandez, Pablo
Universidad de Cantabria, Spain
Márquez, Antonio M.
Universidad de Sevilla, Spain
Rodriguez, Sandra
Universidad Autónoma de Madrid, Spain

Appel, Lisa - ETH Zurich, Switzerland
Asensio Montejo, Cintia - Universidad Autónoma Madrid, Spain
Baptista Santos, Aelton - Institut Laue Langevin - Université Grenoble Alpes, France
Boujon Blanco, Lucas Martín - University of Oviedo, Spain
Contreras, Alexander - Instituto de Catálisis y Petroleoquímica, Spain
Di Muzio, Simone - Consiglio Nazionale Delle Ricerche, Italy
García García, Samuel - Universidad de Oviedo, Spain
Giacomelli, Andrea - Ecole Normale Superieure de Lyon, France

Giardino, Matteo - Politecnico di Torino, Italy
Gómez Arroyo, David - Universidad Autónoma de Madrid, Spain
Gonzalo Alcega, Jorge - University of Zaragoza, Spain
Mitro, Sujon Kumar - University of Bremen, Germany
Molina Nogal, Laura - ICP, CSIC, Spain
Morales Quijano, Miguel - Universidad Autónoma de Madrid, Spain
Nagy, Dániel - University of Oulu, Finland
Olivieri, Jean-François - Université Paris-Saclay, France
Ramos, Carmen - University Jaume I, Spain
Ruiz Aranda, Iris - University of Valencia, Spain
Ruiz Rodas, David - Universidad Autónoma de Madrid, Spain
Saric, Lovro - University of Bern, Switzerland
Shakeri, Mohammad Sadegh – IFJ PAN, Poland
Sobiecki, Piotr - University of Oulu, Finland
Soler Colomina, Sergio - Universitat de Valencia, Spain
Sujal, Sujal - Universidad Del País Vasco, Spain
Vazquez, Mariano - Universidad Autónoma de Madrid, Spain
Xu, Rongrong - Trinity College Dublin, Ireland
Yadav, Anjali - Institut Néel, CNRS, Universite Grenoble Alpes, France

Future directions in non-equilibrium statistical physics



Location: KITS Beijing, China

Webpage : Event webpage

Dates: May 5, 2025 - May 9, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

Recently there has been an explosion of interest in non-equilibrium statistical physics ranging from active matter and biophysics to driven classical and quantum systems [3]. The progress which has been made is impressive but has often been isolated in communities dedicated to specific problems and/or to specific techniques, with little cross interaction or even communication between, e.g., the new developments in classical and quantum systems. The idea of this conference is to bring together a wide variety of physicists working on out of equilibrium systems and to enable the sharing of their ideas and to seek out common ground and challenges. Building on the success of the 2019 workshop on “Soft Matter Out of Equilibrium: from driven to active systems" in Beijing, we envision to facilitate this exchange by inviting leading scientists who will deliver keynote pedagogical talks on challenges and advances, which could then catalyse more detailed and in depth exchanges between the participants.

2. What were the primary outcomes of this workshop, including limitations and open questions?

The workshop / conference brought together a diverse range of speakers from a broad field of nonequilibrium physics - ranging from quantum transport phenomena, classical analytical theory to fluids to soft and biological matter. Due to the large number of speakers that accepted to join the meeting, the meeting eventually turned out to be slightly larger than a typical CECAM workshop and more like a small conference. Regardless, the discussion sessions were well received and lively - discussing topics such as implementation of functional integral techniques, the status of the Onsager variational principle, Lindbladian methods and projection operator techniques as well as novel numerical methods such as rejection free and irreversible Monte Carlo schemes, to list a few among a long list of possibilities. Unfortunately, one of the organizers, Prof. Rudi Podgornik, passed away in December 2024, and the workshop has not be the same without Rudi's active contribution! During the workshop, we have organized a special day where Rudi's collaborators presented with emphasis on the work Rudi had been involved in. The entire meeting was dedicated to his memory.

3. What was the take-home message for the participants?

There is a lot to understand in nonequilibrium statistical physics, but there are also several surprising connections between the topics that traditionally do not talk to each other...

4. Does the outcome(s) of the workshop hold potential for societal benefits?

In principle yes, but this workshop was focused on fundamental questions and while the topics certainly have an important impact on the society, this was not central to the discussions.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The week-long meeting resulted in lively discussions, social gatherings and lots of new ideas and collaboration plans.

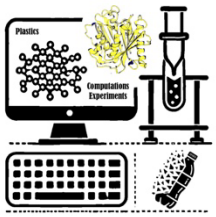
6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

We had a mixture of speakers from all career stages, European and Asian nationalities and both genders. We would wish for a slightly better gender balance, however, several rejections to our invitations and a general difficulty of attracting participants from the USA resulted in the slightly lower percentage of female speakers (about 20).

7. Organiser list

Organisers
Dean, David
University of Bordeaux, France
Dobnikar, Jure
Chinese Academy of Sciences, China
Podgornik, Rudolf
Chinese Academy of Sciences, China

Computations meet Experiments to Advance the Enzymatic Depolymerization of Plastics One Atom at a Time



Location: SISSA, Italy

Webpage : Event webpage

Dates: May 6, 2025 - May 8, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop on enzymatic plastic depolymerization convened researchers and industry experts to advance biocatalytic strategies for plastic pollution and the circular economy. Key themes included enzyme engineering, structure-function characterization, discovery of novel biocatalysts, process upscaling, and sustainable polymer design.

The event reaffirmed the potential of microbial enzymes—such as PET hydrolases, amidases, and wax worm-derived hexamerins—to degrade plastics like PET, polyurethane, and polyethylene under mild conditions. Advances in protein engineering, powered by machine learning, molecular dynamics, and QM/MM simulations, significantly improved enzyme activity and stability. Engineered PHL7 variants achieved over 120-fold activity increases, highlighting industrial potential and the value of integrating computational design with experimental validation.

Techniques like Rosetta modeling, deep learning, and allosteric network analysis provided insights into enzyme–substrate interactions and mutational effects, enabling precise performance tuning beyond active sites.

Enzyme discovery from marine metagenomes, mangrove soil consortia, and insect microbiomes expanded the biocatalytic toolkit. Promiscuous amidases targeting nylon-6 and polyester-polyurethane were identified, while Ancestral Sequence Reconstruction combined with Directed Evolution yielded robust, tailored enzymes.

Sustainable polymer design and upcycling were also key topics. Bio-based polyester synthesis under green chemistry principles, supported by docking and ML-guided ecotoxicity predictions, aligned with “Safe and Sustainable by Design” goals. Enzymatic cascades integrating PET hydrolases with synthetic biology offered new routes to valorize plastic waste.

Mechanistic insights from solution and solid-state NMR, including enzyme–PET–trehalose ternary systems, combined with atomistic MD simulations, clarified how enzymes interact with crystalline and amorphous PET at the molecular level.

High-throughput screening, novel microfluidic assays, and microbial consortia engineering emerged as powerful tools to accelerate development and enable in situ plastic degradation.

In summary, the workshop identified critical challenges and strategic directions for scaling biocatalytic plastic degradation. By combining computational and experimental innovations, the field is advancing toward more efficient, sustainable, and industrially viable solutions to the global plastic waste crisis.

2. What were the primary outcomes of this workshop, including limitations and open questions?

The workshop highlighted significant progress in enzymatic plastic depolymerization while also identifying key limitations and open questions. One major outcome was the successful integration of computational and experimental approaches – machine learning, molecular simulations, and QM/MM methods are now accelerating enzyme engineering by improving activity, thermostability, and substrate specificity. The discovery of novel enzymes from marine environments, mangrove soils, and insect microbiomes expanded the biocatalytic repertoire, with some capable of degrading PET, polyurethane, and nylon-6. New developments in solid- and solution-state NMR, microfluidic assays, and atomistic simulations provided valuable insights into enzyme-substrate interactions at both molecular and systems levels. Additionally, the event underscored the potential of enzyme cascades and bio-based polyester synthesis to contribute to sustainable plastic upcycling within circular economy frameworks.
However, important challenges have been identified. The high crystallinity of PET continues to hinder enzymatic access, and current pre-treatment methods are often energy-intensive, prompting the need for milder, cost-effective alternatives. Efforts to move beyond PET degradation require the identification of new enzyme classes and synergistic cocktails, potentially involving accessory enzymes like LPMOs. A limited understanding of enzyme interactions with polymer surfaces, especially at the mesoscale level, hampers further progress, and the effects of electrostatic environments on catalysis are not yet fully captured in most design models. Finally, despite laboratory successes, translating these innovations into scalable industrial processes remains difficult due to issues of enzyme robustness, substrate variability, and overall process feasibility.
In summary, while the workshop showcased substantial advances and a clear path forward, achieving efficient, eco-friendly, and industrially viable biocatalytic recycling will require deeper mechanistic insights, improved enzyme-surface interaction models, and continued integration of computational and experimental innovations.

3. What was the take-home message for the participants?

The workshop highlighted enzymatic depolymerization as a promising yet inherently interdisciplinary challenge. Tackling barriers will require integrated solutions – combining enzyme engineering, accessory enzymes, scalable bioprocessing, and sustainable design. Advancing the field will depend on cross-disciplinary collaboration to improve enzyme robustness, process economics, and safety.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

The outcomes of the workshop hold strong potential for societal benefits. Advances in enzymatic plastic depolymerization directly contribute to addressing the global plastic waste crisis by offering sustainable, low-energy alternatives to conventional recycling and incineration. Improved biocatalysts for degrading PET, polyurethane, nylon-6, and other polymers under mild conditions could reduce environmental pollution and the reliance on fossil-fuel-based processes. The development of bio-based polyesters and upcycling

strategies further supports circular economy models, promoting resource efficiency and reducing greenhouse gas emissions. Moreover, by integrating green chemistry principles, ecotoxicity prediction, and scalable biotechnologies, the workshop outcomes align with broader goals of environmental protection, climate change mitigation, and sustainable innovation – ultimately benefiting both the environment and society at large.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The workshop is already producing tangible outcomes, including the preparation of a meeting report with a perspective identifying key challenges ahead, planned for publication first on bioRxiv and later in a peer-reviewed journal. Beyond this, it has sparked new collaborations among researchers, fostering discussions around joint project proposals and funding opportunities. For example, the organizers are aware of several scheduled follow-up meetings between participants aimed at exploring collaborations and synergies combining simulations with experiments. These outcomes highlight the workshop's role in advancing both scientific knowledge and practical progress in enzymatic plastic depolymerization.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

We prioritized gender balance and inclusivity by actively inviting women and underrepresented groups, with most sessions chaired by women. Remote access enabled broad geographical participation, including from underrepresented regions. Early-career researchers were given dedicated talk and poster slots to boost visibility. The workshop fostered respectful, inclusive dialogue and supported special needs. To promote informality and personal connection, attendees wrote their names and affiliations on badges with colorful pens. These efforts created a welcoming, diverse environment that enriched collaboration – widely recognized as a highlight of the event.

7. Participant list

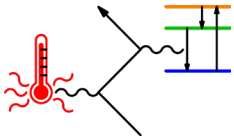
Organisers
Blazquez-Sanchez, Paula
University of Leipzig, Germany
Bussi, Giovanni
Scuola Internazionale Superiore di Studi Avanzati, Italy
Colizzi, Francesco
Institute for Advanced Chemistry of Catalonia- Institute of Marine Sciences, Spain

Ballabio, Federico - National Research Council of Italy, Italy
Bayer, Thomas - University of Greifswald, Germany
Bayer, Kutand - İzmir Institute of Technology, Turkey
Bertocchini, Federica - PlasticEntropy, France

Boukhallat, Manel - Plasticentropy, France
Butenschön, Erik - Leipzig University, Germany
Carosati, Emanuele - University of Trieste, Italy
Cella, Riccardo - University of Trieste, Italy
Concini, Gabriele - University of Trieste, Italy
Danielli, Chiara - University of Trieste, Italy
De Piero, Alessia - UNITS, Italy
Depólo Polêto, Marcelo - Universidade de São Paulo, Brazil
Di Pede - Mattatelli, Ania - Institute of Marine Sciences, Spain
Faggian, Leonardo - University of Padua, Italy
Favaro, Lorenzo - University of Padova, Italy
Fernandes, Pedro A. - Universidade Do Porto, Portugal
Ferretti, Alfonso - Scuola Normale Superiore, Italy
Fojan, Peter - Aalborg University, Denmark
Furlani, Jacopo - University of Trieste, Italy
Gagsteiger, Andreas - University of Bayreuth, Germany
Garcia Ruiz, Eva - Spanish National Research Council , Spain
Gardossi, Lucia - Università degli Studi di Trieste, Italy
Gilioli, Maurizio - SISSA, Italy
Giorgino, Toni - Consiglio Nazionale Delle Ricerche, Italy
Graefe, Norbert - Universität Leipzig, Germany
Guadagnini, Elisa - University of Trieste, Italy
Gunkel, Jonas - Leipzig University, Germany
Hergett, Alexander - Leipzig University, Germany
Jeyaraj Suja, Nitish - Nanyang Technological University, Singapore
Jimenez, Diego - King Abdullah University of Science and Technology, Saudi Arabia
Keller, Malene Billeskov - Technical University of Denmark, Denmark
Künze, Georg - University of Leipzig, Germany
Liberati, Diego - National Research Council of Italy, Italy
Lim, Sierin - Nanyang Technological University, Singapore
Lima, Anderson - Universidade Federal Do Pará, Brazil
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Accurate methods for thermal and excited electrons



Location: CECAM-HQ-EPFL, Switzerland

Webpage : Event webpage

Dates: May 7, 2025 - May 9, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop brought together leading researchers from multiple specialties to share cutting-edge developments and outstanding questions in excited-state electronic structure (wavefunction, ensemble, and density functional), and stochastic (mostly quantum Monte Carlo "QMC") methods. QMC topics included non-zero temperature cases, use of coupled-cluster states to improve auxiliary field and full-CI QMC, and dislocation propagation by PIMC, including across phase boundaries. The most discussed QMC topic was the xi-extrapolation method (the "fictitious identical particle" method), which uses extrapolations from bosonic to fermionic results to avoid the fermion sign problem. Generalization & extension of density functional methods to diverse ensembles (including enabling density matrix embedding) and to regularization that provides well-defined functional derivatives drew attention. Also highlighted was the perhaps under-appreciated relationship of density response to assessment of quality and improvement of exchange-correlation kernels.

Several extensions of high-accuracy ground-state wave-function methods were discussed in detail: to T>0 K (e.g. by thermofield which is another kind of embedding), to ionic-motion time scales rather than electronic fluctuation timescales (e.g. by interpolation-based training on a small set of high-quality electronic structure calculations such as DMRG), and to so-called trans-correlated schemes for multi-reference cases.

As a sign of the Workshop value and a symptom of the difficulty in keeping up with publication, the May 5th arXiv posting of the "Warm Dense Matter Roadmap" perspectives article (with 6 Workshop participants among 75 co-authors) was interesting news to at least half the participants as it occupied several minutes of an open discussion session.

A striking feature to organizers and several participants is the extent to which embedding approaches, conceived of quite generally, are increasingly pursued. Increasingly these methods are being used to apply some comparatively sophisticated but computationally demanding method on some subset of degrees of freedom of a challenging system class and a less-costly methodology on the remainder. The breadth is notable - the degrees of freedom aren't just spatial regions, as was mostly the case 20-30 years ago. Moreover, there is a significant machine-learning aspect of contemporary embedding.

2. What were the primary outcomes of this workshop, including limitations and open questions?

 Undoubtedly the most striking open question category concerned the xi-extrapolation method ("fictitious identical particle") for mapping of bosonic QMC data to fermionic results. Lively discussion session questions included: Is it reliable? (Are there

counter-examples in which the scheme fails? Can analytical properties and/or "safe" canonical forms of the extrapolation be developed? Is there an underlying reason why the scheme works – or from which one can derive limits on applicability? Are there detailed connections with the stochastic coherent state path integral scheme that was presented (it samples both fermions and bosons)?

- A recurring theme was cross-method "borrowing" and comparison, e.g. adsorption from both fixed-node diffusion MC and from coupled-cluster calculations, the aforementioned embedding in diverse contexts, use of high-quality ground-state wavefunctions as a better starting point in auxiliary field QMC. Encouraging developments in conventional PIMC continue to provide benchmarking as well as ingredient functionals for T>0 DFT.
- The need for reliable benchmarking data in thermodynamic state regimes presently inaccessible to QMC was raised several times. There is opportunity and need for finite-T coupled cluster calculations, particularly if tractable on large and/or periodic real material systems.
- Ensembling of density functional theory has advanced sufficiently that a not-fully resolved issue is exposed: systematic relations amongst different ensemble types. A striking example is the Hartree energy definition in excited state ensembles that, superficially at least, differs from the definition in free-energy and ground-state DFT. Another is the extent to which the ensemble work has used some form of grand ensemble (variable particle number) whereas most other methods depend upon or exploit fixed particle number (canonical) or are "N-centered" which is different from both.

3. What was the take-home message for the participants?

Remarkably, in post-meeting email inquiry, two responses were unanimous.
(1) The focused yet informal format enabled participants to engage in open, frank, inter-specialty discussion. They were almost embarrassingly enthusiastic about how the Workshop advanced their own understanding of others' work, pinpointed challenges, and identified new scientific opportunities.
(2) They want to do it again, in preference to other more conventional meetings.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

Responses to this question must be cautious and modest, as societal benefits are difficult to predict, particularly for science which is rather far from engineering implementation, such as in this Workshop. Nevertheless, there was one presentation that included discussion of calculations that have aided the US National Ignition Facility. The work on extracting reliable excited states for large molecular complexes, especially at non-zero temperature, has substantial, realistic potential for calibrating catalysis calculations. Progress on the various kinds of quantum Monte Carlo provides meaningful prospects for real-system validation and calibration of what now are parametrized and/or semi-empirical methods for complicated electronic structure. With those, it is perhaps only a little optimistic to say that we are getting closer to being able to weed out the overgrown collection of density functional approximations. Ensemble DFT calibrated with QMC is making real contributions to planetary science.

Another societal impact is on teaching and training. The face-to-face format created a vibrant and informal environment that encouraged spontaneous, in-depth scientific conversations – many of which went far beyond what would be possible through papers or virtual formats. Researchers repeatedly emphasized how valuable it was to connect personally with peers across sometimes hard-to-access specialties. That increased depth of knowledge almost surely will have an influence on teaching and mentoring.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

A number of new or revived collaborations were reported in response to our post-workshop email query. Several participants initiated discussions on extending the fictitious particle/xi-extrapolation method to systems such as liquid Helium-3, the uniform electron gas, and quantum chemistry applications. Researchers began exploring potential integration of the method into FCIQMC and AFQMC frameworks. Collaborations also were initiated on topics such as compressed fermionic density matrices, conductivity prediction, and orbital-free DFT via inverse Kohn-Sham approaches. Early-career participants connected with leading scientists, setting the stage for academic visits and joint projects. In several cases, these discussions have already resulted in ongoing email exchanges, numerical implementations, and proposal planning. The collaborative spirit of the event – amplified by its interdisciplinary and inter-specialty scope – was a standout feature frequently praised by attendees.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

To foster the richest possible intellectual environment, we asked all invitees to help us identify women researchers from typically under-represented countries who are active in the workshop's focus areas. Several suggestions were received. Geographically, this brought 3 speakers that we were unaware of before. However, most of the female researchers identified were already on our invitation list. As one respondent noted, identifying qualified participants from under-represented countries remains a challenge. The effort was received well, quoting one of the non-male speakers: "I have been to many meetings with a smaller percentage of non-male folks, and I appreciated all of you taking the time to be sure a mixed group of high-quality researchers were not just included in the registrations, but also in the discussions".
The hybrid format – although unofficially – also enabled global participation regardless of travel constraints by distance or by political difficulties.

7. Participant list

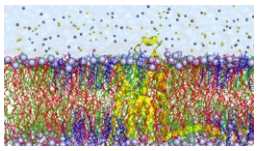
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Membranes and membrane proteins in healthy neurons and in brain diseases: recent advances from multiscale simulation and machine learning

Location: CECAM-SISSA-SNS, Italy



Webpage : Event webpage

Dates: May 12, 2025 - May 14, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The CECAM Flagship Workshop “Membranes and membrane proteins in healthy neurons and in brain diseases: recent advances from multiscale simulation and machine learning” was held from 12 to 14 May 2025 at the Scuola Normale Superiore in Pisa, Italy. The event was organised as a multinodal CECAM workshop involving CECAM-DE-JUELICH, CECAM-ISR, and CECAM-IT-SIMUL.
The workshop brought together researchers in computational biophysics, molecular simulation, structural biology, neuroscience, machine learning, medicinal chemistry, and molecular medicine. It aimed to review recent computational approaches for investigating membrane proteins in neuronal function and disease, while fostering interaction between methodological and application-oriented research communities.
The program covered a broad range of membrane-associated systems and biological questions. Topics included membrane permeation and remodeling, membrane transporters, ion channels, GPCRs, neurotransmitter receptors, amyloid proteins, and protein complexes involved in neuroinflammation.
Several talks focused on disease-associated systems, including potassium channels linked to developmental and epileptic encephalopathies, Kv4.3, the alpha 7 nicotinic acetylcholine receptor, an oxytocin receptor variant associated with brain disorders, autism-linked protein variants, and the NLRP3 inflammasome. These studies addressed how mutations, conformational changes, and molecular interactions influence protein function and disease mechanisms.
Applications to drug discovery and molecular recognition were also discussed, including membrane-protein druggability, allosteric regulation, transporter modulation, and GPCR-G protein coupling.

2. What were the primary outcomes of this workshop, including limitations and open questions?

The workshop resulted in several concrete scientific outcomes.
First, it provided a consolidated overview of current approaches for studying neuronal membrane proteins, allowing participants to compare molecular dynamics, multiscale

simulation, QM/MM, enhanced sampling, Markov state modelling, and machine-learning methodologies across different biological systems.
Second, the presentations established a clear methodological link between physics-based molecular simulation and machine learning. In particular, the contributions on deep learning, generative AI, and machine-learning-assisted molecular simulation illustrated practical opportunities for improving the analysis and exploration of complex conformational landscapes.
Third, the workshop highlighted QM/MM molecular dynamics as an important approach for investigating chemically specific processes in membrane proteins. The presentation from CECAM-DE-JUELICH provided a concrete example of combining QM/MM simulation with machine learning in the study of neuronal membrane proteins.
Fourth, the workshop identified several common computational challenges across different membrane-protein systems, including the treatment of membrane environments, sampling of slow conformational transitions, analysis of disease-associated mutations, and integration of heterogeneous computational methods.
Finally, the multinodal format strengthened scientific exchange between the participating CECAM communities and provided opportunities to identify potential future interactions in computational biophysics, neuroscience, molecular medicine, and machine-learning-based simulation.

3. What was the take-home message for the participants?

The workshop was particularly useful for connecting researchers working on different biosystems and on complementary approaches. Discussions addressed challenges such as conformational sampling, the treatment of complex membrane environments, integration of machine learning with molecular simulation, and the interpretation of disease-associated mutations. Informal discussions provided a productive environment for exchanging ideas and identifying potential areas for future collaboration.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

The workshop provided a focused overview of current computational approaches to membrane proteins in neuronal function and disease. It highlighted the increasing integration of multiscale simulation, QM/MM methods, machine learning, and emerging computational technologies. Beyond the scientific presentations, the event provided a useful forum for comparing methodologies across different biological systems, identifying shared computational challenges, and strengthening interactions between the participating CECAM nodes. The workshop therefore contributed both to the exchange of current scientific knowledge and to the development of new connections between computational biophysics, neuroscience, and molecular medicine.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

Several collaborations and plans for proposals have stemmed from the workshop, favored by the space left for informal scientific discussions and socialization among all participants.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

Organisers have carefully conceived a list of internationally well-known speakers with special attention to the gender balance and have encouraged young researchers at the early stage of their careers to participate by financially supporting some of their local expenses, such as lunches and dinners.

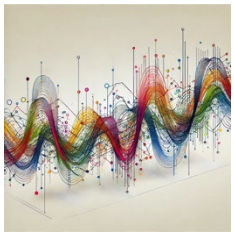
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Stochastics processes: Inferences in complex systems



Location: CECAM-HQ-EPFL, Switzerland

Webpage : Event webpage

Dates: May 14, 2025 - May 16, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

This workshop was dedicated to stochastic processes (SP), addressing both their theoretical foundations, a classical domain within statistical physics, and their applications to complex systems – not only to model random behavior, but also in the context of stochastic inference and learning. The scientific program was designed with this dual perspective in mind, carefully curating topics and speakers to foster meaningful interdisciplinary discussions at the intersection of these fields.

We structured the workshop around three main themes:

1. Theory of SP, featuring leading experts such as G. Schehr, J.-P. Bouchaud, C. Monthus, and O. Bénichou, who presented recent advances on fundamental aspects, such as time of first-passage, domain growth or denoising matrices;
2. Stochastic inference, with invited talks from P. Barucca, M.C. Angelini, A. Braunstein, and A. Altieri, exploring how stochastic frameworks can be used to extract information from data; in this session we had interesting applications in ecology, time-series and the development of stochastic algorithms;
3. Applications of SP, where L. Foini, A.F. Bitbol, M. Michel, and J.M. Parrondo illustrated the versatility of SPs across diverse domains; ranging from quantum mechanics, biology, Monte-Carlo methods and non-equilibrium thermodynamics.

Given the breadth of topics addressed, the workshop revealed several promising and timely research directions that are of broad interest across the field of SP. We were particularly impressed by how deep the connexion was between the different topics and the central role that the understanding of stochasticity implies in each of them. Among the most notable were:

- The deepening connections between theoretical constructs (such as first-passage times, Ornstein-Uhlenbeck processes, etc.) and applied modeling frameworks. A strong theoretical framework enables one to relate an empirical quantity – typically the covariance matrix of a random process – to its denoised reconstruction, correcting for the significant noise that often contaminates the original estimate.
- The use of SP in inverse problems, particularly to infer system parameters from observed trajectories. We had several contributions, for instance the presentation of P. Ronceray, relating the inference performance on a given SP depending on the parameters of the underlying process and the construction of robust estimators based on information theory.
- The role of SP in elucidating the dynamics of complex systems was emphasized, particularly in its dual capacity for interpretability and predictive modeling. A notable example was presented by M.C. Angelini, who demonstrated how the behavior of stochastic gradient algorithms in neural networks can be empirically mapped onto heat-

bath Monte Carlo dynamics, thereby opening new avenues for their analysis through the lens of equilibrium and non-equilibrium statistical mechanics.

2. What were the primary outcomes of this workshop, including limitations and open questions?

This workshop successfully brought together researchers working on stochastic processes (SPs) from a variety of perspectives (mathematical, inferential, and applied) and from different subfields: we had researchers from extreme-event analysis, theory of stochastic process and large deviations, stochastic algorithms, from the spin glass community, etc. A central outcome was the identification of conceptual and methodological links between these traditionally separate approaches. The workshop demonstrated how tools developed in the theoretical study of SPs, such as first-passage analysis, large deviations, or quasi-stationary distributions, are increasingly relevant for stochastic inference – the problem of learning models from noisy data – and for understanding real-world systems across domains such as biology, ecology, and finance.

These sessions revealed a dual role of SPs as both generative models of complex, noisy systems and as tools for inference, especially in contexts where classical machine learning approaches may lack interpretability or robustness.
However, several limitations and open questions common to most of the applications considered were also identified:

- Data limitations: Many inference methods assume abundant or clean data, which is rarely available in practice. Developing robust inference techniques for sparse or noisy time series remains a major challenge.
- Model identifiability and selection: In complex systems, different SPs can yield similar statistical behavior. Determining which model best explains the data – without overfitting – is an unresolved and extremely important problem.
- Multiscale and structured systems: Many real-world systems involve hierarchical time and spatial scales, or structured interactions, that are not adequately described by traditional stochastic models.

Despite these challenges, the workshop fostered interdisciplinary dialogue and sparked new collaborations. A key outcome was the shared recognition that bridging theory, inference, and application is both necessary and achievable, with SPs serving as a unifying framework. The event not only contributed to deepening our understanding across themes but also helped shape a common research agenda for the emerging community at the interface of stochastic processes, statistical physics, and data science.

3. What was the take-home message for the participants?

The workshop underscored that stochastic processes are fundamental to complex systems, emerging in contexts from financial markets and biology to quantum phenomena and algorithms. Rather than mere tools for modeling randomness, they provide essential frameworks for understanding, simulating, and inferring structure in real data. A key message was that the mathematics of noise and fluctuations also underpins learning and prediction, especially when uncertainty is intrinsic. The workshop highlighted the value of interdisciplinary approaches grounded in a shared stochastic language.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

While the topics addressed in this workshop are not directly aimed at immediate societal benefits, they are foundational for advancing our understanding of complex systems – many of which have significant real-world implications. The most relevant societal impact stems from the recognition that stochasticity is an intrinsic feature of complex systems, and that developing rigorous tools to analyze and understand random behavior is essential for progress across multiple domains.
Several talks illustrated how a deeper understanding of SP can have indirect yet meaningful societal implications:

- Ecology: Presentations highlighted how stochastic models can help characterize the dynamics of ecological systems, including the role of environmental fluctuations and random interactions in shaping biodiversity and ecosystem stability. These insights are crucial for informing conservation strategies and predicting ecological responses to environmental change.
- Algorithms and Learning: Several speakers showed how inference and learning algorithms are inherently governed by SP. Understanding and controlling stochasticity in these systems leads to the design of more efficient, stable, and interpretable algorithms – key goals in modern machine learning and data science applications.
- Finance: JP-Bouchaud's talk on financial systems discussed the stochastic nature of markets and how improving the reconstruction of correlations from noisy data enhances our ability to model systemic risk and market behavior – important elements for financial stability and regulation.

While these contributions may not translate into immediate societal benefits, they build a critical scientific foundation to model complexity. In the long term, this kind of fundamental research is indispensable for generating insights and tools that can be adapted to tackle real-world challenges, contributing indirectly but powerfully to societal well-being.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

This workshop will certainly contribute to the development of a new collaboration between some of the participants. We have observed intense scientific discussions during these three days, be it during the day (coffee breaks, lunches, discussion sessions, poster session) or during more mundane events (dinner or the standup event).
As most of the works presented had already been published, we decided not to push for a conference proceeding. However, with the consent of the speakers, half of the talk's slides are publicly available on the CECAM website of the workshop. The recordings made during the talks were kept for private use among the participants.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

We prioritized inclusivity throughout the organization of the workshop. The organizing committee was fully gender-balanced, and we made a concerted effort to invite renowned speakers from diverse backgrounds, geographic regions, and career stages – achieving full gender parity (50% women) among the invited speakers. Despite efforts to promote participation, we received only ~5 applications from women with a profile related to the topic (out of ~40), all of whom were accepted, though some could not attend due to personal reasons. In total, 12 women participated (out of 50 attendees, including organizers). We also ensured geographic diversity, welcoming participants from around 9 countries, including Canada, India, and several European nations. The attendees represented a range of institutions and career stages, from senior researchers to PhD students. While no specific requests were made regarding accessibility, we ensured that the venue was accessible and supportive of all participants within our financial constraints.

7. Participant list

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RNA modelling across scales



Location: SISSA, Italy

Webpage : Event webpage

Dates: May 19, 2025 - May 22, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop was structured around four themes spanning molecular resolution and methodology: (1) quantum methods (QM/QM-MM), (2) atomic-level classical MD, (3) coarse-grained (CG) and multiscale models, and (4) bioinformatics/AI for RNA structure and function.

In QM/QM-MM, talks highlighted how electronic polarization and reactive chemistry shape RNA function, from ligand recognition in repeat RNAs to ribozyme catalysis. Case studies showed that judicious ML-assisted QM/MM can rationalize NMR data and lower barriers in modified active sites, while also underscoring open issues in sampling and the level of theory needed to outperform classical models.

In atomistic MD, the community reviewed the current RNA force fields and the ways we test them. Results on tetraloops, kink-turns and other motifs emphasized that rankings depend strongly on the chosen benchmarks, motivating broader, standardized test sets and thermodynamic targets. New modular developments for modified nucleotides, together with clear analyses of where pairwise additive models succeed (helices, hybrids) and struggle (single-stranded flexibility), refined our view of current accuracy. Ion modeling emerged as a critical bottleneck: divalent binding is often over-stabilized and slow to converge, but targeted LJ tuning, charge scaling and enhanced sampling of Mg^{2+} binding/unbinding can restore realism and predict otherwise hidden binding sites.

CG and multiscale contributions showed top-down advances (SimRNA variants, RNA–solvent/EM integration), a bottom-up coarse-graining method that simplifies RNA motifs into interacting rigid bodies, and hybrid workflows that transfer information across scales – for instance, linking coarse-grained Martini 3 simulations of lipid nanoparticles, genome-scale packaging models, and machine-learning datasets derived from atomistic or quantum simulations.

In bioinformatics/AI, we saw progress on non-canonical base-pair prediction, fragment-based 3D assembly (with and without templates), and dynamic motif vocabularies for next-generation sequence-to-structure models. Several talks connected these tools to ligandability (e.g., curated RNA–ligand structure sets, pocket detection on MD ensembles) and to design (xrRNA engineering, aptamers), stressing data standards and interface with experiments.

Overall, the meeting advanced the state of the art by (i) crystallizing a shared assessment of modeling limits, (ii) surfacing concrete benchmark and dataset needs (thermodynamics/kinetics and ions), and (iii) promoting integrative workflows where physics-based, data-driven and experimental inputs inform one another across scales.

2. What were the primary outcomes of this workshop, including limitations and open questions?

Outcomes.
Community benchmarking agenda. Participants converged on the need for broader, motif-diverse benchmark suites beyond tetranucleotides, with explicit thermodynamic/kinetic targets and ion-sensitive observables. The discussion favored CASP/RNA-Puzzles-like blind exercises for force-field and workflow assessment, especially for modified nucleotides.

- Ion modeling focus. There is emerging consensus that Mg^{2+}/divalent binding is a major source of error and poor convergence in RNA MD. Practical pathways – pair-specific LJ terms, charge scaling, and enhanced sampling protocols that accelerate inner-shell exchange – were shared and compared, with interest in community recipes and reference systems.
- Bridging scales and data. Several groups presented pipelines coupling CG↔AA↔QM and integrating cryo-EM, SHAPE, and NMR constraints. The outcome is a clearer map of where multiscale inference is mature (helices, certain motifs) and where it is nascent (non-canonical networks, flexible ssRNA, lipid–RNA interfaces). Limitations/Open questions.
- Reference data scarcity. Progress is gated by the lack of standardized, high-quality solution thermodynamics/kinetics for simple, reusable RNA systems (including modified bases), and by incomplete ion annotations in high-resolution structures.
- Force-field universality. A single best FF for all RNA contexts may be unattainable; context-dependent performance argues for transparent guidance rather than one-size-fits-all prescriptions.
- Sampling vs. accuracy trade-offs. For QM/MM and ML potentials, finite sampling and uncertain training data (especially in solution) compete with accuracy goals; for classical MD, long trajectories do not automatically resolve systematic biases.
- Non-canonical & modifications. Predictive treatment of non-canonical pairs and widespread chemical modifications remains uneven across AA, CG, and AI tools.

3. What was the take-home message for the participants?

RNA modeling progresses fastest when benchmarks, data, and methods are shared across scales: improve ions and thermodynamics first, use targeted enhanced sampling, prefer standardized, motif-diverse tests over single exemplars, and combine physics-based and data-driven tools with experiment. No single method wins everywhere – integrative, transparent workflows are the path to reliable prediction and design.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

Yes. Health & therapeutics: Better models of RNA structure, ion coupling, and pocket persistence directly support RNA-targeted drug discovery, aptamer/siRNA design, and mRNA/LNP delivery, accelerating routes to antivirals, oncology targets (e.g., receptor-binding aptamers), and safer gene-modulation tools. Data & reproducibility: Shared benchmarks and open protocols will reduce duplication of effort, improve cross-lab reproducibility, and shorten the path from in silico hypotheses to *in vitro/vivo* validation. Education & workforce: The meeting fostered cross-training between computation and

experiment, benefiting students and early-career researchers entering RNA science. Technology spillovers: Advances in multiscale modeling, enhanced sampling, and ML-physics integration are widely transferable (e.g., to DNA nanotech, biosensing, and biomanufacturing). Collectively, these impacts enable more predictive, efficient, and safer RNA technologies with clear societal relevance.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

- Manuscript in preparation: “RNA modeling across scales: Frontiers and Challenges” (meeting report led by the organizers and speakers).
- Future collaboration: A group of participants is preparing a Doctoral Training Network (DTN) proposal to be submitted at the next call deadline.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

We designed the program to be balanced across disciplines and career stages, with more than 70 participants from Europe and the US, and 10 contributed talks selected from abstracts to ensure visibility for early-career researchers and topical diversity. The invited list included academia and industry, spanning physics, chemistry, biology, and informatics. Poster sessions ran daily and remained up over lunch to maximize informal interactions. Session chairs actively encouraged questions from junior attendees. We monitored gender balance when confirming invitations and abstract selections.

7. Participant list

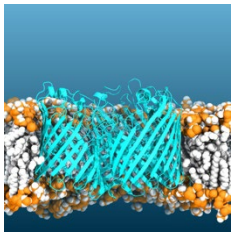
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Nanopores: from basic sciences to applications



Location: Cagliari University, Italy

Webpage : Event webpage

Dates: May 19, 2025 - May 22, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop, held at the University of Cagliari, brought together approximately 40 faculty and 20 students and postdoctoral researchers from France, Germany, Belgium, the Netherlands, India, Italy, Spain, Israel, Switzerland, the UK, and the USA. The scientific program featured seven talks per day for the first three days, followed by six talks and a closing discussion on day 4.

Day 1 (Speakers: Mathé, Montel, Suma, IMEC representative, Howorka, Farci, Jan Behrends)

This day featured experimental and theoretical studies on the translocation of glycosaminoglycans, diffusion through nuclear pores, and structural mechanics of nanopores. Talks examined reverse transcriptase dynamics in extremophiles and introduced “peptide ladders” as a tool to analyze amino acid-specific signals. The importance of nanopores for single-molecule studies of complex biomolecules was strongly emphasized.

Day 2 (Speakers: Biance, Holm, Ritort, Porro, Dekker, Fyta, Mahendran, Wannunu, Aksimentiev)

Focused on computational, technological, and machine learning strategies to enhance nanopore sensing. Topics included nanofluidics, DNA origami-based tunable pores, high-throughput platforms, and alpha-helical barrel design relevant to cancer research. Several talks highlighted collaborations developed in earlier workshops, especially those combining machine learning with experimental data.

Day 3 (Speakers: Amit Meller, Bhattacharya, Orlandini, Mauro Chinappi, Reisner, Keyser)

Blended theory, modeling, and experiments to study mitochondrial DNA, DNA-RNA hybrids, and protein translocation. Presentations employed coarse-grained and all-atom simulations to investigate confinement, knotting, and torsion propagation. These efforts demonstrated the growing synergy between modeling and experiment.

Day 4 (Speakers: Muthukumar, Micheletti, Muccio, Emmerich, Milenkovic, Teng)

Addressed electro-osmotic flow, charge symmetry breaking, and topological influences in macromolecular transport. Talks also included MD and continuum modeling, AI-based current signal prediction, and new bioinspired fabrication strategies for asymmetric nanopores with applications in sensing and energy harvesting.

The topics presented expanded the scope of nanopore research from genomic sequencing toward broader applications in **biophysics, diagnostics, and nanotechnology**.

2. What were the primary outcomes of this workshop, including limitations and open questions?

One of the key outcomes was the clear demonstration that nanopore research is expanding beyond sequencing applications into broader areas, including biophysics, molecular diagnostics, and drug development. The combination of experimental results, theoretical models, and computational simulations provided a comprehensive view of nanopore-based sensing at the single-molecule level.
Several talks highlighted the value of integrating machine learning with experimental nanopore data, enhancing resolution and classification accuracy, especially for peptide identification and post-translational modifications.
The event revealed strong progress in peptide and protein sequencing.
Despite these successes, several limitations and open questions remain. The field continues to face challenges in interpreting complex current signals, particularly for irregular or disordered biomolecules. Many non-equilibrium transport phenomena observed in experiments still lack comprehensive theoretical treatment, requiring further development of multi-scale modeling techniques. Moreover, while AI and machine learning tools show promise, they often require extensive training datasets that are not yet available for many nanopore systems.
Finally, discussions pointed to the need for more systematic comparison across pore types, experimental conditions, and signal processing methods to establish standard benchmarks.

3. What was the take-home message for the participants?

The take-home message was that:
- nanopore science is rapidly evolving towards reliable protein sequencing;
- there is now consensus about the centrality of electroosmotic flow in driving the translocation of all molecules, from charged, to partially charged and neutral;
- multiscale modelling and simulation approaches can be predictive towards the outcome of translocation experiments.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

Yes, the outcomes of the workshop hold clear potential for societal benefits, particularly in the fields of health, diagnostics, and biotechnology. Many of the presentations focused on using nanopores to study biologically relevant molecules – such as mitochondrial DNA, proteins, and glycosaminoglycans – at the single-molecule level. These studies can lead to early disease detection, better understanding of genetic mutations, and the design of targeted therapies.
Several talks addressed applications in **cancer diagnostics**, **viral RNA detection**, and **protein transport relevant to disease pathways**. For example, research on post-translational modifications and amino acid-specific signal analysis could contribute to the development of rapid diagnostic tools.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

 New and ongoing collaborations: Building on partnerships initiated at previous workshops (SISSA 2021, ENS Lyon 2023), the community brought together by the workshop was primed to discuss and plan new collaborative projects during the event. These are expected to lead to joint publications. While output from new collaborations will require its due time to become tangible, we are pleased to report that collaborations seeded in earlier workshops have already appeared in high-impact journals. For example, work by Micheletti, Aksimentiev, and Keyser on DNA supercoiling was recently published in *PRX*. Another example is the collaboration between Behrends and Holm on peptide ladders using machine learning and experimental methods.
 Proposal planning: Organizers initiated discussions for the next CECAM workshop, tentatively planned for 2027 at EPFL, Switzerland. A follow-up Zoom meeting is scheduled to refine the proposal scope.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

We asked every organizer to propose a few names, more than the capacity of our workshop. Thus, we selected a first list and a waiting list, balancing gender and geographical provenance. For the young participants we proposed to all that applied the possibility to have a contributed talk. We had many problems in having female speakers, the selected dates overlapped with almost end of school and some of them could not join for family reasons.

7. Participant list

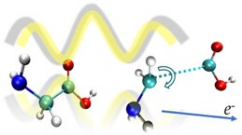
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Ultrafast phenomena in Chemistry: Laser-matter interactions at the femto- and atto-second time scales

Location: CECAM-ES, Spain



Webpage : Event webpage

Dates: May 19, 2025 - May 23, 2025

1. What were the major topics presented in the School?

Our school is structured with practical sessions to learn computational and numerical techniques with realistic applications to current problems of interest in the areas of femto- and atto-chemistry. It is designed in four modules:
Module 1: Introduction to laser technologies.
1.1. (A. Palacios, UAM) Introduction to the fundamentals of light-matter interactions (perturbation theory, time-dependent Schrödinger equation -TDSE- in exact simulations for few-particle systems). Overview of applications exploiting quantum chemistry methods to describe bound and continuum states of molecules (excitation and ionization).
1.2. (J. Biegert lab, ICFO - L. Vamos and W. Gawelda, IMDEA) Comprehensive lectures and hands-on the technical aspects for the characterization of XUV and X-ray laser pulses. This module is presented by experimentalists in the field, experts on attosecond pulses produced by high-harmonic generation (HHG, from ICFO) and produced in free electron lasers (FEL, from IMDEA).
Module 2: Theory on high-order harmonic generation (HHG) techniques.
2.1. (C. Hernández, USAL). Theoretical tools to describe HHG spectra, including the treatment of macroscopic effects. Novel concepts on structured light (e.g., light with angular momenta) are also introduced. Practical sessions are prepared using Jupyter notebooks.
Module 3: Light-induced ultrafast processes in real systems:
3.1. (J. Feist, UAM) Theoretical description of laser pulses in time and frequency domain using open-source codes (htts://github.com/jfeist/laserfields). Extensive module connecting the expressions for laser-matter interactions in the weak-field regime (module 1) with the non-perturbative appraoches to treat high-intense regimes where non-linear phenomena arise (ligh-induced electronic wave packets, dressed states, etc). The lecturer provides pre-made Jupyter notebooks for an efficient practise, using Python libraries and homemade libraries for the large numerical examples.
3.2. (F. Zapata, UCM). Numerical solution of the TDSE using a fortran-based code and python scripts available to the students. This module simulates the photoelectron spectra using attosecond interferometric techniques.
Module 4: Fundamentals of time-dependent density functional theory (TDDFT) and applications
4.1. (A. Castro, U. Valladolid). This module uses OCTOPUS software to treat excitations and strong-field induced problems in large molecules (https://octopus-code.org). A. Castro is one of the main developers of this package and provides an extensive training on this package, which is very well received by the participants.

2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

There were no limitations during the school. We only had a small issue during the practical session on block 3.2., which was quickly solved by the IT responsible from CECAM. There was a small problem related to the virtual machine used by the students in previous editions of the school. The old virtual machine was corrupted, so the IT responsible moved the files to the new machines, and the hands-one session took place with no further problems.
From the anonymous surve realized after the school, we got some feedback from the attendees on which aspects could be improved in the school (we explicitly ask them to identify aspects or ideas that could improve our school for future editions):
"*The half-hour breaks should be broken up into smaller, more frequent breaks. Some professors did this on their own. Perhaps all could at least be advised by the organizers to do so."*
"I found it valualbe to become familiar with different types of simulations ,to connect with professionals in this field, and to receive a broad overview and understanding of the domain"
"The atmosphere was super friendly. The scientific contents were quite well designed, materiasl were helpful. I also like Alicia's emails before the school, which provides useful information about every detail"
"The number of participants is perfect. Timing is great, in terms of when the lecturers start in the morning. Atmosphere is very relaxes. I loved that each professor had sessions in a row so we could really enjoy one topic at a time. The timeline of topics was amazing! Hands-on sessions are exactly what I needed. Topics were perpectly explained with lots of animations. Indeed, it is amazing school with insightful explanations! Well done to lecturers and organizers!"
From these comments (and other similar ones), we can see that participans enjoy the broad overview of methods, while having precise and specific training via practical sessions. This is an important and key aspect in our school to be kept. We will include (for the future, in case new editions take place) to include more small breaks.

3. What was the take-home message for the participants?

The participants received a complete formation on the interaction of light pulses with matter, working with the most advanced methodologies currently employed in attosecond and femtosecond science. These concepts have been introduced in tutorials connected with hands-on sessions. In the words of the attendants (from the survey): "*There was a nice mixture of topics which allowed getting insight into different aspects of the fields - The group dynamics were very good."*

4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

All lecturers made available to the participants their notes, Jupyter notebooks and open-source software:

- Lecture and tutorial notes are available at the CECAM-ES platform in the tab “Documents”. These notes were available for the participants before the class, so they could access the documentation in advance.
- Jupyter notebooks and home-codes are provided to the attendants, so they can keep using them even after the school.
- Attendants employ our libraries for the description of light sources and to reproduce the interaction with simple systems (few-level systems). The software has been developed by the Lecturers and the students have access through notebooks, and libraries available through GitHub (i.e. : https://github.com/jfeist/laserfields).
- Attendants are taught to employ OCTOPUS software, which is installed and available in several centers and computational networks.

5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

Our lecturers come from the main nodes in Spain working on "Ultrafast phenomena in Chemistry", i.e. ICFO, UAM, UCM, USAL, UV and IMDEA, and all have wide international experience, some of them come indeed from abroad (Gawelda, Feist, Biegert). We have female teachers (as role model) and teachers in different career stages (8 to 26 years post PhD).
To promote diversity in our school, we announce it in international distribution lists. In 2025, we have had participants coming from 11 different countries: Germany (8), Spain (4), Czech Republic (2), India (2), UK (2), Sweden (1), Romania (1), Portugal (1), Italy (1), Poland (1) and Iran (1). We had up to 37 applications from 14 different countries (current worldwide situation including USA and last-minute delays in visa prevented some of these students to arrive on time). Gender balance has improved from previous editions (reaching 30%).

6. Participant list

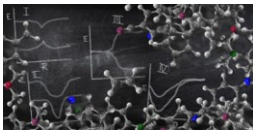
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Lægdsmand, Asbjørn Ørnemark - Universität Kassel, Germany
Macías Labrada, Inés María - InSTEC, Universidad de La Habana, Cuba
Mohamed, Tarek - South Valley University, Egypt
Naum, Diana - ELI-NP, Romania
Ramos, Carmen - University Jaume I, Spain
Riegel, Alexander - University of Tübingen, Germany
Rodriguez, Aude - Instituto de Ciencia de Materiales de Madrid, Spain
Rodriguez, Asensio - UAM, Spain
Saha, Swagato - University College London, United Kingdom
Shaik, Rasheed - Indian Institute of Technology Mandi, India
Shaji, Navya - Louisiana State University, United States
Soler Colomina, Sergio - Universitat de Valencia, Spain
Subramani, Amutha - University of Chemistry and Technology, Czech Republic
Suma Balakrishnan, Sruthil Lal - Pondicherry University, India
Vamos, Lenard - ICFO, Spain
Wülfing, Lasse - TU Dortmund, Germany
Zhou, Qi - Fritz-Haber Institute, Germany

Discussion meeting on molecular benchmarks in nonadiabatic dynamics

Location: University Sorbonne, France



Webpage : Event webpage

Dates: May 22, 2025 - May 23, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

This discussion meeting was a follow-up of the May 2024 CECAM workshop on molecular benchmarks for nonadiabatic dynamics. During that workshop, the community of developers and users of nonadiabatic molecular dynamics met at the CECAM-FR-MOSER to propose, for the first time, the idea of benchmarking in this field. Due to the complexity of nonadiabatic molecular dynamics, the participants of the original workshop proposed a plan of action, or roadmap, to establish the concept of benchmarks in the field. Acting on this roadmap, that was published as a perspective in the Journal of Physical Chemistry A, the discussion meeting initiated the first efforts to construct the benchmark database. Specifically, the purpose was to bring together some of the contributors of the original workshop to evaluate the status of the work after the roadmap article has been finalized and to organize future work. At the same time, we invited 4 speakers whose contributions to the field of nonadiabatic dynamics fall within the scope of our benchmarking initiative.
The major topics discussed at the event were (1) the practical organization of the benchmark work and (2) the identification of the working groups to start acting on the ideas discussed during the 2024 workshop.

2. What were the primary outcomes of this workshop, including limitations and open questions?

The first half day of the discussion meeting was devoted to invited presentations, with an online presentation from the US taking place just after the lunch break. The second and third half days were devoted to discussion sessions animated by the organizers with the scope of proposing the actual organization of the work to develop the first benchmark set of nonadiabatic molecular dynamics data:

- identification of working groups, or task forces, focusing on the different aspects of the problem;
- validation of the systems representing the first benchmark set of the field and related references;
- proposition of a timeline for future meetings of the task forces;
- presentation of the GitLab space hosted by CECAM to store the data envisaging future open access by the community.

All these achievements can be very well viewed as primary outcomes of the discussion meetings as they will ultimately lead to build the GitLab database of molecular benchmarks.

3. What was the take-home message for the participants?

We will have periodic meetings to follow up closely the progress of the work of the task forces.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

During the discussion meeting we did not discuss the potential for societal benefits of our benchmark initiative.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

This discussion meeting allowed us to create a large network of collaborations to establish the benchmark database that will be available and open source on GitLab (hosted by CECAM). For the time being, this network will mainly involve researchers from Europe (France, UK, Germany, Italy, Spain, Sweden, Croatia) but we certainly expect to reach a much broader community once the first database will be published. For instance, the roadmap article that preceded the discussion meeting involved as well participants from the USA, Australia, Argentina, South Korea.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

Due to the short duration of the meeting (one and a half days) we invited participants geographically located in Europe. Only one speaker from the US was invited and attended remotely. Participants of diverse career status attended the meeting, from PhD students to postdocs and junior as well as senior faculties.

7. Participant list

Organisers
Agostini, Federica
University Paris-Saclay - CNRS, France
Le Dé, Brieuc
INSP - Sorbonne Université, France
Spezia, Riccardo

Sorbonne Université - CNRS, France

Akimov, Alexey - University at Buffalo, United States
Albani, Carlo - Chimie ParisTech - PSL, France
Avagliano, Davide - ENSCP ChimieParistech - PSL University, France
Chin, Alex - Insitut des Nanosciences de Paris, France
Cigrang, Leon - University College London, United Kingdom
Coonjobeeharry, Jaymee - UCL, United Kingdom
Curchod, Basile - University of Bristol, United Kingdom
Dhiman, Mukul - Univ Gustave Eiffel, France
Došlić, Nađa - Ruđer Bošković Institute, Croatia
Gómez, Sandra - Universidad Autonoma de Madrid, Spain
Ibele, Lea - Aix-Marseille University - CNRS, France
Joubert-Doriol, Loic - Université Gustave Eiffel, France
Lauvergnat, David - Université Paris Saclay - CNRS, France
List, Nanna Holmgaard - KTH Royal Institute of Technology, Sweden
Loreti, Alessandro - University of Bologna, Italy
Magi, Claudia - University of Bologna, Italy
Mannouch, Jonathan - MPI for the Structure and Dynamics of Matter, Germany
Patra, Sarbani - University College London, United Kingdom
Peláez-Ruiz, Daniel - Université de Lille 1, France
Picconi, David - Heinrich-Heine-Universität Düsseldorf, Germany
Sangiogo Gil, Eduarda - University of Vienna, Austria
Schürger, Peter - MPI for the Physics of Complex Systems, Germany
Toldo, Josene - Université Claude Bernard Lyon 1, France
Worth, Graham - University College London, United Kingdom

COST/ZCAM School on New Computational Methods for Attosecond Molecular Processes

Location: CECAM-ES, Spain

Webpage : Event webpage

Dates: May 26, 2025 - May 30, 2025

1. What were the major topics presented in the School?

The school was motivated by the emerging field of Attosecond Chemistry, which focuses on investigating dynamic processes that take place on the attosecond time scale, the natural time scale of electronic motion in atoms and molecules, using attosecond light pulses. Due to the complexity of these experiments, theoretical support is essential for interpreting the results and guiding the design of new experimental strategies. Thus, new theoretical methods and computational tools have been developed during the last decade. The objective of the school was to offer comprehensive training on these new computational tools, which describe electron and nuclear dynamics triggered by interactions with attosecond pulses or intense IR fields.
The specific topics presented in the school are the following:
1st day: Overview of strong-field and attosecond physics with a tutorial on analytical models for ionization and high-harmonic generation. Hands-on: calculation of high harmonic spectra and photoelectron spectra resulting from the interaction of strong IR fields with simple systems by solving the TDSE for one electron.
2nd day: Merging quantum chemistry approaches with scattering theory methods for strong field ionization of molecules: electronic structure calculations in the ionization continuum. Hands-on: computational packages for strong-field ionization of molecules with correlated electrons, including MO-ADK, TD-RIS and ECS-MP2.
3rd day: Numerical and theoretical challenges associated with the description of strongly driven electrons in the continuum, with the introduction of ir-ECS and t-SURFF methods. Hands-on: Calculations of ionization rates from simple and medium size molecules with the t-SURFF software.
4th day: State-of-the-art methodologies to access attosecond molecular processes driven by attosecond pulses, with emphasis in the hybrid Gaussian/B-spline multi-reference CI method XCHEM. Hands-on: Calculations of photoelectron spectra from simple molecules in the region of Feshbach resonances using the XCHEM computational package.
5th day: Extension of the concepts introduced in the 4th day with emphasis on the UK-Rmol+ methodology (based on R-matrix) for the description of molecular ionization and pump-probe spectroscopy. Hands-on: Calculations of photoelectron spectra in medium-size molecules with the UK-Rmol+ package.

2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

- One of the questions raised this year during the first day was the choice of gauge. The students were curious about why the Strong Field Approximation (SFA) theory framework is not gauge invariant so the speakers explained the reasons and justified why the length gauge was preferred over the velocity gauge within the SFA.
- During the first days, the validity of the Single Electron Approximation (SEA) was also discussed. The speakers pointed out that in some cases, the differences between the SEA calculation and a full-electron calculation can be very substantial.
- The possibility of developing analytical models to describe high-harmonic generation and strong field ionization was also discussed during the first days. However, obtaining analytical solutions became more challenging for the topics covered during the last days of the School.
- Another important topic was the choice of dealing with boundary conditions, to represent the scaping photoelectron wavepacket that travels away from the molecule upon ionization. This aspect was extensively discussed during day 3, when the speaker explained different approaches, such as Complex Absorbing Potential, Exterior Complex Scaling or tSURFF.
- An important point of discussion was the different methods for incorporating nuclear dynamics and its coupling to electronic dynamics. This topic was discussed during days 4 and 5.
- Finally, an important limitation discussed during the School was the extension of the described methods towards larger molecules, i.e. the scalability of the methods and the restrictions due to available computational resources. Some of the tools (e.g. the XCHEM and the UK-Rmol+ packages) are highly accurate in their description of molecular ionization and thus very computationally expensive.

3. What was the take-home message for the participants?

The school offered an overview of the key formalisms, mathematical expressions, and most relevant computational tools currently used in attosecond chemistry. Participants found out about the new challenges in the description of molecules in comparison with atoms. They also learned to identify the most suitable approaches and computational packages for describing specific phenomena across different levels of accuracy. They also received hands-on training in accessing and using these tools.

4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

- Lecture material: most lectures included slide presentations, which were emailed to the participants for their reference.
- Lecture notes: the participants actively took notes of the morning lectures. These lectures mostly consisted of slide presentations, but also included mathematical derivations on the physical whiteboards, which encouraged their active participation.
- XCHEM Software: Participants were provided access to the AMOS Gateway platform where the XCHEM software (4th day) is installed and where it is possible to directly run computational simulations in situ. Thus, they can perform calculations on their

own after the school. This platform also provides access to other computational chemistry packages, such as OpenMolcas or t-Surff (described on the 3rd day). They retained access to the platform after the school.

- R-matrix software: Participants were provided access to Canvas, an online platform where they accessed the R-matrix tutorial (covered on the 5th day). They retained access to the course after the school. The participants were also informed that the UK-Rmol+ software is publicly available in the Zenodo platform.

5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The school was co-funded by the Next COST Action (CA22148) which covered the expenses of the speakers from different countries and career stages. The school was announced through worldwide-popular email distribution lists to ensure that the information was accessible from any geographical region and diverse researcher profiles. Regarding gender balance, 60% of the organizers and 27% of the speakers in the initial program were females (within the participants, 33% of them were presumably females). The school was carried out in a wheelchair-accessible building. The combination of the tangible material, oral lectures and practical training made the content of the school accessible for diverse learning preferences.

6. Participant list

Organisers
Mancini, Giulia Fulvia
University of Pavia, Italy
Martin, Fernando
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Svetina, Cristian
IMDEA Nanociencia, Spain
Vozzi, Caterina
Consiglio Nazionale Delle Ricerche, Italy

Azizi, Sajjad - LRZ, Germany
Batelic Jankovic, Mateja - King's College London, United Kingdom
Binns, Edward - Imperial College London, United Kingdom
Carlström, Stefanos - Lund University, Sweden - Max Born Institute, Germany
Chugh, Pooja - IISER Mohali, India
Dilek, Omer Gurkan - University of Mehmet Akif Ersoy, Turkey
Farhat, Afifa - Max-Planck Institute for the Structure and Dynamics of Matter, Germany
Franco, Enar - Universidad Complutense de Madrid, Spain
González Vázquez, Jesús - Universidad Autónoma de Madrid, Spain
Gorfinkiel, Jimena - The Open University, United Kingdom
Ivanov, Mikhail - Max Born Institute, Germany - Imperial College, Germany
Jana, Susmita - Vienna University of Technology, Austria

Masin, Zdenek - Charles University, Czech Republic
Mohan, Suman - Max Born Institute, Germany
Morales Moreno, Felipe - Max Born Institute, Germany
Patchkovskii, Serguei - Max-Born Institute, Germany
Riegel, Alexander - University of Tübingen, Germany
Saha, Swagato - University College London, United Kingdom
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Stehling, Till - DESY, Germany
Tajouo Tela, Herve - Scuola Normale Superiore di Pisa, Italy
Yi, Sili – Max Born Institute, Germany

Machine Learning in Physical Sciences: Theory and Applications

Location: ENS-Lyon, France

Webpage : Event webpage

Dates: May 26, 2025 - May 30, 2025

1. What were the major topics presented in the School?

The five-day school "*Machine Learning in Physical Sciences with Applications"* aimed to provide comprehensive training in machine learning (ML) techniques relevant to a wide range of physical science disciplines. The school highlighted emerging ML trends that are significantly advancing four key areas: electronic structure calculations, complex porous media, biomolecular science, and method development for atomistic modeling.

Day 1 – May 26:

The morning session, "*Introduction to Machine Learning in Physical Sciences*", provided a foundational overview of ML methods and a presentation of the latest advancements. In the afternoon, two hands-on sessions showcased the extraction of dynamical systems from spatio-temporal data and the use of ML force fields in (bio)molecular simulations.

Day 2 – May 27:

The focus shifted to "*ML Methods for Complex Porous Media*", where ML's predictive power was demonstrated in the analysis of flow behavior, transport properties, and the characterization of geological materials. Afternoon hands-on sessions explored the use of deep learning to classify phase transitions.

Day 3 – May 28:

This day was dedicated to "*ML for many-body systems"*. The morning covered Neural Network Quantum States for continuum systems and their application in assisting electronic wavefunction calculations. In the afternoon, practical examples involving spin systems and the deuteron were used to demonstrate these approaches.

Day 4 – May 29:

The "*ML for Biomolecular Modeling*" day explored how ML can extract valuable insights from large simulation-generated datasets. Algorithms were shown to identify patterns and correlations, offering new understanding of physical and chemical processes.

Day 5 – May 30:

The final day focused on "*The Future of Machine Learning and AI in Physical Sciences"*. Morning sessions addressed the prospective roles of ML in quantum and classical physics and the concept of explainable AI. A roundtable discussion examined the intersection of ML and quantum computing, the implications for education, and the ethical challenges surrounding the misuse of AI.

2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

Throughout the school, several cross-cutting limitations and open questions emerged.

- **Data quality and availability**: Many ML applications suffer from limited, noisy, or costly-to-generate datasets.

- **Generalization**: Models trained on specific systems often fail to transfer to new regimes or materials. Enhancing generalizability remains a major challenge.
- **Validation and benchmarking**: The lack of standard metrics or benchmarking protocols in physical ML limits reproducibility and model comparison.
- **Robustness of ML force fields**: While highly accurate within training sets, ML potentials may fail in unexplored regions, raising concerns for stability and transferability.
- **Small data regimes**: Overfitting is common in domains with limited training data. Incorporating symmetry and prior knowledge is a promising approach.
- **Physical consistency**: ML predictions for flow and transport lack guarantees for physical laws (e.g., conservation principles).
- **Uncertainty quantification**: Biomolecular simulations are noisy; propagating uncertainty through ML models is still underdeveloped.
- **Explainability and trust**: Explainable AI (XAI) is critical but still in early stages in physical sciences.
- **AI in education and research**: The roundtable raised ethical concerns, including AI misuse, authorship dilution, and the growing gap in digital literacy among researchers.

3. What was the take-home message for the participants?

The central message for participants was that **machine learning is rapidly becoming an essential tool across all areas of physical sciences – not as a replacement for traditional methods, but as a complementary framework that enhances modeling, interpretation, and discovery**.

4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

Those are the practical outcomes:
- All the presentations and lecture notes were distributed after the talks using a link.
- The lectures were not recorded but were broadcast live.
- Exercise sessions were given through GitHub repositories.

5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

We are proud to confirm that all applicants were accepted to the school. Due to logistical and financial constraints, in-person participation was limited to 20 students and researchers. To ensure broader access, we transformed the physical workshop into a hybrid event, enabling around 30 additional participants to join online, effectively overcoming visa and financial barriers.
Participants came from 20+ countries, including Brazil, Ethiopia, Ghana, India, Morocco, Pakistan, and the USA. Gender distribution was 51 male and 21 female participants. We welcomed 10 researchers, 30 PhD students, and 10 Master's students.

Our speaker lineup included 15 experts from France, the Czech Republic, Italy, Norway, Spain, Switzerland, Luxembourg, and the USA. All speakers and organizers were professors. No participants identified as having a physical disability.

6. Participant list

Organisers
Cabriolu, Raffaela
Norwegian University of Science and Technology, Norway
Hansen, Alex
Norwegian University of Science and Technology, Norway
Hjorth-Jensen, Morten
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Jónsson, Hannes
University of Iceland, Iceland
Martens, Kirsten
University Grenoble Alpes - CNRS, France
Miettinen, Markus
University of Bergen, Norway

Adegosho, Rehima Sheberu - Addis Ababa University, Ethiopia
Alibakhshi, Amin - SISSA, Italy, Italy
Aljamou, Tareq - Norwegian University of Science and Technology, Norway
Andersson, Stefan - SINTEF Materials and Chemistry, Norway
Aniagyei, Albert - University of Health and Allied Sciences, Ghana
Aznar, Maria - La Laguna University, Spain
Berg, Steffen - Shell Global Solutions International B.V., Netherlands
Bleken, Francesca - SINTEF, Norway
Bragagnolo, Matteo - Università di Ferrara, Italy
Buliyaminu, Ismail - Michigan State University, United States
Carleo, Giuseppe - EPFL, Switzerland
Carneiro Queiroz Da Silva, Guilherme - Université Bourgogne Europe, France
Dieguez, Miguel - Universitat Pompeu Fabra, Spain
Faryad, Muhammad - Lahore University of Management Sciences, Pakistan
Fernández, Estefanía - Instituto de Catálisis y Petroleoquímica, Spain
Flaibani, Matteo - Università di Trieste, Italy
Ghobadpour, Elham - ENS-Lyon, France
Gradisteanu, Valentin - OneAngstrom - Constructor University, France
Grigorev, Petr – CNRS – MatéIS - INSA Lyon, France
Guadagnin Pattaro, Alessia - University of Trento, Italy
Haugland, Tor Strømsem - Norwegian University of Science and Technology, Norway
Korchevaya, Elizaveta - Universitat Pompeu Fabra, Spain
Kutz, Nathan - University of Washington, United States
Li, Ge - Norwegian University of Science and Technology, Norway
Lopez, Marta - Universitat Pompeu Fabra, Spain
Lovato, Alessandro - Argonne National Laboratory, United States
Matre, Bjarte - NTNU, Norway
Medel, Brian - Universitat Pompeu Fabra Barcelona, Spain

Mohammadi, Saber - NTNU, Norway
Naimi, Salma - Mohammed 5 University, Morocco
Ollila, Samuli - Academy of Sciences, Czech Republic
Ortellado, Laureano - Université Grenoble Alpes, France
Osawa, Misaki - Grenoble-Alps, France
Patt, Antoine - Donostia International Physics Center, Spain
Pili, Piero - Elianto Csp, Italy
Pongprayoon, Prapasiri - Kasetsart University, Thailand
Poulain, Pierre - Université Paris Cité, France
Ravichandir, Shashank - Lebniz Institute of Polymer Research, Germany
Rezaee, Mojde - NTNU, Norway
Roitberg, Adrian - University of Florida, United States
Rosas Jimenez, Jose Guadalupe - MPI of Biophysics, Germany
Rozalén Sarmiento, Javier - Institute of Cosmos Sciences, University of Barcelona, Spain
Sahimi, Muhammad - University of Southern California, United States
Sandoval Menjivar, Johanna - University of Valladolid, Spain
Selent, Jana - Hospital Del Mar Medical Research Institute, Spain
Sharma, Anand - Indian Institute of Science Education and Research, India
Sheng, Chenxi - University of Birmingham, United Kingdom
Sidler, Elizaveta - NTNU, Norway
Silvia, Astrid - Norwegian University of Science and Technology, Norway
Smit, Berend - EPFL, Switzerland
Succi, Sauro - IAC - CNR, Italy
Svensson, Oskar - Lund University, Sweden
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Thirion, Louis - University of Erlangen-Nuremberg, Germany
Tkatchenko, Alexandre - University of Luxembourg, Luxembourg
Turchyna, Volha - *, Russian Federation
Vallecorsa, Sofia - CERN, Switzerland
Van Erp, Titus - Norwegian University of Science and Technology, Norway
Vosoughi-Nia, Sakineh - AGH University of Krakow, Poland
Zhang, Xiaoqi - EPFL, Switzerland

YRM 2025 - 21st ETSF Young Researchers' Meeting



Location: CECAM-IT-SISSA-SNS, Italy

Webpage : Event webpage

Dates: May 26, 2025 - May 30, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The Young Researchers' Meeting (YRM) 2025 covered a broad spectrum of cutting-edge topics in condensed matter physics and materials science, with a focus on theoretical and computational approaches. The program was structured around five major themes: (1) Electronic Structure and Methods Development, (2) Optical Properties of Materials, (3) Vibrational Properties and Transport, (4) Strongly Correlated Systems and Magnetism, and (5) High-Performance Computing.

Talks ranged from formal developments in Green's function methods and GW/BSE formalisms to emerging areas such as quantum transport in nanoscale systems, many-body localization, nonlinear optics in 2D materials, and proximity-induced topological phases. Young researchers presented novel applications of density functional theory (DFT), time-dependent DFT, and quantum Monte Carlo, often supported by in-house or community-developed software.

These discussions contributed to advancing the state of the art by encouraging cross-fertilization between different computational approaches and application domains. For example, participants working on time-dependent phenomena and spectroscopy found common ground with researchers developing new many-body methods. The inclusion of high-performance computing as a dedicated session also facilitated technical exchanges on code performance, parallel scaling, and hardware-specific optimization, which are increasingly crucial in materials science.

The event's interdisciplinary breadth and emphasis on early-career scientists ensured a vibrant and dynamic exchange of ideas, contributing meaningfully to the continued innovation in theoretical materials modeling.

2. What were the primary outcomes of this workshop, including limitations and open questions?

YRM 2025 provided a unique and energizing platform for young researchers to exchange ideas, present their work, and connect with peers across Europe and beyond. The event's primary outcome was the reinforcement of a vibrant community of early-career scientists working on theory and simulation of materials — a core objective of the ETSF and CECAM networks.

The workshop helped participants build their confidence in scientific communication and deepen their understanding of topics beyond their immediate expertise. The invited talks, specifically designed to be pedagogical and accessible, introduced complex areas of theoretical physics (such as GW/BSE, TDDFT, quantum transport, or electron-phonon

coupling) in a way that invited engagement from students and junior postdocs. The presence of multiple invited speakers per session allowed for diverse angles on shared themes, often sparking continued discussion during breaks and social events.
Another important outcome was the exposure to adjacent subfields. Talks on machine learning potentials, strongly correlated systems, or high-performance computing techniques were followed by informal conversations among participants who recognized potential for synergy. While no formal collaborations or publications emerged during the event, several participants reported follow-up exchanges after the meeting.
However, the compressed schedule also introduced limitations. Some sessions were significantly longer than others, while a few had only limited contributed content. Balancing the topic distribution across days – while accommodating speaker availability and maintaining thematic coherence – proved challenging. In a few cases, talks were placed in less-than-ideal sessions in order to preserve the overall structure of the program.

3. What was the take-home message for the participants?

YRM is a safe and supportive environment where young researchers begin developing their communication and collaboration skills. It encourages informal exchange, cross-field exposure, and discussions driven by peers – helping participants connect with new topics, new people, and new ideas at a formative stage in their careers.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

While YRM 2025 was primarily a scientific and training-focused event, its outcomes carry important indirect societal benefits. By offering a platform tailored to early-career researchers, the meeting supported the development of essential skills such as scientific communication, interdisciplinary thinking, and community building – all of which are critical for long-term progress in science and technology.
The workshop brought together young scientists working on topics that are highly relevant to societal challenges, including computational modeling for materials used in energy, photonics, and quantum technologies. Although these contributions may not translate immediately to applied outcomes, they help build the foundational knowledge and human capital needed to address broader issues such as sustainability, digital innovation, and future clean technologies.
By cultivating scientific maturity, peer support networks, and a sense of international community among young researchers, YRM plays a role in creating a more open, collaborative, and globally connected scientific culture – with clear long-term benefits for society.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

As a meeting primarily aimed at early-stage researchers, YRM 2025 did not lead to immediate tangible outcomes such as publications or proposals. However, several

participants initiated informal discussions that may evolve into future collaborations. The event helped young scientists discover shared interests and complementary methods, which is a critical first step toward joint work later in their careers.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

YRM 2025 placed strong emphasis on inclusivity, particularly in promoting early-career researchers at all stages, including Master's and PhD students. We achieved the best gender balance of recent editions, with 50% female invited speakers. We also ensured broad geographical representation, welcoming participants from across Europe as well as from Turkey, India, and Australia. The atmosphere was welcoming and accessible, fostering open exchange across backgrounds and career stages.

7. Participant list

Organisers
Dutta, Sarbajit
Ecole Polytechnique, France
Fabbro, Gabriele
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Azizi, Maryam - UCLouvain, Belgium
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El Sahili, Abdallah - Ecole Polytechnique-CEA, France
Maliyov, Ivan - EPFL, Switzerland
Monti, Marta - The Abdus Salam International Centre for Theoretical Physics, Italy
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Paoletti, Francesca - Universität Würzburg, Germany
Serrano Richaud, Elisa - Paris Saclay, Onera, Cnrs,lem, France
Zivkovic, Aleksandar - Utrecht University, Netherlands

Chemical reactivity in aerosols and at air-water interfaces



Location: Ecole Normale Supérieure, France

Webpage Event webpage

Dates: May 26, 2025 - May 28, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop was devoted to chemical reactivity in aqueous microdroplets, aerosol particles and at air-water interfaces, a field in which evidence for anomalous reactivity has accumulated far faster than its molecular modeling and interpretation. Twenty invited lectures, six contributed talks and five discussion sessions were organised around five themes, running from the properties of the interface to the chemistry they are invoked to explain.

 Properties of droplet interfaces: structure, dynamics and electric fields. Sylvie Roke and Heather Allen quantified interfacial structure, water orientation and electrostatics of aqueous interfaces by nonlinear spectroscopy; Ali Hassanali examined hydrophobic interfaces; Simone Pezzotti showed that electrified metal-water interfaces display air-water-like behaviour; and Yair Litman established that entropy governs water dissociation under strong fields. Together these moved interfacial electric fields from qualitative invocation to a measurable or computable quantity.

 Surface composition: ion propensity, partitioning and acidity. Xiangrui Kong compared atomic and molecular ions as drivers of surface reactivity, Chris Mundy went beyond simple ions to complexation, Miguel de la Puente revisited Henry's law in finite droplets, and Nonne Prisle demonstrated shifted protonation equilibria of atmospheric acids and bases at aqueous surfaces, with consequences for cloud droplet chemistry and climate. The recurring conclusion: the outermost layers, not the bulk, set the relevant reactant concentrations.

 Reactivity: radical formation, solvated electrons and oxidation. Jan Verlet and Gilbert Nathanson presented the dynamics, creation and reaction of solvated electrons at the water surface; Maria Angelaki addressed spontaneous OH formation in inorganic and organic droplets; James Donaldson surveyed "spontaneous" interfacial oxidation; Markus Ammann traced oxidation from surface to bulk; and Imon Mandal, mechanisms at seawater surfaces.

 Reaction acceleration, and the artifact question. Kevin Wilson, Teresa Head-Gordon and Shinichi Enami confronted reported rate enhancements with quantitative kinetic modelling, while Himanshu Mishra's re-examination of "spontaneous" H_2O_2 formation was programd deliberately alongside them, separating robust observations from other factors.

 Measurement, aerosol ageing and applications. Ruth Signorell, Bryan Bzdek and Ulrich Krieger presented femtolitre- and picolitre-droplet techniques giving access to reaction monitoring, surface tension and viscosity in single particles; Thorsten Hoffmann, Liwu Zhang and Celine Toubin connected these to size-selective aerosol processing, pollution and freezing; and Joakim Halldin Stenlid proposed nanodroplet-based removal of CH_4 and N_2O.

The state of the art was advanced by confronting experiment and simulation on the same observables, not merely the same phenomena.

2. What were the primary outcomes of this workshop, including limitations and open questions?

The central outcome was a substantially clarified and more critical consensus. Participants agreed that interfacial and droplet effects on reactivity are real and can be large, but that they are heterogeneous in origin: no single mechanism, whether dangling OH groups, partial solvation, low interfacial permittivity, strong electric fields, excess charge, confinement, shifted pH or evaporative preconcentration, accounts for the full body of observations. Several widely cited accelerations were shown to be partly attributable to experimental artifacts. The discussion sessions converged on the need for standardised reporting of droplet size, charge state, generation method, gas-phase composition and reaction kinetics, without which reported enhancements spanning several orders of magnitude simply cannot be compared.

A second outcome was methodological. The workshop made explicit that spectroscopic, mass-spectrometric and simulation probes interrogate different interfacial depths and different timescales, so that apparent disagreements are often definitional rather than physical. Agreeing on an operational definition of the "interface", and on benchmark systems on which experiment and theory can be compared quantitatively, emerged as the community's clearest priority.

Concrete follow-up actions were agreed during the meeting and have since materialised: an invited Perspective article for the Journal of the American Chemical Society, to be written by the three organisers together with Prof. Joseph S. Francisco; a follow-up conference held in Shanghai, China in April 2026, which attracted more than 200 participants; and the creation of a new Gordon Research Conference, "Fundamental to Applied Chemical Reactivity Across Interfaces and Droplets", whose inaugural edition will be held on 21-26 February 2027 in California.

Important limitations and open questions remain. The quantitative link between model microdroplets and atmospheric aerosols, which are multicomponent, viscous and often organic-rich, is still missing. The pH and the charge state of small droplets remain difficult both to measure and to define. Reactive simulations are limited by the cost of ab initio molecular dynamics and by the accuracy and transferability of machine-learning potentials, and the lengthscales they access still fall short of the systems probed experimentally. There is no consensus on how droplet effects scale with size, nor on whether interfacial catalysis can be exploited synthetically at scale. Finally, the workshop did not resolve the controversy over spontaneous H_2O_2 formation, although it did establish the experimental conditions under which the question must henceforth be posed.

3. What was the take-home message for the participants?

Interfacial and droplet effects on chemical reactivity are real and consequential, but there is no single mechanism and no substitute for careful control experiments. Progress now depends on the community agreeing on benchmark systems, on reporting droplet size,

charge and generation conditions systematically, and on comparing experiment and simulation on the same observable rather than on the same phenomenon.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

Yes, on three distinct fronts.
Climate and air quality. Aerosol chemistry and aerosol-cloud interactions remain the largest source of uncertainty in the radiative forcing estimates underpinning climate projections. Several contributions delivered parameters that feed directly into atmospheric models: shifted protonation equilibria of atmospheric acids and bases at droplet surfaces and their consequences for cloud droplet chemistry, revised Henry's law behaviour in finite droplets, surface tension and viscosity of individual picolitre particles, and the surface-to-bulk progression of oxidative ageing. Better constrained interfacial parameters mean better constrained predictions of cloud formation, aerosol lifetime and pollutant fate. Work on air-water interfacial mechanisms in atmospheric pollution processes and on the heterogeneous processing of organic aerosols bears directly on particulate matter toxicity and therefore on respiratory and cardiovascular health.
Green chemistry and sustainable synthesis. If reaction acceleration in microdroplets can be understood mechanistically and controlled, it offers a route to chemical synthesis with reduced solvent use, milder conditions and fewer catalysts. The workshop's critical scrutiny of which accelerations are genuine is a precondition for any credible scale-up, and protects the field from building on artifacts.
Finally, the meeting contributed to training: six contributed talks and the poster session were reserved for doctoral students and early-career researchers, who debated directly with the field's established figures.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

Publication. The organisers, together with Prof. Joseph S. Francisco, have been invited to write a Perspective article for the Journal of the American Chemical Society, drawing on the discussions held during the workshop. The article is in preparation.
Follow-up events. 1) A follow-up conference was held in Shanghai, China in April 2026 and attracted more than 200 participants, confirming the rapid growth and international reach of the community assembled in Paris. 2) A new Gordon Research Conference. The discussions initiated at this workshop led to a successful proposal for a new Gordon Research Conference "Fundamental to Applied Chemical Reactivity Across Interfaces and Droplets". Its inaugural meeting, "Interfacial and Droplet Reactivity: Mechanisms, Measurement, and Applications", will take place in February 2027 and be chaired by Profs. Head-Gordon and Zhang, two of our invited speakers. The creation of a GRC is the clearest possible institutional recognition for this new field.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

Inclusivity was addressed at the program design stage. The 20 invited speakers were based in 12 countries across Europe, North America, Asia and the Middle East, deliberately reaching beyond the usual European and North American core. Six invited speakers were women (30%), as were three of the six session chairs (50%), and a woman chaired a session on each of the three days.
Six short talks were selected competitively from submitted abstracts and reserved for doctoral students and early-career researchers, programd within the main sessions rather than in a separate junior slot; the poster session was open to all. CECAM support covered travel and accommodation for junior participants who could not otherwise have attended. Of the 44 registered participants, 13 were women and 15 were PhD students or postdocs, from 13 countries. The Ecole Normale Superieure venue is wheelchair accessible and dietary requirements were collected in advance.

7. Participant list

Organisers
George, Christian
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Wilson, Kevin - Lawrence Berkeley National Laboratory, United States
Zhang, Liwu - Fudan University, China
Zhou, Qi - Fritz-Haber Institute, Germany

Advanced SIESTA Workshop 2025

Location: ICN2, Spain
Webpage : Event webpage

Dates: Jun 2, 2025 - Jun 5, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The topics discussed in the event were:

- Electrochemical properties using TranSIESTA and Quantum Mechanics / Molecular Mechanics (QM/MM).
- Electronic transport.
- Postprocessing of data using sisl and external control of SIESTA through LUA.
- Magnetism: from spin-orbit couplints to TB2J and beyond.
- Superconductivity.
- Dynamical Mean Field Theory (DMFT).
- Anharmonic phonons and thermal conductivity with TDEP and SIESTA.
- Electron-lattice interactions.
- Lindhard response function in relation to Fermi surface nesting.
- SIESTA workflows and interoperability.
- Using SIESTA in exascale computers: solvers for large systems, tips and tricks for GPU usage.
- Molecular Dynamics acceleration in SIESTA using Machine Learning.
- The role of SIESTA in future Machine-Learning-based technologies.
- Recent and future developments in SIESTA.
- Challenges of high throughput calculations.

The workshop addressed recent advances in the SIESTA ecosystem, combining invited scientific presentations, technical demonstrations, tutorials, and community discussions. Major themes included large-scale parallel electronic-structure solvers; machine-learning-assisted acceleration of self-consistent-field calculations with graph2mat; post-processing and on-the-fly control using sisl and Lua; and interoperability with specialised tools for magnetism, DMFT, quantum transport, Lindhard-response, or finite-temperature phonon calculations with TDEP, among others. These examples demonstrated that SIESTA has evolved from a stand-alone DFT code into a flexible platform able to support advanced, domain-specific simulations.

A central discussion concerned how such capabilities can be combined into reproducible everyday research workflows. AiiDA, jobflow, atomate and custom Python scripts were considered as a possible workflow-management frameworks, although no universal solution has yet emerged. This diversity reflects the active search for robust approaches to handle heterogeneous calculations, manage data, and connect multiple simulation stages. Code modularisation and the adoption of community-maintained libraries were identified as key enablers of this evolution, facilitating code maintenance, validation, reuse, and the incorporation of new methods.

The workshop also considered the growing influence of AI and machine learning on electronic-structure research, stressing that interoperable interfaces, modular infrastructure, transparent workflows, and reliable documentation are prerequisites for

their responsible uptake. Finally, participants discussed strengthening the SIESTA community through improved branding, tutorials, documentation, Discord and other communication channels, and more active engagement with GitLab through bug reports, feature requests, and merge requests. Together, these actions support sustainable software development and accelerate the translation of methodological advances into broadly usable research capabilities.

2. What were the primary outcomes of this workshop, including limitations and open questions?

A principal outcome of the workshop was a shared recognition of SIESTA's distinctive scientific and practical value. Its efficient local-orbital approach enables simulations that can be difficult or computationally prohibitive with other DFT implementations, particularly for large and complex systems. This efficiency has helped democratize access to electronic-structure modelling by lowering computational-resource requirements and enabling researchers, including those with limited access to large-scale computing infrastructures, to undertake competitive first-principles research. Participants also identified a mature and expanding ecosystem of capabilities for scalable calculations, specialised analyses, scripting, and coupling to external methods/utilities/codes.
At the same time, the discussions identified limitations that require collective action. Although SIESTA is well established scientifically, it is not always perceived as a default reference code by potential users, who may be concerned about reliability relative to widely used plane-wave implementations. A priority is therefore to communicate validation results, benchmark protocols, methodological strengths, and appropriate domains of applicability more systematically. Better branding, documentation, tutorials, workshops, schools, and sustained dissemination are needed to make these strengths visible and to lower barriers for new users.
A further open question concerns how to engage the broader network of users and developers beyond the formal core team, and how to connect available tools into reliable packages. The call from a new generation of developers for a more dynamic and participatory environment was an especially positive outcome. Strengthening communication channels and contribution pathways can turn this renewed energy into sustained software development, wider validation, and new scientific functionality. The overall message was forward-looking: SIESTA has both a distinctive technical niche and an emerging community ready to expand it.

3. What was the take-home message for the participants?

SIESTA is an actively developed and maintained atomistic simulation software that is constantly incorporating new functionalities. There is also an ecosystem of other softwares that are interoperable with SIESTA and that broaden the scientific scope of its applications. The workshop also included a surprise celebration to mark the 30th anniversary of SIESTA, paying tribute to its founders and the project's evolution since its launch.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

Although the workshop was focused on fundamental computational materials science with SIESTA, it has a clear enabling and long-term societal benefit. SIESTA methodology, based on local-orbital with efficient linear-scaling algorithms enables accurate first-principles calculations at a substantially lower computational footprint than other approaches requiring more demanding resources to address comparable problems with similar accuracy. From the very beginning of the SIESTA project, this has helped democratize access to DFT modelling, allowing groups without routine access to large HPC facilities to undertake competitive research in electronic structure. The tutorials, hands-on and documentation prepared specifically for the Workshop contributes to lowering technical and training barriers for researchers worldwide.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The workshop did not produce a dedicated publication, but it generated several outputs. The sessions included hands-on tutorials and practical training materials, while new and improved user documentation was made available through the SIESTA web resources and documentation portal: https://siesta-project.org/siesta/events/Advanced_SIESTA_Workshop-2025/Sessions.html
The discussions and poster session also created opportunities for new scientific collaborations among users, developers, and researchers working on related methods and applications. Although these collaborations are still emerging, at least three SIESTA-related proposals were submitted to the most recent Spanish call for research projects, reflecting the capacity of the workshop to stimulate cooperation. The event also reinforced communication channels between the wider user and developer communities, creating a basis for further code contributions, documentation improvements, and joint training or dissemination activities.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The workshop promoted inclusivity across gender and career stage through both its organization and program design. Women represented approximately 20% of participants, while 2 out of the 5 organizers were women. The speakers included junior postdoctoral researchers alongside established scientists, creating visibility for researchers at different career stages.
The program was designed to encourage broad participation beyond formal presentations. Round-table discussions, poster sessions – with awards for outstanding student and postdoctoral presentations – and shared coffee-breaks and lunches created opportunities for early-career researchers, users, and developers to exchange ideas directly with senior participants. Despite limited travel-support resources, the workshop included 2 participants based outside Europe and sought to foster an open, collaborative environment for the wider SIESTA community.

7. Participant list

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Virtual Materials Design: AI, Simulation, and Workflows

Location: Karlsruhe Institute of Technology, Germany

Webpage : Event webpage

Dates: Jun 2, 2025 - Jun 5, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

106 scientists from 17 nations and various disciplines discussed recent developments in Virtual Materials Design, Accelerated Materials Design, Quantum Materials, High-Performance Computing, Multiscale Modelling, Artificial Intelligence and Machine Learning, Research Data Management and Data Science.
The framework of the workshop consisted of 10 thematic sessions with 37 talks with intensive discussion, featuring talks of 15 internationally renowned invited speakers. The workshop character was fostered by

- two poster sessions featuring 30 posters,
- two optional lab visits:

grid computing (https://www.scc.kit.edu/en/research/gridka.php)
and self-driving labs (https://www.chemasap.kit.edu/index.php)

- and two world-café discussion rounds to current key issues “Operating systems for Materials Accelerating Platforms - status and perspectives” and “Research Data Management - which tools are actually being used?”.

The workshop was complemented by four parallel half-day hands-on tutorials on the “4C multiphysics framework” (https://www.4c-multiphysics.org), “all-electron DFT code FLEUR” (https://www.flapw.de/MaX-8.0/), “Karlsruhe Data Infrastructure for Material Sciences Kadi4Mat” (https://kadi.iam.kit.edu/) and “Workflows for Virtual Materials Design with SimStack and Beyond” (https://www.simstack.de/). The developers of these freely accessible software tools explained the functions of the respective software to the attendees and helped them to solve their own research questions with these software tools.

2. What were the primary outcomes of this workshop, including limitations and open questions?

The workshop provided a surprisingly successful venue to bring together experimentalists to explore and understand the existing challenges and to discuss ways to overcome them. From the experimental colleagues the issue of many theoretical methods is their lack of robustness. Slight changes in the parameters often result in unexpected outcomes. In addition, there are gaps in the method spectrum, in particular for processing / synthesis questions. There was ample discussion regarding the potential of AI to close these gaps, which then led to discussions of the need for high-quality training data. From the theorists' perspective, there is a lack of systematic experimentation to validate methods or to train ML models. Most experiments are "one-of-a-kind" and even experiments on the same application, e.g. batteries, yield very different outcomes in different laboratories. Overall,

however, there was a sense of progression of the method, also with regard to multiscale and AI guided approaches to virtual materials design and several invited speakers provided high-level success stories as examples.

3. What was the take-home message for the participants?

Virtual Materials Design has an increasing number of success stories which enable interested parties to evaluate the potential of this approach, combining multiscale simulation and AI guided design, for a broad range of applications.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

In Virtual Materials Design long test series give way to algorithms and computational models. This can drastically shorten the cycle of developing novel materials or chemical compounds. New functional materials and devices are the key for mastering many societal and environmental challenges, ranging from energy conversion and storage, automotive or communication technologies to healthcare devices or new pharmaceuticals. The technological readiness of the presented theoretical methods was discussed with the participants from industry, e.g. BASF, FEHRMANN Materials, and CuspAI for accelerating materials development, or IBM and ParTec for developing supercomputers.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

There were several software-related workshops which were very well attended and are likely to lead to better dissemination of the software. We know from discussions that new collaborations are planned between several participants but the organizers did not attempt to follow up on this on a formal level.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

We allowed all applicants from abroad and limited the participation of employees of the host institution KIT. We provided personalized invitation letters to all applicants from overseas three months before the workshop to facilitate the visa procedure. Due to the high level of personal interaction, the workshop was designed as an on-site face-to-face workshop, but we made it possible for one participant with visa issues to give her presentation online. 65 participants were German, 27 from other European countries and 14 participants came from overseas.
We encouraged the invited speakers to bring students who were given the chance to present a poster, and the various event formats made the workshop attractive for participants at all career levels.

19% of the participants, 17% of the poster presenters and 13% of the speakers were female. This roughly corresponds to the gender ratio among students and professors in these research fields. Increasing this ratio is a focus for our next workshop.

7. Participant list

Organisers
Blügel, Stefan
Forschungszentrum Jülich, Germany
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Karlsruhe Institute of Technology, Germany
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Multiscale Molecular Dynamics with MiMiC: Optimizing the Performance on Modern Supercomputers

Location: CECAM-DE-JUELICH

Webpage : Event webpage

Dates: Jun 2, 2025 - Jun 6, 2025

1. What were the major topics presented in the School?

The school covered a range of topics in multiscale molecular simulations, with a focus on quantum mechanics/molecular mechanics (QM/MM) methodologies and their efficient execution on modern high-performance computing (HPC) systems. The core of the program introduced participants to the theory and practice of QM/MM molecular dynamics.

Specifically, participants were trained on the MiMiC framework, a flexible and high-performance software environment for QM/MM simulations that couples widely used quantum and molecular mechanics packages. Through lectures and hands-on tutorials, students learned how to set up and execute simulations, from basic QM/MM protocols to tasks such as system preparation, parameter selection, and simulation control.

Another major component of the program focused on the practical use of HPC infrastructures. Lectures addressed the architecture and programming models of current and upcoming supercomputers, including GPU/CPU hybrid systems. Tutorials guided participants through benchmarking and resource optimization for scalable QM/MM simulations, equipping them with the tools to make efficient use of supercomputing resources with MiMiC.

The program also explored advanced simulation techniques such as enhanced sampling methods and rare-event algorithms. Students were introduced to tools like PLUMED for coupling with QM/MM simulations to access rare events. Finally, applications of the MiMiC framework to real biochemical problems were showcased.

2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

In addition to having dedicated Q&A moments after each lecture, we also dedicated the last session of this school to discuss open questions and feedback from the students. Some of the topics that came up during Q&A sessions and the reflection session:

- How to streamline the format of exercises for future users on the public-facing page, with notes on executables to use at the top to make it more general
- Request for read-at-home information and pointers on how to improve knowledge about electronic structure methods (specifically DFT) for students who were less familiar with these topics.
- Discussion on further examples of rare-event sampling within biochemical systems and how we might model those using MiMiC-based simulations.

- Individual discussions about the HPC architectures that students will encounter at home. We gave pointers for the use of computing resources at their home institutes.
- Individual discussions about the systems of interest for the students. For example, if they plan to model an enzymatic process, we would discuss with them ideas for selecting a relevant quantum region within the system.
- We ended the school with a discussion of the features students would like to see as part of the MiMiC framework in the future such as different codes (e.g., LAMMPS), different scales of simulation (e.g., coarse graining), and additional types of quantum mechanical calculations (e.g., wave function-based methods).

3. What was the take-home message for the participants?

The school highlighted how multiscale modeling software leveraging modern HPC infrastructures enables state-of-the-art simulations of biochemical processes. Participants learned how the MiMiC framework provides a powerful and flexible platform to efficiently perform such simulations by coupling quantum and classical codes on heterogeneous architectures.

4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

- Lecture notes available for the students on the CECAM event website.
- Recording of the lectures will be published on the MiMiC YouTube channel (https://www.youtube.com/@mimicproject).
- Hands-on tutorials are collected on the MiMiC GitLab repository and will be accessible through the MiMiC website.

5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

We paid close attention to gender balance and a broad geographical representation among both participants and speakers, as illustrated by the statistics below.
A total of 48 participants attended the school:
- 38 participants (28 onsite, 10 remote). 14 females, 24 males.
- 10 speakers (9 onsite, 1 remote). 3 female, 7 male.

Attendees represented institutes from 14 countries: Colombia, Denmark, Egypt, Germany, Ireland, Italy, Netherlands, Norway, Sweden, Switzerland, Taiwan, Turkey, UK, US.
Countries of origin included: Ecuador, Egypt, Denmark, Germany, India, Italy, Spain, Mexico, Portugal, US, Vietnam.
Participants comprised master and PhD students, postdoctoral researchers, faculty members, and permanent scientific staff.

6. Participant list

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Wieduwilt, Erna - University of Southern Denmark, Denmark
Wiley, Brian - University of Bath, United Kingdom

Advancing biochar molecular models – from experiments to model construction and application

Location: CECAM-HQ-EPFL, Switzerland



Webpage : Event webpage

Dates: Jun 4, 2025 - Jun 6, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

This workshop focused on bridging experimental and computational approaches to advance biochar molecular modeling and the potential use of this tool in the design of new carbonization processes and products. [*Fig. 1 shows the word cloud of 25 presentation titles - could not insert figure*] Key topics included: (1) integrating experimental characterization techniques, such as solid-state NMR, Raman spectroscopy, and BET analysis, with atomistic modeling to develop realistic biochar models; (2) constructing molecular models that account for biochar's heterogeneous structure, including porosity, defects, and cross-linking; (3) establishing structure-property relationships to optimize biochar for applications like carbon sequestration, water purification, and energy storage; and (4) potential to exploring density functional theory (DFT) and machine learning (ML) to enhance model's accuracy and scalability. We surveyed the participants with a questionnaire; the responses highlighted their interest in the discussions on modeling mesopores, surface area, and biochar's porosity, as well as the challenges of incorporating experimental data to predict properties such as FTIR, XPS spectra, and gas sorption isotherms.

These discussions advanced the state of the art by fostering collaboration between experimentalists and modelers, addressing longstanding challenges in biochar modeling and experimental analysis. Historically, biochar models oversimplified its complex, feedstock-dependent structure, limiting their predictive power. The workshop built on recent advancements in carbon material modeling (e.g., kerogens, graphene-based materials) by integrating large-scale experimental datasets with computational tools like classical and reactive molecular dynamics (MD) and DFT. Participants noted that linking experimental data with simulations enables more accurate representations of biochar's molecular complexity, particularly surface chemistry, polyaromatic ring structures, porosity and defect structures. The discussions also covered the need for the need to use of ML-driven approaches and standardized workflows to streamline model development, reducing reliance on trial-and-error approaches. By identifying bottlenecks in both modeling and experimental characterization, the workshop aims to set a roadmap for developing truthful models of biochar materials, advancing the use of computational chemistry in sustainable material design and environmental applications.

2. What were the primary outcomes of this workshop, including limitations and open questions?

The workshop yielded several key outcomes. It facilitated new collaborations between experimentalists and computational scientists, with participants reporting plans for joint publications, including a perspective article on biochar molecular modeling (led by organizers) and a review paper on pitfalls in biochar physicochemical analysis (led by one of the invited speakers). We also had discussions on EU funding opportunities, such as COST and MSCA, and there are initiatives for collaborative research proposals for both schemes.
Participants gained insights into advanced methodologies, including DFT for reaction mechanisms, classical and reactive MD for pore structure modeling, and development of databases for predicting biochar properties. The workshop also highlighted the importance of integrating experimental data (e.g., NMR, Raman) with simulations to capture biochar's heterogeneity, enhancing model accuracy for adsorption applications, carbon sequestration, etc.
Limitations identified included the challenge of standardizing modeling workflows due to biochar's diverse compositions and production conditions, as well as defining models targeting different usages. This is a limitation not for the developers in the modeling community, but rather for the community that would like to apply those models. Modelers also highlighted difficulties in representing defects induced by inorganics or during post-treatments. Open questions included: (1) how to develop scalable, validated models that account for feedstock variability; (2) how to integrate molecular and mesoscale models to capture biochar's behavior in real-world environments, such as soil systems; and (3) how to train models with accurate experimental data to predict long-term biochar transformations. These unresolved issues underscore the need for shared databases and standardized measurement and modeling protocols, which participants proposed addressing through collaborative frameworks like EU-funded projects. The workshop's emphasis on interdisciplinary approaches and community-building initiatives, such as Round Robin tests for surface analysis, laid the groundwork for tackling these challenges. We hope this workshop is the key steppingstone to fostering a cohesive biochar research community. The workshop also highlighted the need for more joint work between modelers and experimentalists to advancing our understanding of the evolution of solid structures (from biomass to biochar) during carbonization.

3. What was the take-home message for the participants?

Collaboration between experimentalists and modelers is essential for developing realistic biochar atomistic and molecular models. Integrating experimental data with advanced computational techniques enables accurate prediction of biochar properties, optimizing its use in environmental and industrial applications. More collaborative work is also needed to better understand the gradual evolution of the structure of the solid and the mechanisms of biochar formation.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

The workshop's outcomes have significant potential for societal benefits, particularly in environmental sustainability and climate mitigation. The conversion of biomass carbon into stabilized biochar structures has great potential to fight global warming. By advancing

the development of predictive biochar molecular models, the workshop supports the optimisation of biochar for applications like C-sequestration, water purification, soil enhancement, and energy storage. Participants emphasised biochar's role in fighting global warming through carbon sequestration and improving soil fertility for agricultural productivity, which could enhance food security, especially in developing regions. Improved models for adsorption (e.g., gases like CO_2, or pollutants like PFAS) could lead to more effective environmental remediation technologies, addressing water and soil contamination. The focus on structure-property relationships enables tailored biochar production, reducing costs and increasing efficiency for industrial applications.
The workshop's collaborative initiatives, such as plans for perspective/review articles and EU-funded projects, could also influence policy and industry by providing expert insights to guide sustainable practices. However, realizing these benefits requires translating scientific outcomes into cross-sector partnerships and clear application pathways. Challenges like scaling models to industrial processes and ensuring equitable access to biochar technologies must be addressed. Participants noted that moving further, involving stakeholders from application-focused fields (e.g., agriculture) could strengthen the impact. By fostering a multidisciplinary community, the workshop laid a foundation for innovations that could drive environmental protection, resource utilization, and sustainable development.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

Tangible outcomes include plans for a perspective article (led by organizers) on biochar molecular modeling and a review paper (led by a speaker) on pitfalls in biochar physicochemical analysis.
New collaborations emerged, with participants initiating discussions for joint research projects and the creation of databases and training materials. Proposals for EU funding (COST and MSCA) were outlined to support structured collaborations. Participants reported intentions to apply new learned methodologies in their research. These outcomes reflect the workshop's success in fostering actionable research initiatives.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The w/sh promoted inclusivity through a balanced selection of speakers, which naturally ensured gender diversity. This is particularly notable in computational sciences where women are underrepresented. Participants and speakers represented diverse regions (17 countries: UK–11, Italy–5, Fra/USA–5, Germ–4, Ind/Can/Belg/Swe–2, and Aust/Col/Indon/ Kenya/Neth/Pakis/Tur-1, from 20 institutions). Though the survey feedback it was suggested to increasing representation from Africa, S. Asia, and L. America. We note that with CECAM fellowship we funded a participant from Kenya, who unfortunately could not secure a visa. We also covered hotel for participants from Colombia and Pakistan. Hybrid participation ensured accessibility for remote attendees, unable to travel for various reasons. Suggestions for improvement included more outreach to diverse regions and more posters for ECRs.

7. Participant list

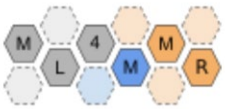
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School on Machine Learning for Molecules and Materials Research

Location: Zadar, Croatia



Webpage : Event webpage

Dates: Jun 9, 2025 - Jun 13, 2025

1. What were the major topics presented in the School?

This event offered a comprehensive overview of cutting-edge machine learning methods, data-driven modeling, and atomistic simulations applied to materials and molecular sciences. Through a series of lectures and hands-on tutorials, participants were introduced to both foundational concepts and advanced tools currently transforming computational chemistry, materials design, and soft matter research.
The school covered each topic through an introductory lecture and hands-on tutorial showcasing a realistic scenario. The lectures and tutorials were complemented by selected oral contributions from early-career participants. A block concerned the exploration of large chemical spaces, generally accounting for equilibrium or ensemble-averaged information, utilizing an array of methods that range from materials and chemo-informatics approaches to those closer to artificial intelligence. Another block of lectures illustrated the key role of dynamics in determining the properties of a material, a molecule, or an experimental measurement. Also for this case, a diverse set of methodologies was considered, also in relation to a multi-scale vision.
Topics covered included high-throughput materials discovery using DFT and beyond, Bayesian optimization and active learning strategies, machine learning potentials and force fields, generative models and autonomous agents – including large language models and embeddings for property prediction – data integration and structure determination, physics-informed ML architectures for experimental observables and nonadiabatic dynamics, as well as transferable coarse-grained models for multiscale simulations.
State-of-the-art equivariant graph neural networks were explored for modeling complex chemical systems and addressing industrial-scale challenges. The “materials genes” concept was highlighted as a promising approach to bridge atomistic simulations with experimental efforts. The application of ML in industry was showcased through the example of structure determination in the pharmaceutical sector, reflecting the emerging start-up ecosystem around ML for materials.
Participants gained hands-on experience with modern ML libraries and simulation tools, acquired practical skills in model training, validation, and fine-tuning, and learned how to effectively integrate computational and experimental data to accelerate discovery across multiple scales and material systems.

2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

Several key limitations were identified throughout the event, broadly categorized into data-related challenges, scalability and computational cost, and issues concerning model

generalizability and transferability. These were identified during Q&A, panel, and poster sessions.
In the context of high-throughput discovery using DFT, participants discussed the prohibitive computational cost of high-fidelity methods such as hybrid functionals and GW, which scale poorly with system size. Additionally, the lack of standardization across datasets – due to variations in pseudopotentials, exchange-correlation functionals, and calculation settings – raises concerns about data interoperability. Incorporating environmental effects (e.g., solvent, temperature, pH) into high-throughput workflows remains a significant open challenge.
For machine learning potentials and force fields, the need for large, diverse, and high-quality DFT-level datasets was emphasized, alongside current limitations in model transferability and robustness across different chemical environments. While state-of-the-art equivariant graph neural networks (e.g., NequIP, MACE) show excellent accuracy, they are computationally expensive and memory-intensive to train. Moreover, datasets relevant to industrial applications or extreme conditions are often scarce or difficult to generate reliably. Open questions bridging the atomistic one - hence involving learning electronic structure solutions (e.g. Hamiltonian learning) or coarse grained representation - were also identified.
The importance of uncertainty quantification – especially via Bayesian methods – was highlighted as a critical component for both prediction reliability and decision-making in ML-guided materials design.
Regarding generative models and autonomous agents, concerns were raised about the chemical validity and safety of generated structures, particularly in models lacking physical constraints or domain-specific priors. Purely data-driven generative approaches were contrasted with physics-informed machine learning, leaving open questions about the achievable accuracy, interpretability, and reliability of these methods over the next few years.

3. What was the take-home message for the participants?

Key takeaways included the shift toward foundation models and acceleration via ML/MD pipelines, as well as the transformative role of generative models. Future directions emphasize integrating computational and experimental data, handling uncertainties, and using ML to overcome DFT and broader physics limits. Career advice stressed lifelong learning, curiosity, and readiness to solve complex, real-world problems across academic and industrial domains.

4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

Yes, several tangible outcomes are made available after the school.
- The GitHub repository rbi-mtm/ml4mmr provides 10 curated tutorials covering key topics in machine learning for molecules and materials research. Each tutorial includes its own kernel/environment specification, ensuring reproducibility and ease of setup. For several tutorials, an additional Google Colab link is provided, enabling participants to run the notebooks directly in the cloud without local installation.

- Recordings of the lectures, tutorials, oral presentations, and panel discussions are available on a DAEMON COST YouTube channel: https://www.youtube.com/@DAEMON-COST-action/playlists.
- the video recordings will be soon added to the Lhumos platform too.

5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

We actively promoted inclusivity by ensuring gender balance and diversity in the selection of speakers, organizers, and participants. Excluding organizers and invited speakers, out of 66 participants, 22 (1/3) were women. Out of 15 lecturers, 4 were women, while out of 10 tutors, 1 was a woman. Due to the program constraints and cancellation from some tutors, the final gender ratio of tutors does not fully reflect our efforts to promote representation and diversity. The program featured early-career and senior researchers from 17 countries across Europe and beyond. Special attention was given to including participants from EU13 countries and non-EU countries in the region. The call for participation was widely distributed through open channels and COST Action networks, encouraging applications from diverse backgrounds and career stages. Online materials are made available for those with limited on-site access. We also emphasized inclusive communication and a respectful environment through our code of conduct.

6. Participant list

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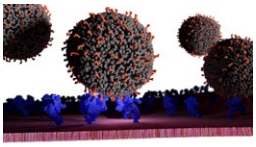
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The role of multivalency and superselectivity in the regulation of the immune system

Location: CECAM-HQ-EPFL, Switzerland



Webpage : Event webpage

Dates: Jun 16, 2025 - Jun 18, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The talks examined **multivalency,** the simultaneous binding of multiple ligands to multiple receptors, as a central principle of immune recognition and signaling. A related effect, **superselectivity**, where small changes in affinity or receptor density trigger disproportionate binding outcomes, was highlighted as critical for immune discrimination.
Contributions spanned multiple perspectives:
1. Theoretical and computational models of multivalent binding
2. Statistical mechanics and physics-based approaches to immunity
3. Experimental tools to probe receptor activation
4. Roles of crowding and spatial organization in signaling
5. Nanotechnology and synthetic biology to manipulate immune processes
6. The importance of glycans, mucins, and other modulators

This diversity of approaches created fertile ground for interdisciplinary connections. Discussion converged on **four priority themes**:

1. Mechanisms of B-cell and adaptive immune activation

How does multivalency shape B-cell activation, tolerance, and differentiation? Can multivalent self-antigens drive activation of autoreactive B cells? Do NK cells also exploit multivalency? How does antigen spatial organization (e.g. on viral particles) affect immune outcomes? What roles do hydrodynamic interactions and collective receptor dynamics play, and which tools are best suited to probe these mechanisms?

2. Information processing in the immune system

Does the immune system use temporal correlations to improve discrimination? How can principles from physics and information theory illuminate decision-making? What frameworks can better integrate physics-based modelling with immunology?

3. Nanotechnology and simplified model systems

How can nanomaterials provide new probes or synthetic platforms? What constitutes an "ideal" simplified model – capturing essential biology while remaining tractable?

4. Glycans and mucins in immune regulation

How do glycans and mucins suppress or modulate immune responses? How do viral glycans influence B-cell receptor superselectivity? Which experimental models best test these hypotheses?

Together, these discussions underscored the need for multidisciplinary strategies that combine modelling, simulation, quantitative experiments, and materials science to advance understanding of immune regulation.

2. What were the primary outcomes of this workshop, including limitations and open questions?

The CECAM workshop in Lausanne successfully fostered dialogue across disciplinary boundaries, creating a common language between physicists, immunologists, and nanotechnologists. The meeting started from ideas about the role of *multivalency and superselectivity,* but the final discussion was much broader and clearly stressed the need for tighter collaboration between physicists, immunologists and nanotechnologists to better understand the immune system regulation, where very fundamental questions still remain unanswered. As one participant highlighted “Immunology is a bit like physics at the beginning of 1900[CY1] ”. In other words, a lot is known, but a revolution is possibly coming. CECAM role in this should be to facilitate further discussion around the topics previously mentioned, as they seem to be those where the most impact can be achieved. In this regard, the identified open questions provide a roadmap for future efforts. By addressing these challenges, the community can move toward a deeper understanding of immune activation and regulation – knowledge with profound implications for vaccines, immunotherapies, and nanomedicine.

3. What was the take-home message for the participants?

As one participant highlighted “Immunology is a bit like physics at the beginning of 1900”. In other words, a lot is known, but a revolution is possibly coming. CECAM role in this should be to facilitate further discussion around the topics previously mentioned, as they seem to be those where the most impact can be achieved. In this regard, the identified open questions provide a roadmap for future efforts. By addressing these challenges, the community can move toward a deeper understanding of immune activation and regulation – knowledge with profound implications for vaccines, immunotherapies, and nanomedicine.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

Progress in fundamental understanding of the physical mechanisms behind the immune system response obviously has an enormous social impact as it opens new possibilities to design disease treatments and strategies to control and regulate the immune response. Moreover, it has an impact on many other areas in biomedical technology.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

There are several new collaborations emerging from the discussions during the workshop - on top of the already existing ones.
We decided to put together a special issue on the topic, and we also discussed a possibility to propose a European doctoral training network on the topic. This would be a

great opportunity to further consolidate the community and train young scientists in this interdisciplinary field, for which the traditional doctoral programs are lacking in content. The activities along these ideas have started and we expect to prepare a proposal in 2026.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

We took great care to promote inclusivity on all levels: in the composition of the organizational committee, in inviting participants/speakers, and in accepting participants.

7. Participant list

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Structure, Stress, Strain & Stretching Flows



Location: Monash University Prato Centre, Italy

Webpage : Event webpage

Dates: Jun 18, 2025 - Jun 20, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The Workshop *Structure, Stress, Strain & Stretching Flows* (Prato, June 18–20, 2025) convened researchers across simulation, theory, and experiment to address a central challenge in complex fluids: connecting microstructural dynamics to macroscopic flow behavior. Over three days, the meeting traced the arc from detailed mesoscale simulations, through constitutive modeling, to macroscopic flow experiments and machine-learning-enabled coarse-graining.

Day 1 explored *mesoscale simulations as a bridge between theory and experiment*. Talks addressed single-polymer dynamics in turbulence, Brownian dynamics of wormlike micelles, ring polymer dynamics, and network fracture under elongation. These studies demonstrated how mesoscale simulations now yield detailed insights into configuration statistics, stress fluctuations, and hydrodynamic interactions, especially in extension-dominated flows where classical models often fail.

Day 2 focused on *constructing and testing constitutive models* informed by microstructure. Speakers examined the successes and limitations of slip-link, tube, and kinetic theories, and emphasized the need for benchmark flows covering shear, extension, and mixed kinematics. New rheometric methods such as CHEW waveforms and tethered swimming probes were presented. Multiple talks highlighted divergences between model predictions in extensional flows, underscoring the need for better experimental discrimination.

Day 3 turned to *macroscopic modeling and multiscale challenges*, including flows of gels, granular suspensions, and soft glasses. Talks ranged from yielding and memory in soft materials to viscoplastic flow simulations and hybrid micro-macro approaches. Several speakers showcased emerging data-driven constitutive frameworks that integrate physics-based insight with machine learning. The concluding panel discussion emphasized three forward-looking themes: (1) the need for validated benchmark problems; (2) the promise of data-informed modeling; and (3) the challenge of unifying steady and transient behaviors across diverse flow types.

Overall, the workshop underscored the value of integrating mesoscale simulations, advanced rheometry, and statistical modeling. It brought clarity to long-standing modeling challenges, fostered new collaborations, and helped chart a path toward predictive rheology for complex fluids.

2. What were the primary outcomes of this workshop, including limitations and open questions?

Several key outcomes emerged.
First, there was consensus that extension-dominated and kinematically mixed flows are the most stringent tests for constitutive models. Traditional benchmarks like steady shear are inadequate. Many participants called for shared benchmark problems – transient, steady, and mixed – that enable systematic cross-validation between simulations and experiments.
Second, the limitations of current constitutive models were emphasized. Even advanced slip-link and tube models diverge in extensional flows or fail outside calibrated regimes. This reinforced the need for closures grounded in configurational statistics or simulation-informed models.
Third, mesoscale simulations have become indispensable for probing microstructure–stress relations. However, they remain sensitive to parameters, lack validation in complex geometries, and face scaling challenges in multicomponent systems like biofluids and FMCGs.
Fourth, data-driven approaches – though promising – must be anchored in physical insight. Talks by Ellero, Graham, and others explored hybrid strategies: physics-informed neural networks, reduced-order modeling, and data-assisted closures. These drew strong interest, though concerns about robustness and generalizability remain.
Fifth, several talks examined the complexity of materials with nested or hierarchical microstructures. Geri, speaking on dense suspensions and materials like cement, highlighted the need to understand systems without clear scale separation. These *hypercomplex* materials may require *microstructure-agnostic constitutive models*, as discussed by Rogers and Ewoldt, who proposed modeling based on nonlinear response surfaces, memory effects, and dispersity rather than fixed molecular structure.
Finally, too often, theory, simulation, and experiment proceed in isolation. Participants strongly supported creating collaborative platforms and shared datasets to accelerate model testing and refinement.
In sum, the workshop clarified pressing priorities, catalyzed new collaborations, and crystallized a central challenge: how do we construct models that faithfully predict flow in nonlinear, history-dependent, multiscale materials – not by oversimplifying microstructure, but by learning when and how to abstract from it?

3. What was the take-home message for the participants?

To model complex fluids meaningfully, we must move beyond traditional constitutive equations and embrace approaches that integrate mesoscale insight, experimental nuance, and data-driven abstraction. Extension-dominated and mixed flows offer critical tests, and for hypercomplex materials, microstructure-agnostic frameworks may be essential. Predictive rheology demands collaboration across theory, simulation, and experiment.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

Yes. The outcomes of the workshop hold significant potential for societal benefits, particularly in sectors that rely on the processing and performance of complex fluids and soft materials. These include industries such as pharmaceuticals, food and beverages,

cosmetics, consumer goods (FMCGs), paints and coatings, and construction materials such as cement and concrete.
Participants highlighted that predictive models of flow behavior are essential for designing *energy-efficient and sustainable processes*, reducing waste, and improving material performance. For example, understanding extensional flows in polymer solutions directly informs the manufacturing of biodegradable plastics and high-performance fibers. Similarly, insights into dense suspensions and yield-stress materials – such as those discussed in the context of concrete, gels, and emulsions – can lead to better formulations and more resilient infrastructure.
The potential for *data-driven, simulation-informed rheology* to reduce costly experimental trials and accelerate formulation development was repeatedly emphasized. Such approaches can also assist in *personalized medicine* (e.g., injectable drug delivery), *nutrition for vulnerable populations* (e.g. texture-modified foods for dysphagia), and the optimization of *sustainable packaging materials*.
Importantly, the concept of *microstructure-agnostic modeling*, discussed in relation to hypercomplex materials, offers a new paradigm for understanding poorly characterized systems – critical for emerging technologies and circular economy applications.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

Yes. A perspective review article is being planned for the *Journal of Non-Newtonian Fluid Mechanics*, synthesizing insights from the workshop and outlining future directions. A novel suggestion by Prabhakar – viewing capillary breakup as the *simplest complex flow* – was widely appreciated as a crucial test case for microstructure-based models in extension-dominated regimes. Plans are also underway to initiate an *interlaboratory collaborative experiment* using standardized test polymer solutions across benchmark flows (e.g., 4:1 contraction, planar extension). This would generate high-quality experimental data for validating competing models. Several new collaborations were seeded across simulation, theory, and rheometry, and participants expressed interest in coordinated proposal submissions to support this work.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

We promoted inclusivity across gender, geography, and career stage. Six women gave talks at the workshop, contributing key perspectives across theory, experiment, and simulation. We ensured broad geographical representation, with participants from Europe, North America, Asia, and Australia. Early-career researchers were included among speakers and poster presenters, and informal networking at meals and the poster session encouraged open dialogue. While the number of posters was smaller than anticipated, the event fostered inclusive discussion and cross-disciplinary exchange. The venue was fully accessible, and we accommodated specific needs as they arose. Diversity of intellectual approach was a key priority, and the program intentionally combined established leaders with emerging voices across continents.

7. Participant list

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The atomic simulation environment ecosystem: Present and perspectives



Location: CECAM-HQ-EPFL, Switzerland

Webpage : Event webpage

Dates: Jun 23, 2025 - Jun 27, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop brought together a diverse community of users, developers, and contributors to the Atomic Simulation Environment (ASE) package and its broader ecosystem of dependent packages to critically assess the current state of the software and collaboratively shape its future. Major topics included:

- **Modularisation and plug-ability:** Participants strongly supported making components like visualisers, IO, calculators, and even low-level algorithms (e.g., neighbour lists) plug-able. This reflects a broader trend in scientific software towards modular, maintainable architectures that can evolve with community needs.
- **Decoupling core components:** A key technical discussion focused on decoupling core components, for example by implementing more interfaces like Optimizable that provide generic functionality, and by increasing the code's usage of the Single Responsibility Principle, e.g. by separating the Atoms and Calculator classes. This would allow for more flexible workflows, better integration with machine learning potentials, and support for multiple calculators per structure – an increasingly common requirement in modern computational materials science.
- **Improving usability and documentation:** There was a clear consensus on the need to improve tutorials and documentation. This is essential for lowering the barrier to entry for new users and contributors, and for ensuring the long-term sustainability of ASE.
- **Governance and community practices:** Participants proposed adopting enhancement proposals (akin to Python's PEPs) and establishing clearer boundaries for core vs. plugin functionality. These discussions aim to foster a more inclusive and transparent development culture.
- Future Development Priorities: A ranked poll identified top priorities such as moving functionality to plugins, improving error handling, and supporting additional computed properties (e.g., Hessians). These priorities reflect a mature and forward-looking vision for ASE's evolution.

The format for the event comprised two days of invited talks by key users and developers of packages in the ASE ecosystem, followed by a challenge development session with pitches from facilitators for three working groups. The working groups then broke out to focus on the development of a plugin infrastructure for ASE, redesigning the Atoms/Calculator interface, and improving the documentation for the package. On the final day each group presented an update on its findings to all participants, feeding into a road map generation session. This format worked very well.

2. What were the primary outcomes of this workshop, including limitations and open questions?

The workshop yielded several concrete outcomes:

- **Prioritised development roadmap:** Through ranked polling, the community established a clear set of development priorities, including decoupling core components, improving documentation, and enhancing error handling.
- **Consensus on modularisation:** There was strong agreement on the need to modularise ASE, with many participants advocating for a rewrite of the core to support a plugin-based architecture. This would enable faster innovation and easier maintenance.
- **Community-driven proposals:** The idea of using ASE Enhancement Proposals (AEPs) to formalise and discuss major changes was well received. This could lead to more structured and transparent decision-making.
- **Governance structure:** There was a clear consensus around establishing a Steering Committee for ASE. The initial membership of this committee will comprise the organiser and invited speakers of the workshop. Draft terms of references were discussed and agreed. The first meeting is planned for later this summer.

Open Questions :

- How to balance modularity with usability for new users?
- How to ensure backward compatibility while modernising the codebase?

Limitations :

- The workshop was limited in time and could not fully explore all technical proposals.
- Some key stakeholders were not present, potentially limiting the representativeness of the consensus. Further consultation will be needed before making breaking changes to the code.
- While many ideas were proposed, concrete implementation plans (e.g., funding, timelines) remain to be developed.

Despite these limitations, the workshop succeeded in identifying critical issues, building consensus, and laying the groundwork for future development.

3. What was the take-home message for the participants?

ASE is a critical piece of research infrastructure with a broad and vibrant community behind it. To fully deliver on its promise, the package must continue to evolve to remain sustainable: modularisation, better documentation, and community-driven governance are essential to support future scientific innovation and broader participation.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

Yes. ASE is a foundational tool in computational materials science, used in fields ranging from energy storage to catalysis and quantum computing. By improving its usability, modularity, and extensibility, the workshop outcomes can:

- **Accelerate scientific discovery:** Easier integration of new methods (e.g., ML potentials) will enable faster development of materials for clean energy, electronics, and more.

 Enhance education and training: Improved documentation and tutorials will make ASE more accessible to students and researchers worldwide.
 Promote open science: A more inclusive and transparent development process aligns with the principles of open science, fostering collaboration and reproducibility.
 Support innovation: Modular design will allow industry and academia to build custom workflows, reducing duplication and increasing efficiency.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

Yes:
 A Steering Committee is being established.
 A prioritised roadmap for ASE development.
 Community consensus on modularisation and governance.
 Plans for regular hackathons and improved release cycles.
 Potential collaborations around GUI development and ML integration.
 Ideas for funding proposals, including a follow up workshop in one year to be held at a CECAM node. A proposal for this has been developed by early career attendees of the present workshop and submitted.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The workshop ensured inclusivity by:
 Encouraging participation across career stages (PhD to faculty).
 Using anonymous polling in the discussion session to give all voices equal weight.
 Including contributors from diverse geographical and institutional backgrounds.
 Highlighting accessibility and documentation as key future priorities.
 Promoting open discussion on governance and contribution barriers.

7. Participant list

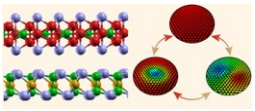
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Magnetic interactions and topological spin textures in 2D van der Waals magnets and heterostructures

Location: CECAM-FR-GSO, France



Webpage : Event webpage

Dates: Jun 25, 2025 - Jun 27, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

One of the key topics discussed during the workshop was the systematic development of spin models for 2D van der Waals magnets going beyond the standard spin model including pair-wise exchange, Dzyaloshinskii-Moriya interaction, and magnetocrystalline anisotropy. The first talk of the workshop by Stefan Blügel (Forschungszentrum Jülich, Germany) addressed this topic. Another major topic addressed by many speakers concerned the first-principles calculation of magnetic interaction constants for atomistic spin models. In particular, different methods to obtain exchange constants were discussed. Here, it was suggested that a comparison of different approaches and density functional theory (DFT) codes would be desirable in the future. Magnetic interactions and spin models were also the topic of the “Open discussions” on the first day. Another important topic at the workshop concerned the stabilization and lifetime of different types of topological spin textures in van der Waals magnets and their verification by transport measurements or microscopy experiments.

2. What were the primary outcomes of this workshop, including limitations and open questions?

Topological spin textures in 2D van der Waals magnets and heterostructures constitute an exciting and rapidly advancing research field with many opportunities. However, there is an urgent need to systematically compare different DFT-based spin models and their parameterization, e.g. the exchange constants, with respect to each other and to work more closely together with experimentalists in order to test the theoretical methods by direct comparisons. It also became apparent that in many van der Waals magnets one must go beyond the standard spin model and that in certain cases it can be crucial to use extensions of DFT such as DMFT to explain experimental observations. The participants of the workshop used the opportunity for intense discussions during the sessions and in the breaks and to start new collaborations between different theory groups and between theoreticians and experimentalists.

3. What was the take-home message for the participants?

- “Topological magnetism in 2D materials” is an emerging area in condensed matter physics, materials science, and nanoscience.
- Going beyond the standard spin model is essential in many 2D magnets.
- Benchmark studies for the calculation of spin interactions are needed.
- We should collaborate more closely with experimentalists.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

During the workshop fundamental aspects of complex topological spin textures in 2D van der Waals magnets and heterostructures were discussed. Since the field is still relatively young and rapidly developing, many challenges still lie ahead in particular in terms of technological applications. The workshop has helped to identify the challenges as well as the opportunities and to bring researchers from different fields of cutting-edge theory and advanced experimental techniques together. There are great prospects for future technology since energy efficient spintronic devices could be realized based on 2D van der Waals magnets.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

Since there were many intense discussions among the participants of the workshop, we anticipate that a number of collaborations will arise from this event which may lead to joint publications and project proposals. The opportunity to get to know each other personally was very often mentioned by participants as an important result of the workshop. The mixture of researchers from theory and experiment at the workshop was another important aspect since a closer collaboration between these areas was identified as central to develop the field of topological spin textures in 2D van der Waals magnets in the future.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

We had a total of more than 50 participants. As expected, the majority were from Europe. However, unexpectedly, we also had around 10 participants from Asia, including China and Japan. In addition, there were 3 participants from Africa and 2 from the US. We also provided financial support to two researchers (one female and one male) from Africa to attend our workshop. In addition, we invited three early-career researchers (at the assistant professor level) to give invited talks.

7. Participant list

Organisers
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Chen, Zefeng - Fudan University, China
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Reusable libraries for quantum chemistry (ReLibQC) – WATOC satellite meeting 2025

Location: CECAM-FI, Finland

Webpage : Event webpage

Dates: Jun 29, 2025 - Jul 3, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The main topic of the meeting was software development for quantum chemistry: specifically, how to make quantum chemistry software more sustainable by using best practices, motivated by the recent call to arms in doi:10.1063/5.0175165. The goal was to advance the field by increasing awareness of the reusable libraries that are already available, as well as to advance cooperation to achieve common goals through the development of new reusable libraries. Important aspects discussed herein were problems where libraries are not yet available, as well as discussions on the major hurdles of creating new libraries. The major contribution of the meeting was thus to draw attention to the importance of reusable libraries, and to start a conversation on the topic and allow the formation of new communities.

A poll was performed to address this and other questions for the scientific report. Out of the 72 attendees, 16 replied; many were key software developers. Analysis of the replies indicated the major topics discussed at the meeting to also have included interfaces and interoperability between program packages, general-purpose graphics processing unit computing, numerical quadrature, and the standardization of wave function formats and tensor contractions. Software development best practices (e.g., CI testing/documentation, code review, not using deprecated language features) were also discussed at the meeting. The issues with managing dependencies were identified to be hugely important in practice; some strategies to avoid them were also discussed at the meeting (e.g. packaging simple libraries in a single compilation unit that can be bundled in other codes or pulling the library in a git submodule pinned to a specific version in CMake). Other notable topics discussed at the meeting included libraries for automatically deriving new quantum chemical methods, as well as for orbital optimization.

The meeting started a process of finding conventions and standardization to improve interoperability between different software packages and improving the reproducibility of research through discussions regarding the use of libraries in our programs and use of the open-source framework for development and maintenance. Discussions regarding common standards and field-specific challenges (especially regarding various basis set ordering, phase, and normalization conventions) were also pivotal to the meeting.

Some attendees drew attention to the issue of the lack of common standards for data formats, which challenges the development of developing and interfacing to new libraries. It was found useful that several lead developers of various quantum chemistry packages were present during the presentations on libraries that face these challenges. The conference thus succeeded not only in raising awareness but also led to cooperation on improving the interoperability of some packages.

2. What were the primary outcomes of this workshop, including limitations and open questions?

We furthered networking within the quantum chemistry community on reusable libraries, convincing the participants that they are not alone with their struggles: problems in software development are common. The most important thing in new collaborations is often the handshake: meeting people in person. The conference was extremely successful: we got quantum chemistry software developers together with the developers and maintainers of various other codes. People were also assured that others also care about software development: it is important to write maintainable code, instead of being satisfied by code that just works somehow.
We also seeded the ground for the development of new libraries to improve the situation. Despite the lack of tangible outcomes in initiatives like this in previous years, there now seems to be a will and the ability to increase the amount of sharing of data and code. The answers to the poll indicate that participants learned about new ways to approach / solve their problems by reusing existing solutions. The answers indicate a strengthened desire to share code and to interface to libraries: people at the meeting seemed willing to make efforts to adopt libraries proposed by others.
We spread the message about existing libraries. The interoperability challenge of reusing and exchanging wave function data was considered as solved during this conference: we have good open-source tools for exchanging wave function data among quantum chemistry packages: the TREXIO library, https://trex-coe.github.io/trexio/. It gained interfaces to DIRAC and PyMolpro at the meeting and will likely be adopted by many more codes thanks to the increased visibility through the meeting. Some tools to generate formulae and generate code automatically were also discussed.
Although some initial answers were formulated, open questions were identified regarding the concrete details of the conventions / standardization. It will take more than a single meeting to change the status quo that has lasted several decades. Practical issues include discoverability (one needs to know about libraries to use them), issues with package and dependency management, and the (lack of) proper documentation. There is a proliferation of reinvented libraries on some topics (e.g., integral evaluation), and the question is how to settle into a single (or at least fewer) standard solution.
Some practical limitations were identified in the poll replies. As is well known, many scientific developers lack software engineering experience, and there is also a lack of recognition for developing libraries, which results in difficulties in finding funding. Time management is a further issue: software is generally developed for a limited scope of the original author's usecase, while academic culture only rarely appreciates the development effort needed to make a library more generally useful by modifications to the original project.

3. What was the take-home message for the participants?

Don't reinvent the wheel; avoid code duplication by collaboration. Before starting a project, check if a library already exists. Starting from scratch can lead to reproducibility issues and suboptimal performance. New functionalities should be reusable, as others likely have similar needs and your project could gain wider adoption. Break up your project

into reusable modules and consider adopting functionalities from existing or upcoming libraries. Use open standards for data transfer.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

The workshop helped to accelerate the development of reusable libraries, which in turn helps to accelerate the usability of quantum chemistry methods that are commonly used for applications in many areas of societal interest. The conference helped inspire quantum chemists to collaborate more on the issues of generating code to avoid both code and effort duplication in problems that have already been solved. If more collaborations in software development are created to reduce code duplication, the consolidation around existing solutions will lead to more efficient / cost-effective development. We expect that the community will keep up the momentum in the near future. The availability of new tools should result in an increase in developer productivity, thanks to not reinventing the wheel. Hence, money spent on software development will either be reduced or funneled towards more useful outcomes.
Already at the meeting people seemed to agree on using TREXIO as a standard, and it will be a big benefit for data exchange between codes that has been so far from a big problem that has prevented interoperability between programs. There are therefore immediate benefits for the community of computational chemists involved in software development. These changes will also benefit others later on. Improving open-source solutions has the potential to improve a wide variety of quantum chemistry programs and their downstream applications, as opposed to siloed improvements to individual quantum chemistry codes. Hence, the field of quantum chemistry will be able to use (public) funding in a more efficient way to do actual research.
Quantum chemistry software has a huge role to play in the discovery of drugs and materials, and the improvement (including environmental) in the manufacture of bulk and fine chemicals. Quantum chemical simulations are used to steer and explain experimental chemistry in a variety of fields including pharmaceuticals, catalysis, battery design, and critical material recovery. With access to more reusable libraries, we expect quantum chemistry to become more powerful and to accelerate the rate of progress.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The participants are now aware of libraries that help them to develop software. The conference also helped cement the need to renew codebases, to further standardize interfaces, and to make the build processes easier. Poll replies also indicated the formation of many new collaborations, especially for TREXIO that was one of the flagstone projects of the meeting: there are reports of new connections to several projects, including Psi4, Molpro, MOKIT, Dirac, and OpenMolcas.
There will be an invited perspective paper in the Journal of Chemical Theory and Computation for in-depth discussion of the topics at the meeting. While people are usually very active during conferences and have a lot of ideas on what they could collaborate on, when people go back to their usual tasks they often no longer have time. We hope that the paper will motivate the participants to spend time on reusability. We also intend to start a website and a GitHub repository to coordinate future efforts.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

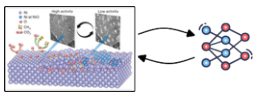
We promoted inclusivity by preferring an open-door policy: we only invited the 6 keynote speakers (2 of which were women), and the rest of the conference program was open for abstract submissions; almost everyone got their request. The conference location was accessible, allowing for potential disabilities.
Although we had room for 100 participants (or even a bit more), at the end the meeting had 72 participants of various genders, geographical origin and career stage. Piggybacking on the WATOC meeting made it easier for people coming from other continents to attend; still, many participants did not attend WATOC and only came for our meeting.
Inclusivity in terms of career stage was furthermore promoted by having lengthy discussion sessions for all talks. The presentation time was limited to 2/3 of talk, and 1/3 of discussion. The increased audience contributions were found to be appreciated and was considered the most beneficial part of this type of an event.

7. Organiser list

Lehtola, Susi
University of Helsinki, Finland
Sundholm, Dage
University of Helsinki, Finland, Finland

From operando electron microscopy images to atomistic models: Machine Learning assisted analysis in the age of big data

Location: Zuse Institute Berlin, Germany



Webpage : Event webpage

Dates: Jul 2, 2025 - Jul 4, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The focus was at the intersection of electron microscopy, machine learning, and atomistic modeling. Presentations were grouped into key thematic areas reflecting the workshop's focus.

1. Machine Learning for Automated EM Data Analysis: This theme explored advanced ML techniques to automate and accelerate interpretation of large-scale EM datasets.

Scalable machine learning methods were presented for examining large electron microscopy datasets, enabling detailed characterization of various nanoparticle groups. Self-supervised vision transformers were introduced for label-free feature detection and real-time microscopy control. Investigations into the performance of neural networks under varying conditions provided insights for the effective application of ML in atomic-level HRTEM analysis. Methods for generating synthetic data for temporal segmentation models demonstrated that temporally coherent data significantly enhances the accuracy of material change tracking.

2. Real-Time and High-Throughput Data Processing:

This category focused on tools and workflows for live analysis and feedback. LiberTEM-live, an open-source framework, was introduced to enable distributed processing of large EM datasets and real-time feedback between data processing and instrument control. Automated SEM data collection workflows were demonstrated for long-term operando experiments, facilitating continuous monitoring. Dual magnification automation in ESEM was presented as a novel means to improve data collection efficiency.

3. Linking EM to Atomistic Models and Simulations: Speakers demonstrated how to bridge experimental data with simulations to gain atomistic insights: Cecilia Clementi created a flexible model using deep learning on detailed simulations, which allows for quick modeling of protein movements in new sequences. Aditya A. Sesh combined quantum computing and physics-informed neural networks to accelerate multiphysics CFD simulations for silicon crystal growth.

4. Applications in Catalysis, Energy Materials, and Quantum Devices: This category addressed domain-specific advancements enabled by ML-assisted electron microscopy analysis. A combined STEM and ML approach was developed for automated analysis of semiconductor heterostructures. In situ electron microscopy techniques were employed to observe electrochemical processes in energy materials, enabling real-time studies of battery systems. An integrated workflow combining experiments, analysis, and simulations was established to track the behavior of individual catalyst particles, informing catalyst design. A 1000-hour operando microscopy study on CO_2 hydrogenation yielded a pattern library for ML-based analysis of catalytic processes. Machine learning was also

applied to identify active sites and reaction pathways in Pd and Pt catalysts on ceria, contributing to the understanding of complex catalytic systems.

2. What were the primary outcomes of this workshop, including limitations and open questions?

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1. Establishment of Machine Learning Pipelines for EM Analysis: The workshop showed how ML techniques like convolutional neural networks, U-Nets, and vision transformers can be used to automatically find features, separate parts, and rebuild images in large EM datasets. These advances demonstrated the feasibility of minimizing human intervention and accelerating analysis workflows across disciplines.
2. Integration of Experiment and Simulation: Several presentations showed systems that link real-time EM data to atom-level modeling, making it possible to create predictions for changing processes in catalysis, energy materials, and protein systems. This integration offers the potential to discover mechanistic insights that are otherwise experimentally inaccessible.
3. Real-Time Data Processing and Closed-Loop Control: Tools such as LiberTEM-live exemplified the potential for real-time analysis of streaming EM data and supported adaptive experiments. This capability lays the groundwork for autonomous, self-optimizing experimental setups that respond dynamically to evolving sample conditions.
4. Community Building and Knowledge Sharing: The event successfully brought together experimentalists, computational scientists, and ML researchers, fostering new collaborations and a shared vocabulary across traditionally siloed disciplines.

3. What was the take-home message for the participants?

The workshop's take-home message emphasized the transformative potential of integrating machine learning with operando electron microscopy and atomistic modeling. Participants recognized that automated, data-driven workflows can unlock unprecedented insights into dynamic material behaviors. However, achieving robust, interpretable, and generalizable solutions requires overcoming current limitations in data quality, model transferability, and interdisciplinary collaboration.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

The outcomes of the workshop hold significant potential for societal benefits across multiple domains. By using machine learning to better analyze electron microscopy data and linking it to atom-level modeling, the participants showed ways to quickly generate new ideas in energy, health, and environmental technologies.

In energy materials, automated analysis of dynamic processes at the nanoscale can drive the development of more efficient batteries, fuel cells, and catalytic systems. Real-time insights into material degradation and transformation enable the design of longer-lasting and safer energy storage devices, supporting the global transition to renewable energy and sustainable transportation.

In health and biotechnology, methods like cryo-electron tomography used with deep learning give very detailed views of complex biological systems in their natural settings. This has direct applications in drug discovery, structural biology, and the design of novel therapeutics, potentially improving treatment outcomes and reducing development timelines.

In environmental monitoring and sustainability, ML-enhanced EM can be used to understand and control catalytic processes for pollutant degradation, carbon capture, and green chemical synthesis. Automating long-term operando studies allows researchers to explore environmentally friendly catalysts and processes with unprecedented efficiency.

By fostering interdisciplinary collaboration, the event created a foundation for tackling complex global issues where materials science, data science, and experimental innovation intersect.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The workshop created a fertile ground for future developments. Several participants expressed interest in pursuing collaborative projects that integrate machine learning with operando electron microscopy workflows. There is also potential for joint software development efforts and coordinated grant applications to advance these ideas. Additionally, some of the presented work may lead to publications as during the discussions interesting perspectives at the intersection between data acquisition and machine learning predictions emerged.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The workshop organizers took several measures to promote inclusivity. Efforts were made to ensure gender diversity among invited speakers and participants, resulting in balanced representation across sessions. The program included speakers and attendees from diverse geographical regions, including Europe and North America, fostering a global perspective. Early-career researchers were actively encouraged to present their work through talks and posters, supporting career development. The venue provided full accessibility for individuals with disabilities, and hybrid participation options were explored to accommodate those unable to travel. These measures collectively aimed to create an open and welcoming environment for all participants, regardless of background or career stage.

7. Participant list

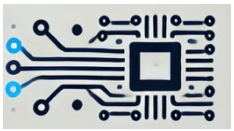
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Open software for neural wavefunctions

Location: CECAM-HQ-EPFL, Switzerland



Webpage : Event webpage

Dates: Jul 2, 2025 - Jul 4, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop connected advances in neural quantum states (NQS) with the software needed to make them reproducible and usable beyond individual research groups. The program covered JAX and distributed computing, fermionic simulations with jVMC, QMCTorch, a JAX-based ab initio QMC package, Pfaffian wavefunctions, finite-range embeddings, transcorrelated methods and optimisation.

Applications ranged from correlated lattice models and molecular electronic structure to nuclear systems and open-system dynamics. These developments address complementary bottlenecks. Finite-range embeddings reduce the cost of electronic neural-wavefunction calculations by restricting costly electron-electron features. Pfaffian-based ansatzes provide a flexible description of fermionic pairing and correlation. New optimisation strategies address the practical difficulty of reaching accurate variational states, rather than increasing expressivity alone.

Transcorrelated approaches offer another route to reducing computational demands by treating short-range correlations explicitly. The implementation discussions placed these methods in the context of automatic differentiation, just-in-time compilation and accelerator parallelism. These tools can simplify derivatives and enable larger calculations, but require algorithms and data layouts suited to the hardware.

A further theme was the sharing of neural-network architectures, trained parameters and reusable software components, together with the maintenance of open research codes. The contribution of this combination was to bring methodological progress and implementation experience into the same forum: techniques for improving accuracy could be considered alongside their sampling cost, optimisation stability, reproducibility and computational requirements.

2. What were the primary outcomes of this workshop, including limitations and open questions?

The main immediate outcome was an exchange of practical expertise between neural-wavefunction developers and the wider quantum Monte Carlo community. Presentations were complemented by dedicated project-kickstart/hackathon sessions, discussion and a concluding roundtable, providing opportunities to examine implementation issues with developers and explore contributions across existing projects.

A tangible subsequent development within the participating community is jQMC. Its software paper explicitly acknowledges discussions with workshop organisers Giuseppe Carleo and Filippo Vicentini about JAX implementation and its application to ab initio QMC. This illustrates the value of exchanges between communities that share computational

techniques but often develop separate software. The next step is to turn such exchanges into reusable implementations and reproducible workflows.
Sharing trained models requires more than distributing parameter arrays: the architecture, physical conventions, Hamiltonian, numerical settings and software versions must also be recoverable. Interoperability should preserve the physical meaning of a calculation, not merely provide compatible file formats. Important limitations remain. A flexible ansatz does not by itself ensure reliable stochastic optimisation; comparisons should account for both statistical uncertainty and variational accuracy. Accelerator speedups depend on memory use, vectorisation and workload, and do not remove unfavourable system-size scaling. Success on one benchmark does not establish transferability to other Hamiltonians or particle numbers.
Open questions include which components can be shared across lattice and continuum problems, how to compare optimisers fairly under sampling noise, how best to distribute reusable trained states, and how to sustain maintenance and testing. Addressing these questions requires continued development and validation beyond the workshop.

3. What was the take-home message for the participants?

Accuracy, sampling, optimisation and implementation must be developed together. Shared, tested software and reproducible benchmarks are essential for turning neural-wavefunction advances into tools that other groups can verify and extend. JAX and modern accelerators provide a common technical foundation, but collaboration and long-term maintenance determine its scientific value.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

Yes. The potential benefits are primarily enabling and long-term. More accurate and affordable simulations of correlated electrons could improve our understanding of molecular bonding and functional materials, including systems for which simpler electronic-structure approximations are unreliable. Advances in neural wavefunctions and quantum Monte Carlo could thereby support future research in chemistry and materials science.
Open implementations also offer a public-research benefit: methods can be inspected, independently checked and reused, rather than remaining tied to a single group. Documented code and examples can make advanced computational methods more accessible for education and for researchers without the resources to build a complete software stack.
Better use of accelerators and reduced duplication of software development can lower the effort needed for a given scientific task. Access to high-performance hardware nevertheless remains a practical barrier. The workshop's contribution is foundational: stronger research capabilities, reproducibility and transferable computational skills, with prospective downstream benefits rather than an immediate technological application.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

A concrete software development associated with the workshop is jQMC, by Kousuke Nakano and Michele Casula. Presented by Nakano at the meeting and subsequently described in arXiv:2607.13781 (2026), this open JAX-based ab initio QMC package provides GPU-capable variational and lattice-regularised diffusion Monte Carlo, automatic differentiation, public code and documentation.
A related later output from the participating community is lrux, by Ao Chen and Christopher Roth (arXiv:2602.05255, 2026), a reusable JAX library for differentiable low-rank updates of determinants and Pfaffians. It is closely related to the computational needs of the Pfaffian NQS presented by Roth at the workshop. Both outputs are aligned with the workshop's emphasis on reusable components and shared computational infrastructure.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

We advertised an open call explicitly welcoming students, new researchers and newcomers to open-source development alongside experienced contributors. Talks, posters, discussions and hands-on project sessions offered different ways to contribute and interact across levels of experience.
Participation was international, with institutions in Europe, Asia and North America. Remote attendance was available and is recorded for participants based in India, Singapore, Turkey, Italy and the UK, providing a route to participation without travel. The EPFL community could also attend individual lectures without registering for the full event. These measures broadened access through career-stage inclusion, geographic reach and flexible participation formats.

7. Participant list

Organisers
Carleo, Giuseppe
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Machine Learning Advances for Molecular and Materials Property Prediction

Location: CECAM-US-CENTRAL, United States



Webpage : Event webpage

Dates: Jul 7, 2025 - Jul 9, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop brought together an interdisciplinary group of researchers working at the intersection of machine learning (ML), computational chemistry, molecular sciences, and materials modeling. Discussions during the event were framed around several core themes that reflect both current challenges and emerging opportunities in the field.

1) ML-based Interatomic Potentials and Enhanced Sampling

One of the central topics of the workshop was the integration of ML-based interatomic potentials (such as neural network potentials) into molecular simulations. Presentations and discussions highlighted practical challenges, including transferability, data efficiency, and stability of ML potentials. New developments in active learning strategies and hybrid approaches that combine physics-based and data-driven components, e.g., the incorporation of long-range interactions, were discussed as promising solutions.

2) Featurization and Exploration of Chemical/Materials Spaces

The development of effective molecular and materials representations remains a central concern for predictive modeling. The workshop featured presentations on emerging representations, such as resonance invariant graph representations, along with approaches to integrate domain knowledge into featurization pipelines. Discussions emphasized the importance of physically motivated descriptors, especially for extrapolation tasks and property prediction in diverse chemical spaces, and the merit of hybrid approaches was also debated (e.g., the use of hidden representations of graph neural networks pre-trained on descriptor datasets).

3) ML in Data-Sparse Regimes

A recurring theme was the challenge of making accurate predictions in data-scarce regions of chemical and materials space. Participants discussed various strategies, including transfer learning, few-shot learning, and the incorporation of physical priors to mitigate data scarcity. Emphasis was placed, among others, on uncertainty quantification as a critical component of ML model development in this context. These discussions reflected a growing shift toward robust and reliable ML in real-world scientific settings.

2. What were the primary outcomes of this workshop, including limitations and open questions?

The main outcome of the workshop was the introduction of a disparate group of researchers from different disciplines working on various aspects of machine learning to

each other. Many of the presenters knew of other presenters by name and reputation but had not met in person. This was especially true for the graduate students and postdocs. The workshop helped foster connections that will lead to fruitful collaborations down the road. Technical outcomes included: a robust discussion of ways of developing and applying MLIPs, where a major focus was on accuracy, especially for long range forces; descriptions and implementations of effective molecular and materials representations (featurization) for predictions, with an emphasis on interpretability and hybrid approaches; and discussions on the use of ML in data-sparse regimes, focusing on how to make accurate predictions and quantify uncertainty in those regions of the chemical/materials space.
In addition, early career researchers (graduate students and postdoctoral researchers) presented their work during the poster sessions, interacting with leaders in the field and receiving feedback from them.

3. What was the take-home message for the participants?

The biggest take-home message was that the field of machine learning for molecular and materials properly prediction is moving extremely fast. Significant advancements are occurring on an almost weekly basis, and it is difficult to predict exactly where the field is headed. This area is a particular bright spot for students and junior faculty, given the rapidly evolving state of the field and that powerful new predictive methods are leapfrogging established computational approaches.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

The primary focus of the workshop was on advancing fundamental science at the interface of machine learning (ML), chemistry, and materials science. By developing and refining ML models for molecular and materials property prediction, participants addressed key challenges in understanding complex chemical systems and simulation techniques. These fundamental advances improve how we model, interpret, and predict molecular behavior with higher accuracy and efficiency.
While the immediate outcomes are foundational, their long-term societal impact is significant. Enhanced ML-driven simulations and interatomic potentials can accelerate the discovery of new materials and catalysts, supporting sustainable energy solutions, cleaner chemical processes, and advanced materials for technology and health. Improved ML tools for spectroscopy and molecular characterization have the potential to speed drug discovery and enable personalized medicine.
The workshop also highlighted efforts in data curation and FAIR principles, promoting open, reproducible science that benefits academia, industry, and policymakers. Addressing data-scarce regimes expands accessibility of advanced modeling to a broader scientific community. Additionally, advances in interpretability and integration of large language models can enhance knowledge extraction and scientific communication. Overall, by pushing the boundaries of fundamental ML methodologies in molecular sciences, this workshop paves the way for innovations that can ultimately lead to cleaner technologies, improved healthcare, and more sustainable industrial practices, generating lasting societal benefits.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The workshop facilitated extensive and fruitful discussions not only during formal sessions but also throughout social events such as lunches and the conference dinner. These informal interactions proved invaluable for exchanging ideas, identifying common interests, and fostering connections across disciplines and career stages.
While it is still early to identify concrete outcomes, we anticipate that several new collaborations will emerge from these interactions. Participants expressed strong interest in pursuing joint research projects, co-authoring publications, and exploring funding opportunities together. The workshop thus laid a solid foundation for future collaborative efforts in advancing machine learning applications in molecular and materials sciences.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

Inclusivity was a key priority in organizing the workshop. We ensured a diverse speaker lineup, with gender balance as an explicit goal. Several leading women scientists were invited, and early-career researchers were actively included through contributed talks. A dedicated poster session for attending postdocs and PhD students, to enable them to showcase their work as well. Geographical diversity was also emphasized, with participants from both Europe and North America. These measures promoted broad, equitable participation across gender, career stage, and geography.

7. Participant list

Organisers
Cersonsky, Rose
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Frontiers in Simulation of Photoresponsive Biological Systems

Location: University of Siena, Italy



Webpage : Event webpage

Dates: Jul 7, 2025 - Jul 10, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The main focus of the workshop was on biological systems that interact with light. This encompassed both natural systems - such as photoactive proteins, chromophores, and nucleobases - and artificial systems designed to mimic or enhance these interactions. Participants included both method developers and users from across the fields of computational photochemistry and photobiology.
Method developers presented recently implemented techniques in various computational packages, with a particular focus on the treatment of environmental polarization effects. Invited and contributed talks focused on applications provided an overview of specific systems of current and future interest, highlighting key topics and open questions. In addition to the theoretical and computational contributions, experimentalists also attended the workshop and presented their latest findings. Furthermore, the workshop was joined by two representatives from Algorithmiq, offering a company perspective on the topic.
This kind of interdisciplinary interaction can significantly advance the state of the art. The workshop served as a platform for researchers in computational photochemistry and photobiology to stay informed about cutting-edge developments and to engage directly with method developers. In turn, developers benefited from exposure to new systems and real-world challenges encountered by users, which can drive future methodological improvements.
These exchanges are essential for the development of robust and advanced computational protocols, fostered through community feedback and collaboration. Moreover, the direct exchange with experimentalists allowed theoreticians to stay up to date with the latest experimental trends and to provide timely, constructive feedback. Such integration of theory, computation, and experiment is crucial for achieving more accurate simulations of light-matter interactions in complex biological environments.

2. What were the primary outcomes of this workshop, including limitations and open questions?

The major outcome of the workshop was the direct interaction between computational scientists studying photoresponsive systems and method developers creating tools for the same purpose. This close exchange allowed participants to align methodological developments with current research needs, fostering collaboration and mutual understanding. Another significant strength of the workshop was the productive dialogue between theoretical and computational researchers and experimentalists, which enriched the discussion by bridging different perspectives and approaches. The success of this

interdisciplinary interaction was evident throughout the workshop: participants showed a consistently high level of interest, actively engaging in talks and discussions. Sessions were marked by lively and insightful exchanges, demonstrating the strong expertise and enthusiasm of the community. During Q&A sessions and open discussions, numerous valuable insights and questions emerged from the audience. Overall, the workshop facilitated a dynamic exchange of ideas that is expected to inspire new collaborations and research directions in the field.

3. What was the take-home message for the participants?

Key take-home messages include:

- new polarizable embedding methods are now available in several software packages;
- experimentalists presented novel photosensitive systems, highlighting the need for complementary computational studies;
- beyond established targets like photoactive proteins, new systems - such as molecular solids of small biomolecules - are emerging as promising candidates.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

Several of the topics discussed during the workshop have the potential to make a significant impact on society. One example is the development of optogenetic tools, which allow precise control of cellular processes using light. These tools are increasingly being used to better understand the molecular basis of various diseases and may ultimately contribute to the development of novel therapeutic approaches.
Another important area is the study of how light interacts with genetic material, such as DNA and RNA. A deeper understanding of the mechanisms underlying light-induced damage to nucleic acids can inform strategies for cancer prevention, particularly in the context of UV exposure and phototherapy.
In addition, artificial photosynthesis is a promising field with long-term implications. By mimicking the natural process of converting sunlight into chemical energy, artificial photosynthesis aims to produce clean fuels and valuable chemicals in a sustainable way. Advances in this area could play a crucial role in addressing energy challenges and reducing our dependence on fossil fuels, thereby contributing to climate change mitigation and the transition to a greener economy.
Collectively, these topics highlight the broader relevance of fundamental research on light-matter interactions in biological and chemical systems, demonstrating its potential to drive innovation in medicine, energy, and environmental sustainability.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

One tangible outcome of the workshop is the initiative to publish a Perspective article focused on the workshop topics, highlighting recent progress in method development and computational protocols. One of the organizers, Rosa Di Felice, has already received an

invitation from the editors of The Journal of Physical Chemistry Letters to contribute such an article. All workshop participants were invited to take part in this collaborative effort, and the final session of the workshop was dedicated to planning the content and structure of the manuscript. The article is expected to be published in early 2026.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

To promote gender equality and inclusive policies, we invited speakers with attention to gender balance and representation across different career stages. Furthermore, we have encouraged and adopted bottom-up suggestions from young researchers on how to make further progress in the field, and how to best organize the JPCL Perspective article. Young scientists who contributed a poster to the workshop were given the opportunity to briefly present their work in a dedicated session prior to the poster presentations, thereby increasing the visibility of their contributions. The social dinner was offered to all participants and there was an excellent balance between junior and senior generations at all tables. Overall, there was a very balanced social and scientific vibe, with everybody talking to everybody during coffee breaks, lunches and other self-organized moments.

7. Participant list

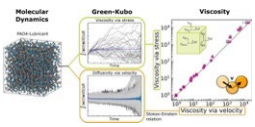
Organisers
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Zhong, Dongping - Shanghai Jiao Tong University, China

Summer School on Sampling High-Dimensional Probability Measures with Applications in (Non)Equilibrium Molecular Dynamics and Statistics

Location: University of Birmingham, United Kingdom



Webpage : Event webpage

Dates: Jul 7, 2025 - Jul 11, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The topic of the summer school was the computation of transport coefficients using methods from molecular dynamics. Our aim was to present the state of the art for the various classes of methods which are currently the most common, namely

- nonequilibrium molecular dynamics methods (NEMD)
- Green-Kubo and Einstein formulas
- This was also the opportunity to present alternative approaches, which are currently not so well known, such as
- alternative fluctuation formulas
- dual methods to NEMD (based on fixing the response and measuring the average forcing)
- transient methods, for instance based on relaxing an initial perturbation.

In fact, the school started by a first day where the basics of molecular dynamics and sampling methods were presented; then lectures focusing on error estimates for equilibrium quantities; next lectures on error estimates for transport coefficients; and finally, a presentation of Molly.jl, a software to perform molecular dynamics in Julia.

2. What were the primary outcomes of this workshop, including limitations and open questions?

This workshop was in fact a research school. The material which was presented was therefore stabilized in terms of scientific content. However, the review which was provided to the participants (and which should be published as a preprint in the coming months) clearly indicated the need for further work to efficiently estimate transport coefficients. A major current limitation lies in the reduction of the variance of the various estimators under consideration.

The discussions and exchanges among the participants and with the speakers also indicated that it is useful to disseminate good practices, and overcome biases and habits which can depend on the subdomain researchers are active in.

Moreover, the Julia notebooks used in the hands-on sessions will be uploaded to the OSSCAR (Open Software Services for Classrooms and Research) platform

https://www.osscar.org/courses/index.html with the title "Computation of Transport Coefficients"; and the recordings of the lectures will be published on the Lhumos portal.

3. What was the take-home message for the participants?

The main message was that statistical and systematic errors can and need to be quantified, the statistical error being usually the dominant one due to the scaling of the asymptotic variance, whatever the numerical method used to compute transport coefficients (e.g., linear response of nonequilibrium molecular dynamics, Green-Kubo approaches, transient methods).

4. Does the outcome(s) of the workshop hold potential for societal benefits?

The main social benefit of the event is to train a new generation of young and enthusiastic researchers in molecular dynamics. Most of them had background in physics/chemistry/biology, so a key point of the training was to provide them with an appropriate mathematical background, allowing them in particular to better assess and quantify numerical errors in simulation results in general, and for time averages and integrated correlation functions in particular.
A side benefit was to advertise the field of nonequilibrium dynamics in general, and computation of transport coefficients in particular, not only to the attendees but also to some of the speakers. We indeed strongly believe that much remains to be done in this field.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The preparation of the school catalyzed the writing of Julia notebooks which can serve as introductory materials for courses and training on nonequilibrium dynamics: an introductory one on toy two dimensional systems, one on the computation of thermal conductivity for atom chains (a not so known example, which is in our opinion an excellent case to test the scalability of methods), and a more realistic one on the computation of shear viscosity in Lennard-Jones fluids using Molly.jl.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The School of Mathematics at the University of Birmingham imposes a 30% proportion of female speakers, which further motivated us to include various female presenters in the program, both for actual lectures and also for hands-on sessions. We also mixed more junior and more experienced speakers, in particular relying on PhD students and postdocs to take care of the hands-on sessions and present their research when hosting the session, in order to give them a maximal visibility.

Concerning the audience, as this was a summer school, it was composed only of younger researchers.
For geographical provenance and gender, we accepted all applications from students with relevant background. No specific effort was made for gender balance, and we fortunately had various female attendees.

7. Participant list

Organisers
Shang, Xiaocheng
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Zhao, Peiyuan - University of Birmingham, United Kingdom

Biomolecular Dynamics in the Age of Machine Learning



Location: University of Wisconsin-Madison, United States

Webpage : Event webpage

Dates: Jul 14, 2025 - Jul 16, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

Our CECAM workshop brought together leading experts to explore the rapidly evolving intersection of machine learning (ML) and biomolecular dynamics. The major topics reflected the state of the art in both theoretical development and practical application:

- **Markov State Models (MSMs)** to decode complex conformational dynamics underlying protein folding, allostery, and molecular recognition.
- **Non-Markovian dynamic models** based on the Generalized Master Equation and Generalized Langevin Equation, addressing limitations of traditional Markovian assumptions. Novel ML algorithms to infer such behaviors were presented.
- **Generative AI methods** that learn latent representations of molecular conformational landscapes, enabling efficient sampling of rare events. This includes techniques leveraging GNNs, flow-based models, and latent thermodynamic flows.
- **Adaptive sampling strategies** enhanced by ML to accelerate exploration of biomolecular phase space by guiding simulations toward under-sampled regions. These advances impact studies of complex systems such as protein-protein interactions and cryptic binding pockets.
- The **integration of computational models with experimental data (e.g., NMR data)** to refine understanding of biomolecular dynamics.
- The crucial **balance between physics-based principles and data-driven ML models**, ensuring ML complements rather than replaces mechanistic insight. This was exemplified in talks combining enhanced sampling, Bayesian reweighting, and mechanistic modeling.

Together, these topics represent a vibrant, multidisciplinary effort to push the boundaries of ML, computational chemistry, and biophysics. By addressing key methodological challenges and fostering cross-disciplinary dialogue, the workshop significantly advanced the state of the art in modeling biomolecular dynamics with ML.

2. What were the primary outcomes of this workshop, including limitations and open questions?

Major outcomes:

- **Integration of ML with established physical models** (e.g., MSMs & GME). This synergy improves the accuracy and interpretability of kinetic models describing biomolecular dynamics.

- **Emerging ML-Driven Sampling Techniques:** Participants showcased innovative AI generative models and adaptive sampling strategies that enable efficient exploration of high-dimensional conformational landscapes and rare events. These methods have the potential to significantly reduce computational costs and enhance the sampling of biologically relevant states, especially in large and complex systems.
- **Community Building:** By bringing together experts from diverse fields (chemistry, physics, applied mathematics, computer science, and structural biology), the workshop fostered collaborations that will drive future innovations. The community agrees to work together to curate MD simulations datasets to train ML models.

Open Questions :

- **Interpretability and Mechanistic Insight:** Ensuring that ML-models for protein dynamics are interpretable and physically meaningful continues to be an open area of research.
- **Training data Quality:** There is still lack of high-quality MD simulation data to train ML models for biomolecular dynamics.
- **Generalizability and Transferability:** Open questions persist regarding how best to transfer learned representations and adapt models to new proteins, complexes, or environmental contexts.

3. What was the take-home message for the participants?

ML is transforming the study of biomolecular dynamics, not by replacing physical models, but by enhancing them. Integrating data-driven methods with experimental and mechanistic insights offers a powerful path forward to unravel complex biological processes. Continued collaboration across disciplines is essential to tackle challenges in ML for biomolecular dynamics.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

Yes, the outcomes of the workshop hold potential for societal benefits, particularly in the fields of health, biotechnology, and drug discovery. Understanding biomolecular dynamics is central to deciphering the mechanisms of diseases, identifying therapeutic targets, and designing more effective drugs. ML–enhanced dynamics modeling can accelerate these processes by enabling faster, more accurate predictions of mutation effects, drug binding pockets, etc. Beyond drug design, these tools have broader implications in synthetic biology, and biomaterials science, where understanding and engineering biomolecular function is key. By bringing together experts from computational chemistry, ML, and biophysics, the workshop catalyzed cross-disciplinary collaboration that is essential for translating scientific advances into societal impact.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The workshop resulted in several tangible outcomes. New collaborations were initiated among participants. There were also informal agreements for the workshop participants

to work together to curate a MD simulation data containing representative protein systems for the training of the ML model. We are also exploring the idea of creating a focus collection in the journal "Machine Learning: Science and Technology" around the topic of the CECAM workshop on ML for biomolecular dynamics. Finally, we plan to apply for a CECAM flagship workshop in Berlin on a similar topic in two years.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

We actively prioritized inclusivity in both speaker invitations and participant selection. The workshop achieved strong gender representation, with over one-third of invited speakers identifying as women (8 out of 21). As a US-CENTRAL-Node event, we fostered transatlantic interactions by having 9 invited speakers from European countries, 11 from the USA, and 1 from Asia. Participants reflected broad geographical diversity, including Europe, North America, and Asia. We also ensured representation across career stages, from senior faculty to early-career researchers and postdocs.

7. Participant list

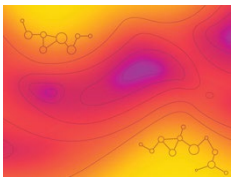
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Shastry, Shashank - UIUC, United States
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Advancing simulation, analysis and prediction of complex chemical systems using modern chemical graph theory and computational topology

Location: CECAM-HQ-EPFL, Switzerland



Webpage Event webpage

Dates: Jul 16, 2025 - Jul 18, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The event highlighted a set of interrelated themes at the frontier of computational chemistry, mathematics, and data science. A central focus was the use of graph-theoretical frameworks to represent chemical systems. Talks demonstrated how chemical graph theory can capture the complexity of hydrogen-bonding networks, energy landscapes, and other structural motifs in a way that preserves both connectivity and physical interpretability. By mapping molecular interactions and potential surfaces into graph structures, researchers showcased how longstanding problems in chemistry can be reframed with mathematical clarity.

Building upon this, topological data analysis (TDA) emerged as a powerful tool for navigating high-dimensional chemical spaces. Persistent homology and related methods were applied to probe rugged potential energy surfaces, reveal configurational heterogeneity, and compare datasets that resist conventional descriptors. These approaches provided new ways to quantify the shape and connectivity of complex landscapes, offering insights into sampling challenges and structural diversity.

A third major theme was the integration of machine learning and ML with graph- and topology-based descriptors. Presentations showed how embedding persistent homology features or spectral graph measures into ML pipelines enables both more efficient sampling and more robust predictive models. These advances not only accelerate computational workflows but also maintain interpretability, allowing physical meaning to remain central while harnessing the power of data-driven methods.

Together, these topics represent significant contributions to the state of the art**.** The event fostered genuine cross-disciplinary dialogue, bridging abstract mathematics and algorithm development with domain-specific challenges in chemistry and physics. Novel descriptors derived from graph theory and topology are expanding the toolkit available for analyzing chemical complexity, while scale-bridging methodologies point toward simulations that are both faster and more faithful across molecular to mesoscale regimes. Most importantly, the discussions underscored that progress arises not only from applying mathematics to chemistry, but from **co-**developing methods where both fields advance in tandem. By coupling physical questions with innovative mathematical frameworks, the event demonstrated new pathways to represent, compare, and predict the behavior of complex chemical systems – pushing beyond the boundaries of conventional simulation.

2. What were the primary outcomes of this workshop, including limitations and open questions?

First, participants gained new methodological insights, particularly into how graph spectral measures and topological data analysis (TDA) can enrich our understanding of chemical systems. Persistent homology, for example, was shown to reveal topology-driven features of configuration spaces and transition pathways, offering perspectives that traditional descriptors often miss.

A second outcome was the advancement of computational tools. Talks and poster sessions, including those devoted to algorithms and software prototypes, highlighted practical implementations of graph- and topology-based approaches. These developments provide an initial foundation for broader adoption, with potential to evolve into robust platforms that enhance both analysis and predictive modeling.

Equally important was the workshop's role in interdisciplinary networking. By convening experts from chemistry, mathematics, materials science, and ML, the event catalyzed collaborations aimed at uniting mathematical rigor with chemical relevance. These new connections lay the groundwork for shared projects and community-building around emerging techniques.

The discussions further revealed some important limitations and open questions in the area. A major challenge is **scalability**: applying graph and TDA methods to very large molecular assemblies or high-dimensional datasets remains computationally demanding. Another issue is the trade-off between interpretability and performance**.** While ML and neural-network-based methods show promise, there is concern that physical insight may be obscured in the pursuit of predictive accuracy. Finally, participants emphasized the need for a unified, community-accessible software infrastructure that can integrate diverse graph-theory-based codes into a coherent ecosystem, ensuring reproducibility and broader impact.

Together, these outcomes underscore both the promise and the hurdles in leveraging mathematics and ML for chemical discovery. The workshop not only identified new directions for research but also clarified the challenges that must be addressed to translate methodological advances into practical, scalable, and interpretable tools for the wider community.

3. What was the take-home message for the participants?

Graph-theoretic and topological methods, especially when coupled with ML and multiscale modeling, offer powerful and interpretable tools for analyzing complex chemical systems. Their full potential will be realized through scalable implementations and sustained collaboration across chemistry, mathematics, and computer science.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

Yes – this workshop's outcomes hold substantial potential for societal benefit. One of the clearest impacts lies in accelerated materials and drug design. By leveraging graph- and topology-based descriptors, researchers can more efficiently screen vast chemical

spaces, identifying promising candidates for catalysts, advanced materials, or therapeutics. Such acceleration directly benefits healthcare, energy, and sustainability by shortening the path from discovery to application.
The methods also advance our understanding of complex systems. Persistent homology and spectral graph descriptors provide new ways to characterize spatial heterogeneity, configurational diversity, and dynamic phase behavior in both materials and biomolecular systems. These insights are essential for tackling pressing challenges, such as designing more efficient energy storage devices, improving environmental remediation strategies, or engineering biomolecules with novel functions.
Equally important is the workshop's contribution to fostering interdisciplinary research and knowledge. By equipping participants with mathematical, ML, and chemical toolsets, the event strengthens a workforce capable of tackling the multifaceted problems at the interface of science and technology. This integrated expertise will be a key driver of future innovation, ensuring that advances in fundamental research translate into practical solutions for society.
In sum, the workshop demonstrated that the cross-pollination of graph theory, topology, and computational chemistry does more than enrich academic understanding – it creates pathways for tangible progress in medicine, energy, and sustainability, while cultivating the human expertise needed to realize those advances.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The workshop helped to establish potential collaborations between researchers from math, computer science and chemistry. A new website is being developed that will house computational codes in this area.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The workshop achieved broad geographical representation, with participants from Europe, North America, and Asia, including institutions. Efforts toward career-stage balance ensured visibility for both senior leaders (e.g., Herbert Edelsbrunner, Lee Cronin) and early-career researchers, who were supported through poster and contributed presentations. The program also emphasized interdisciplinary breadth, drawing participants from applied mathematics, computational chemistry, and materials science to foster exchange across fields. This spectrum of inclusivity led to a very natural equity in gender representation. Accessibility was further supported by methodological and software tutorials, designed to equip participants at varying levels of expertise.

7. Participant list

Organisers
Bougueroua, Sana
University Evry Paris Saclay, France

Clark, Aurora
University of Utah, United States
Gaigeot, Marie-Pierre
Université D'Evry Val D'Essonne - Université Paris-Saclay, France
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Xia, Kelin
Nanyang Technological University, Singapore

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Assalmi, Hassan - Mohammed V University, Morocco
Barthel, Senja - Vrije Universiteit Amsterdam, Netherlands
Batista, Victor - Yale, United States
Bilsky, Joshua - University of Utah, United States
Bleile, Yossi - Institute of Science and Technology Austria, Austria
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Cherupilil Sajeev, Madhav - Institute Polytechnique de Paris, France
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Cronin, Lee - University of Glasgow, United Kingdom
Dogra, Riya - Vrije Universiteit Amsterdam, Netherlands
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Vidal, Laurent - Laboratoire David, Université Versailles Saint-Quentin, France
Wales, David - Cambridge University, United Kingdom
Zens, Coralie - DAVID - Université Versailles Saint-Quentin, France
Zerbato, Elena - University of Geneva, Switzerland

CCP5 Summer School

Location: Newcastle University, United Kingdom



Webpage : Event webpage

Dates: Jul 21, 2025 - Jul 31, 2025

1. What were the major topics presented in the School?

School is an introductory intensive and comprehensive training program for early-career researchers, primarily new PhD students, in the field of molecular simulation. The curriculum is designed to provide a solid foundation in the theoretical underpinnings of simulation techniques, complemented by extensive hands-on practical sessions. Main topics are

- **Statistical Mechanics:** The theoretical framework upon which molecular simulation is built. Students are introduced to key concepts such as ensembles, partition functions, and the relationship between microscopic states and macroscopic thermodynamic properties.
- **Molecular Dynamics (MD):** A powerful simulation technique that models the time evolution of a system of interacting particles. Lectures cover the basic algorithms for integrating the equations of motion, the implementation of thermostats and barostats, and the analysis of trajectories to calculate various properties.
- **Monte Carlo (MC) Methods:** This section explores a range of stochastic simulation techniques based on random sampling. Participants learn about the Metropolis algorithm; different Monte Carlo moves for various ensembles.
- **Force Fields:** A critical component of classical simulations, lectures on force fields delve into their parameterization, validation, and the different types available for various systems.
- **Free energy methods**: usage of rare events methods for modelling.

Advanced topics discussed :

- **First-Principles (Ab Initio) Methods:** An introduction to quantum mechanical simulation techniques, such as Density Functional Theory, which allow for the study of electronic structure and chemical bonding without empirical parameters.
- **Mesoscale Methods:** This module focuses on simulation techniques that bridge the gap between the atomic and macroscopic scales, such as Dissipative Particle Dynamics and the Lattice Boltzmann method, which are essential for studying complex fluids.
- **Biomolecular Simulation:** Tailored for those interested in biological systems.
- **Machine Learning for Interatomic Potentials:** Reflecting the latest trends in the field, this increasingly popular module explores how machine learning techniques can be used to develop highly accurate and efficient interatomic potentials from quantum mechanical data. In addition to these students, get to attend research seminars, present their research during a poster session with prizes and selected few presents during a student research seminar.

2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

In general school is very well received with students appreciating the breadth of the subjects discussed. This is very important since there is a modern tendency for early specialisation. Limitations noticed by lecturers in general relate around variable level of mathematics showed by participants. This can make courses around statistical mechanics or advanced molecular dynamics and Monte Carlo challenging. During hands on sessions there are few problems reported mainly due to the movement to cloud environments which allowed us to remove previsible issues. Some students prefer more in-depth exercises with writing the code; however, this is not a time effective solution for all the cohort who in general are not very well versed in programming.
Advanced courses are positively received since they align much better with current research topics of the students. One issue raised is related to the fact some students expect to learn how to use a code, rather than the methodology underpinning.

3. What was the take-home message for the participants?

Molecular and Materials modelling is a diverse field that can model very diverse systems with various levels of accuracy.

4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

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all material for the school is available online for students to study independently. https://ccp5.gitlab.io/summerschool/
Lectures are circulated separately into electronic format.

5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

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75 students from UK and oversees took part this year with a roughly 50/50 split. Gender split was approx. 45% female and 55% male. , with the first two days being dedicated to computer programming classes, Fortran and Python, which students choosing one of them. No real need other than blind review of applications was needed to achieve this. By choosing students from different fields means we need to accommodate to different levels of hard skills in computing and mathematics.

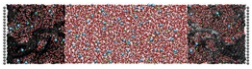
6. Organiser list

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Simulations of electrochemical storage devices: from quantum to classical descriptions

Location: CECAM-FR-MOSER, France



Webpage : Event webpage

Dates: Jul 21, 2025 - Jul 24, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop brought together leading experts working at the interface between quantum and classical modeling of electrochemical energy storage systems, with a particular focus on batteries, supercapacitors, and electrocatalytic interfaces. Major topics included the development and application of advanced electronic structure methods to electrochemical environments, the integration of machine learning with quantum simulations, recent developments in the constant potential approach in classical molecular dynamics, and multiscale modeling approaches bridging atomistic and continuum descriptions.

A key theme was the growing role of AI and data-driven methods in electrochemistry. Talks highlighted recent progress in neural network-based machine learning potentials tailored to solid and liquid electrolytes. Another central topic was the accurate modeling of electrode/electrolyte interfaces, including quantum capacitance, interfacial structure, and charge transfer processes. Presentations demonstrated how first-principles simulations can now resolve phenomena such as field-driven water dissociation, phase transitions at electrified interfaces, and the formation of the solid–electrolyte interphase with unprecedented detail.

The program also covered multiscale frameworks that combine DFT, QM/MM, and classical molecular dynamics, enabling simulations that capture electronic effects while allowing sufficient sampling of the phase space. These approaches are essential to connect microscopic descriptors (e.g., solvation structure, ion correlations) with macroscopic properties such as ionic transport and capacitance. Several contributions showcased how these methods are used to interpret experimental observations and guide materials design, for example in optimizing solid electrolytes, tailoring interfacial chemistry, or accelerating the discovery of new energy materials.

Overall, the discussions revealed a rapidly evolving landscape in which quantum accuracy, machine learning efficiency, and multiscale realism are being combined to address the complexity of electrochemical systems. This convergence is pushing the state of the art towards predictive modeling of realistic electrochemical devices, providing powerful tools for designing next-generation energy storage and conversion technologies.

2. What were the primary outcomes of this workshop, including limitations and open questions?

The workshop highlighted significant methodological advances that are reshaping the modeling of electrochemical systems. A key outcome was the recognition that the traditional gap between electronic structure methods (e.g., DFT) and classical or continuum approaches is rapidly narrowing. Whereas these domains used to be largely disjoint – electronic structure theory focusing on small systems at high accuracy, and molecular mechanics or continuum models treating large scales with limited resolution – the community now benefits from a continuum of techniques that connect quantum and classical descriptions. These include machine-learning potentials trained on ab initio data, QM/MM frameworks, constant-potential molecular dynamics parameterized from DFT calculations, and emerging multiscale simulation schemes. Together, they enable more seamless transfer of information across scales, allowing for realistic modeling of electrode/electrolyte interfaces, solid–liquid boundaries, and device-level phenomena.
However, despite recent progress, it remains challenging to achieve quantum-level accuracy for large, realistic systems over relevant timescales. Current methods often involve trade-offs between accuracy, transferability, and computational cost. For example, machine learning potentials promise quantum accuracy at lower cost but require extensive, carefully curated training data and may face limitations in describing rare events or chemical reactivity. From the methodological point of view, "conventional" machine learning potentials are often not sufficient for electrochemical systems as they lack long-range electrostatic effects.
Open questions therefore emerged regarding how best to systematically couple methods across scales, maintain consistency of electrochemical observables (e.g., potential, capacitance), and integrate electronic structure, statistical mechanics, and data-driven approaches into coherent frameworks.

3. What was the take-home message for the participants?

Participants emphasized the need for community benchmarks, shared datasets, and open software to accelerate progress. Addressing this will require both methodological innovation and closer collaboration across traditionally separate communities.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

The outcomes of the workshop clearly hold significant potential for societal benefits, given the central role of electrochemical systems in the global energy transition. Batteries, supercapacitors, and electrocatalytic devices are key enablers of renewable energy integration, electrified transportation, and sustainable chemical production. Progress in their design and optimization directly impacts the development of cleaner and more efficient energy technologies.
The workshop showcased methodological advances that bring us closer to predictive, multiscale modeling of electrochemical systems, enabling accelerated discovery and improvement of materials and interfaces for energy storage and conversion. By bridging electronic-structure and large-scale modeling, the emerging approaches discussed can help shorten development cycles, reduce the need for costly trial-and-error experiments, and provide fundamental insights into degradation mechanisms, efficiency limits, and interfacial phenomena.

As the field grows rapidly, the tools and collaborations strengthened during this workshop contribute to faster innovation pipelines for next-generation batteries, fuel cells, and electrolysers. Ultimately, this knowledge will support technologies essential for decarbonization, improved energy security, and sustainable economic development.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The workshop participants have agreed to collaborate in the writing of a perspective article on this topic.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

Particular attention was given to gender balance when selecting invited speakers. As a result, one third of the speakers were women, in line if not slightly higher than the current gender distribution in this research field. Efforts were also made to ensure broad geographical representation among both speakers and participants. Attendees came from 15 different countries, mostly from Europe but also from the US, China, Rwanda, Korea, and Japan (one invited speaker from China participated online due to visa issues). In terms of career stage, the organising committee included established and early carrier researchers, and the program combined presentations by leading experts with contributions from postdoctoral fellows and recently established group leaders, giving visibility to emerging voices in the community and fostering intergenerational exchanges. Several PhD students were also present. This mix encouraged dynamic discussions and networking opportunities across different generations of scientists.

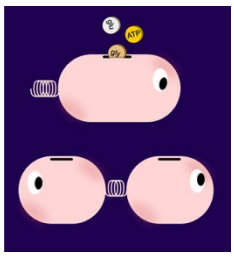
7. Participant list

Organisers
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Economic Principles in Cell Biology



Location: University of Vienna, Austria

Webpage : Event webpage

Dates: Jul 23, 2025 - Jul 26, 2025

1. What were the major topics presented in the School?

The summer school offered an in-depth introduction to systems modeling of cellular behavior, with a particular focus on understanding how cells manage their limited resources. In other words, how they make “economic” decisions to balance growth, maintenance, and efficiency. Through a combination of lectures and hands-on computer exercises, participants explored key principles shaping cellular strategies, such as metabolic optimization, trade-offs in enzyme allocation, and the coordination of growth. The course content was closely aligned with our collaborative open-access textbook “Economic Principles in Cell Biology” (https://principlescellphysiology.org/book-economic-principles/index.html), with each session corresponding to a specific chapter. Our introductory lectures built a solid foundation in key concepts and modeling techniques for studying cellular systems. By providing an overview of core principles in cell biology, metabolism, and growth, they prepared participants to engage with more advanced and research-driven topics later in the week, including:

- Modeling interactions within microbial communities
- Understanding the impact of cell-to-cell variability
- Investigating how cells schedule their behavior over time
- Exploring the economic principles underlying organ structure and function in multicellular organisms, illustrated through the example of the human lung.

These sessions offered participants a glimpse into ongoing research questions and demonstrated how economic principles can be applied across different scales of biological organization.

The lectures were accompanied by hands-on computer exercises using Jupyter notebooks, which were specifically developed for this course. These interactive notebooks are freely available via the associated Git repository. After a session introducing Python and Jupyter for participants with little programming experience, the remaining exercises aligned closely with individual lectures. Each session was designed to reinforce and apply the concepts covered in the corresponding lecture, helping participants deepen their understanding through practical implementation. These sessions enabled participants to explore modeling techniques first-hand and gain experience with tools commonly used in systems biology research. An overview of lectures, computer exercises session, and all course materials is available on the course website at https://principlescellphysiology.org/summer-school-2025/

2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

Throughout the summer school, many of the lectures concluded with a critical reflection on the strengths and weaknesses of the presented modeling approaches, helping participants understand not only what can be modeled effectively, but also where current methods fall short. Several key limitations and open questions emerged across sessions and discussions:

- Model complexity vs. interpretability: Simplified models like Flux Balance Analysis offer tractable predictions but sacrifice biological realism. Striking the right balance remains a core challenge.
- Data limitations: Mechanistic models often require difficult-to-measure parameters. Strategies like optimization and comparative modeling were explored as workarounds.
- Dynamic behavior: Capturing temporal processes, especially in fluctuating environments, is still an open problem.
- From cells to communities: Single-cell models fall short in explaining emergent behaviors like cooperation and cross-feeding in microbial consortia.
- Scaling up: Extending economic principles to multicellular systems poses conceptual and technical hurdles.
- Linking biology and economics: While “cellular economics” was introduced, deeper integration with economic theory (e.g., pricing, market dynamics) is needed.

These open questions also reflect the current limited scope of the open-access textbook Economic Principles in Cell Biology, which is primarily focused on bacterial systems and standard modeling frameworks. The course highlighted the need to expand this foundation to include:

- Microbial communities and their internal “economies”
- Eukaryotic cells and compartmentalised structures
- Multicellular organisms and tissue-level optimization
- Clearer cross-disciplinary links between cell biology and economics

We plan to develop these themes for future editions of the textbook and include them in future summer schools.

3. What was the take-home message for the participants?

The summer school introduced participants to the concept of the economy of the cell: how cells manage resources efficiently. It showed that this behavior can be explored through mathematical modeling, using various approaches and tools, many of which were practiced hands-on. Participants were invited to actively contribute to and shape the Economic Principles in Cell Physiology community, for example, through the “Young Scholars” group for students and early-career researchers.

4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

The summer school produced a range of openly accessible resources to support ongoing learning and long-term impact. These include:

1. Course content and lecture materials

- The lectures were based on our open-access textbook Economic Principles in Cell Biology, available at https://principlescellphysiology.org/book-economic-principles/index.html
- To complement the textbook, all lecture slides from the summer school have been published at https://principlescellphysiology.org/summer-school-2025/lectures.html
- Recordings of the 2025 lectures are currently being processed and will be uploaded to the same platform. Meanwhile, recordings from 2024 are available at https://principlescellphysiology.org/summer-school-2024/presentations.html

2. Practical resources
- All Jupyter notebooks used during the hands-on sessions are publicly available and documented. To support reproducibility, a preconfigured Docker container has also been provided. These materials can be accessed at https://principlescellphysiology.org/book-economic-principles/problems.html

3. Educational videos
- During the summer school, ten participating educators recorded short instructional videos at the University of Vienna's Center for Teaching and Learning. The videos are currently being edited and will form part of a free open-access online course, further expanding the educational reach of the program.

5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

We aimed for inclusivity in gender, geography, and career stage. Speakers were primarily authors of our textbook, most of whom are in advanced career stages. The structural imbalances in our field resulted in a gender skew (5 women, 13 men). We are actively working to improve this balance from year to year. We were pleased to include three invited teachers from Latin America, supporting broader geographic representation. Among on-site participants, we achieved near gender parity (21 female, 17 male, 2 undisclosed). We selected participants from 18 countries, prioritized non-European applicants. No fees were charged except a €25 student union fee (required by UniVie) to ensure access. Despite these efforts, all accepted African participants faced visa and travel barriers, and we lacked funding to offer travel support. Last-minute cancellations were filled by Austrian applicants. Remote participation was possible, and all materials are freely available online.

6. Participant list

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Noor, Elad - Weizmann Institute of Science, Israel
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Correlations and Topology in Moiré Materials: Theory vs. Experiments



Location: ETH Zurich Monte Verita, Switzerland

Webpage : https://www.cecam.org/workshop

Dates: Jul 27, 2025 - Jul 30, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The focus of this workshop was on the physics of moiré materials, and the strongly correlated phases that emerge in them. Moiré materials are materials made of a few atomically thin layers of a two-dimensional material (such as graphene or 2D semiconductors such as transition metal dichalcogenide). The slight mismatch between the different layers creates an interference pattern, a superlattice or 'moiré' pattern on a length scale 10 to 100 times larger than the distance between atoms. In turn, a well chosen such moiré pattern can result in a suppressed kinetic energy for the conduction electrons, allowing electron-electron interactions to play a major role. This situation leads to new phases of matter, which can be detected experimentally, and need to be understood theoretically.
Several experimental methods were discussed, including mesoscopic transport, optical pumping, absorption, photoluminescence, scanning tunneling microscopy and spectroscopy. These techniques were applied to study the following moiré materials: 2, 3, 4, 5 layers of graphene with rhombohedral alignment, or with a rotation to magic angle, twisted bilayer WSe2, twisted bilayer MoTe2. Phases such as superconductivity, fractional Chern insulators, strange metals, correlated insulators with exotic order were discussed. On the theoretical side, we discussed how to best model these materials and understand their phase diagrams, using computational methods such as ab initio downfolding, DMFT (Dynamical Mean Field Theory), Hartree-Fock, Quantum Monte Carlo, DMRG (Density Matrix Renormalization Group), and exact diagonalization.

2. What were the primary outcomes of this workshop, including limitations and open questions?

Moiré materials are a relatively young field, which has known a rapid expansion since 2018. In the past 2-3 years, experimentalists in this field have worked very hard to improve the quality of their devices, which led to an important increase in the fraction of devices showcasing strongly correlated phases. This has permitted the observation of especially exotic phases never observed before, such as fractional Chern insulators. In parallel, the improvement in device quality has increased the reliability and reproducibility of experiments. This general trend should help bridge the gap between theory and experiment. Compared to most strongly correlated materials, moiré materials appear as very controllable, and the potential for a good theory-experiment match is very strong. This is clear from such successes as understanding the key role of strain in magic angle

twisted bilayer graphene, and predicting the emergence of incommensurate spiral Kekulé order, later confirmed by experiments. Another example is the discovery of the fractional quantum anomalous Hall effect in twisted MoTe2, following great progress in the theory of fractional Chern insulators.
Some open questions laid out by the workshop are: what are the symmetry and mechanism of pairing in the superconducting phases of twisted bilayer graphene and other moiré materials? Is it possible to realize (time-reversal preserving) fractional topological insulators in twisted TMDs? And non-abelian fractional Chern insulators? What is the origin of the disappearance of the anomalous Hall metal in twisted MoTe2?

3. What was the take-home message for the participants?

The complexity of moiré materials requires the combination of many experimental and theoretical techniques. This effort is worthwhile and has already offered unprecedented results in the field of correlated quantum condensed matter, while leaving many open questions to be explored.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

The greater understanding of fundamental material science through this workshop can be considered a societal benefit.
Beyond fundamental science, sensors and electronics based on moiré materials have been suggested and are a possibility. For example, the possibility of using magic-angle graphene as a sensor to detect single magnetic vortices was discussed during the workshop. Additionally, moiré materials based on TMDs can be manipulated with light, opening the possibility to create memories with optical read-out and optical addressing.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

There will be new collaborations thanks to the workshop. It is too early to tell whether there will be other tangible outcomes.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

We invited a diverse mix of invited speakers, and we communicated directly with potential participants from less represented backgrounds through personalized emails. We made the selection of contributed oral presentations in the same spirit. Overall, the female/male ratio was 8/42 – 2/4 organizers, 3/9 invited speakers, 2/12 contributed talks. This is a comparable ratio (19%), probably a little bit higher than the typical ratio in the quantum condensed matter community.

The generous funding helped us reduce the cost of accommodation (350CHF for full board accommodation for three days) and even made it possible to offer free accommodation to 3 participants in addition to the invited speakers. During the workshop, we fostered a friendly atmosphere and were vigilant to include more junior members in scientific as well as more informal discussions.

7. Organiser list

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Wagner, Glenn
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Entropy of Soft Matter Systems



Location: ISTA, Austria

Webpage : Event webpage

Dates: Aug 27, 2025 - Aug 29, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

We discussed the usefulness of entropy and whether it adds more to understanding biomolecular behavior than simply knowing the free energy. We compared and contrasted in turn the many ways to decompose entropy and assess their meaning, either in terms of coordinates, experimental measurables or other quantities. The modern methods discussed included *k*-th nearest neighbor, maximum information spanning tree, inhomogeneous solvation theory, and multiscale cell correlation.
The need for benchmarking and validation is clear. While groups often have their own codes for calculating entropy, consistent validation so that the accuracy of these calculations can be determined and compared to other methods and software would improve the field.
We sought to identify where there might be synergy between computational and experimental approaches. Experimentalists do not always know what systems have been studied computationally, and computational scientists can struggle to find experimental validation for the systems they choose.

2. What were the primary outcomes of this workshop, including limitations and open questions?

Some of the early career participants noted that it can be difficult for new researchers to know what software is available and which methods would be best to use. The lack of training and tutorials showing how to calculate entropy is a barrier to using these methods. A comprehensive survey of the available software including the pros, cons, and special requirements of each one, ideally linked to validation and benchmarking results, would aid researchers. If all the software was readily accessible and documented, people could avoid replication of coding work and focus the available software development effort on adding new features and improving the user-friendliness. Sharing the existing methods is not as exciting as creating new algorithms but is important and useful.
Computational and experimental scientists struggle to talk to each other and to make the connections that are necessary to work together. This is a challenge when we are trying to validate simulation results by comparing them to experiments and the systems simulated do not already have experimental data.

3. What was the take-home message for the participants?

Entropy is as fascinating as it is complex. We should continue to do great science and collaborate as much as possible.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

The main interest in this topic is academics who enjoy thermodynamics. History has shown that better understanding of the thermodynamics leads to better design of materials and pharmaceuticals, enabling applications in key areas such as modern drug discovery and energy materials.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

There are plans for creating a software review article in a “living journal” style publication so that it can be updated in the future as software develops. This will serve as a guide for exploring the software choices available and will include efforts for benchmarking and validating the software.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

We tried to invite speakers from diverse backgrounds (including experimentalists as well as computational scientists). Most of the participants (invited and applied) came from Europe because of the impact and costs of travel. With the sponsorship from CCPBioSim we were able to give a few early career researchers travel support to attend the workshop.

7. Participant list

Organisers
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Peptide Computational Methods and Applications



Location: CECAM-IRL, Ireland

Webpage : Event webpage

Dates: Sep 1, 2025 - Sep 2, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The Peptide Computational Methods and Applications Flagship Workshop brought together leading researchers from academia and industry to address the challenges and opportunities at the interface of state-of-the-art artificial intelligence and peptide science. The event highlighted several major themes that collectively contribute to advancing the state of the art in this rapidly evolving field.

The start of the first day was focused on predicting and modelling bioactive peptides. Talks by Denis Shields and Martin Zacharias set the stage by addressing peptide activity prediction and cyclic peptide modelling, two areas where computational innovation can impact drug discovery. Advances in modelling peptide-protein interactions, as presented by Ioana Ilie and Niklas Halbwedl, underscored the importance of combining structural biology with computational engineering to design peptides that can modulate critical biological processes.

The workshop also placed strong emphasis on AI-driven generative approaches. Presentations from researchers such as Nuno Costa and Wolfgang Banzhaf demonstrated how frontier generative models and evolutionary computation can unlock discovery of new peptides, even in cases prone to aggregation or structural instability. These methods not only enhance the diversity of candidate peptides but also accelerate the design process, reducing the reliance on trial-and-error laboratory experiments.

Another recurring theme was handling uncertainty and data scarcity. Raul Fernandez-Diaz and Raquel Rodriguez Perez discussed frameworks for partitioning, representation, automation, and uncertainty estimation. This is vital since peptide datasets are often small and heterogeneous compared to protein datasets. Addressing uncertainty is key for making AI predictions interpretable and trustworthy, especially in contexts where decisions impact therapeutic development.

The hands-on sessions on the second day reinforced the importance of applied AI methods. Participants worked on machine learning prediction for peptides and explored generative modelling approaches, enabling direct experience with the tools and fostering collaboration. Pierre Tuffery's talk on scoring functions using AlphaFold further connected the latest advances in structural AI with peptide-specific challenges, highlighting cross-fertilization between protein modelling and peptide design.

By integrating structural biology, machine learning, generative AI, and applied computational design, the workshop advanced the state of the art in peptide research. It highlighted both technical innovations - such as uncertainty-aware generative models - and community priorities, including collaboration, reproducibility, and user-friendly software. Collectively, these contributions pave the way for faster, safer, and more efficient peptide discovery pipelines, bridging the gap between AI innovation and therapeutic application.

2. What were the primary outcomes of this workshop, including limitations and open questions?

A key outcome was the consolidation of a shared understanding of the current capabilities and challenges in peptide-focused AI. The presentations demonstrated clear progress in areas such as cyclic peptide modelling, generative design of peptide candidates, and uncertainty-aware prediction frameworks. By bringing together structural biologists, AI researchers, and industrial practitioners, the workshop fostered a cross-disciplinary dialogue that clarified which computational approaches are most promising and where experimental validation remains essential.

Another outcome was the recognition of generative AI as a central driver of innovation. Multiple talks and the hands-on sessions showed how conditional generative models and protein language models can accelerate peptide discovery. Participants identified opportunities to use these methods not only for structural prediction but also for functional optimisation, particularly for peptides with unusual amino acids or multifunctional properties.

The workshop also highlighted the importance of addressing data limitations. Discussions repeatedly returned to the challenge of small and fragmented peptide datasets, especially compared to datasets available in industry. The emphasis on uncertainty estimation and explainable AI was another outcome, reflecting the community's recognition that model interpretability and robustness are as important as predictive accuracy.

However, several limitations and open questions were acknowledged. One limitation is the lack of widely accessible, standardised benchmarks for peptide AI, which hampers fair evaluation of different methods. Questions also remain about how best to integrate experimental feedback loops into computational pipelines, and how to balance speed of discovery with safety considerations such as toxicity and stability.

The workshop concluded that while technical progress is strong, building a sustainable research ecosystem requires community action: open-source tool development, improved visualization and user interface design, and mechanisms for secure collaboration across academic and industrial partners. These were seen as essential to overcoming the hurdles of data scarcity and ensuring that AI-enabled peptide discovery can transition smoothly from research to therapeutic application.

Overall, the primary outcomes were the demonstration of state-of-the-art computational methods, the identification of generative AI and uncertainty modelling as critical future directions, and the articulation of clear limitations that demand collective solutions. The open questions – how to standardise data and how to scale discovery safely – set a focused agenda for future work.

3. What was the take-home message for the participants?

The key takeaway was that advancing peptide science now depends on integrating cutting-edge AI (especially generative models, uncertainty-aware prediction, and collaborative data strategies) with experimental research. Participants left with a shared vision that interdisciplinary collaboration, open tools, and innovative approaches are essential to overcome data limitations and accelerate the discovery and design of functional, safe, and effective peptides.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

Peptides are increasingly central to modern therapeutics, with applications ranging from cancer treatments to metabolic disorders and infectious diseases. The workshop demonstrated how advances in artificial intelligence – particularly generative models, protein language models, and uncertainty-aware prediction – can accelerate the discovery of novel peptides, making drug development more efficient, less costly, and more targeted.

The emphasis on open-source tools and human-centered design also carries societal value by democratizing access to advanced computational methods. This ensures that not only large pharmaceutical companies, but also smaller biotech startups and academic groups, can contribute to and benefit from innovation in peptide science. The resulting ecosystem can drive broader participation and more rapid translation of research into therapeutic and diagnostic applications.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

One of the most important outcomes was the formation of new collaborations between academic researchers, industry representatives, and applied AI specialists. These collaborations may lead to joint projects that integrate expertise in structural biology, peptide chemistry, and advanced machine learning.

The hands-on sessions seeded practical outcomes by exposing participants to available tools for peptide prediction and generative modelling. This not only built technical capacity but also identified gaps where further software development is needed. While obviously no publications have to date resulted directly from the workshop, the shared commitment to collaboration, tool development, and coordinated proposal submissions ensures that its impact will extend well beyond the two days of meetings.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

Inclusivity was embedded in both the organising committee and the workshop program. The committee itself was diverse in career stage and gender, ensuring broad perspectives in planning. The invited speakers and participants represented a balance of male and female researchers, spanning early-career scientists, established academics, and industry leaders from Ireland, Europe, and the USA. The event was held in accessible UCD venues with step-free entry and clear signage, and registration was free of charge to reduce financial barriers. By combining talks with interactive sessions, the workshop created space for meaningful participation across levels of expertise, fostering an inclusive and collaborative environment.

7. Participant list

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Quantum computing for classical complex systems: Opportunities and challenges from soft matter to life sciences.

Location: CECAM-IT-SISSA-SNS, Italy



Webpage : Event webpage

Dates: Sep 1, 2025 - Sep 3, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop, held at **CECAM-IT-SISSA-SNS (SISSA, Trieste)** on **1–3 September 2025**, ran over three days with eight talks on Day 1, eight on Day 2, and six on Day 3. The program connected quantum hardware/control, annealing and gate-model algorithms, and quantum-inspired optimization to concrete problems in soft matter and the life sciences, from polymers and fluids to protein folding/design and biomolecular condensates. Across sessions, the meeting advanced: (i) problem-to-hardware mappings (Ising/QUBO, qudit encodings) tuned to preserve physical constraints; (ii) credible hybrid workflows where quantum subroutines seed or warm-start powerful classical samplers/optimizers; (iii) observable-centric metrics (structures, rates, critical behavior) replacing "anecdotal" speedups.

Day 1 (Speakers: Schmidt-Kaler, Fazio, Moller, Zecchina, Dalmonte, Slongo, Panizza, Irbäck)
Schmidt-Kaler and Fazio outlined device capabilities and control-theoretic routes beyond annealing for state preparation and optimization on near-term platforms. Moller introduced quantum computational fluid dynamics. Zecchina discussed optimization frameworks at the interface with AI. Dalmonte presented data-mining of quantum simulators. Slongo showed how quantum-inspired encodings accelerate stochastic sampling in soft matter. Panizza and Irbäck focused on biomolecular applications.

Day 2 (Speakers: Roggero, Mazzola, Ghamari, Orland, Santoro, Succi, Carobene, Bolhuis)
Mazzola analyzed bottlenecks for digital quantum advantage on classical problems and discussed quantum-enhanced sampling prospects. Bolhuis and Ghamari discussed transition path sampling and hybrid rare-event pipelines. Orland provided a statistical-physics backbone for the optimal transport problem and Schrödinger bridges. Santoro detailed quantum control strategies that generalize annealing for optimization/state preparation. Succi explored Carleman Lattice Boltzmann formulations aimed at quantum execution of fluid dynamics. Carobene introduced local fermion-to-qudit mappings relevant for superconducting-qudit platforms.

Day 3 (Speakers: Stella, Teza, Chan, Meuser, Reha)
Stella addressed quantum simulations of molecular excitations in photoactivated drugs. Teza showed how calibrated annealers can sample effective Boltzmann distributions. Chan presented analytical approaches for field-theoretic models of biomolecular condensates. Meuser described de novo design of protein-binding peptides using hybrid

quantum/classical optimization. Reha closed the meeting by outlining further applications and open problems.

2. What were the primary outcomes of this workshop, including limitations and open questions?

Discussions converged on hybrid pipelines where quantum subroutines, including annealing schedules, variational or control-based state preparation, and compact qudit encodings, seed or warm-start strong classical optimizers and samplers. Case studies covered lattice protein folding and sequence design, peptide–target binding, dense-polymer and soft-matter sampling, rare-event pathways in complex landscapes, and fluid or continuum surrogates. The emphasis shifted from raw speed to observable-level gains, for example improved structures, rates, and phase behavior, and to measurable reductions in classical search once a quantum step supplies high-quality initial states or constraints. The hybrid framing also made clear the engineering levers that matter most, namely embeddings, schedule tuning, calibration, and error-robust update rules.
A second outcome was participants compared QUBO formulations for polymers and lattice proteins, constraint encodings for self-avoidance, contact patterns, and side-chain specificity, coarse-grained reactive networks for rare events, and local fermion-to-qudit mappings that reduce gate overhead relative to standard fermionic encodings. Alongside these mappings came practical guidance on minor embeddings and connectivity limits, penalty calibration and schedule design, compiler and optimizer choices, and when quantum-inspired solvers provide the right classical baseline.
Limitations and open questions were addressed directly. Demonstrations of advantage remain not fully conclusive and instance dependent, with outcomes sensitive to calibration drift, noise, connectivity, and depth. Compact encodings can drop crucial physics, for example solvent or side-chain effects, so the balance between fidelity and tractability must be managed explicitly. Preparing the correct initial state is a major bottleneck even for problems with formal advantage. Mapping annealing or controlled dynamics to finite-temperature and kinetic observables, with quantified uncertainties, remains difficult. Data scarcity limits ML surrogates beyond a few systems.

3. What was the take-home message for the participants?

- Important improvements would follow from designing compilers and algorithmic optimizers to defining benchmark problems with scientific output.
- Advantages of QC in physically relevant problems are still to be reaped; even where quantum advantage has been theoretically demonstrated, the preparation of the initial quantum state may still pose a formidable challenge.
- Quantum computing is also forcing us to take an entirely new look at established physical problems and models.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

The workshop helped overview the state-of-the-art of quantum computing for numerous challenging problems at the interface of physics, chemistry, data science, and biophysics. These included problems aimed at breakthrough with societal benefits:
Materials & soft matter: Ising/QUBO encodings and quantum-inspired solvers accelerate searches in polymers, gels, and self-assembled systems, with tailored properties.
Engineering: Quantum-amenable fluid models could help design new microfluidic devices and better understand the multiscale effects of turbulence.
Health & biomedicine: Hybrid pipelines for protein and peptide folding and design can shorten discovery cycles for therapeutics, including photoactivated drugs and binders with improved specificity. Better rare-event sampling supports predictions of misfolding and aggregation.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

New collaborations were seeded during and after the meeting, and the workshop, which was the first of its kind in this area, helped kickstart a community by creating first contact among physicists approaching quantum computing from different angles and parent disciplines. Thanks to the workshop, several participants became aware of relevant work done in other groups and established connections for sharing results and potential future collaborations. Most participants felt it appropriate to propose a follow-up edition in two to three years, somewhere in Europe.
Tangible outcomes include the large set of presentation slides that were uploaded on the activity webpage for the benefit of the wider scientific community.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

We promoted inclusivity by giving the broadest possible publicity to the activity through the CECAM network and multiple scientific mailing lists spanning soft matter, statistical physics, biophysics, and quantum computing. We accepted **all** participation requests, thus ensuring the broadest possible coverage for seniority, gender, or geographic provenance. This ensured a diverse mix of participants and speakers across career stages and geographical backgrounds.

7. Participant list

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CECAM/ALC/CCP9 Spectroscopy Masterclass

Location: CECAM-UK-DARESBURY, United Kingdom



Webpage : Event webpage

Dates: Sep 1, 2025 - Sep 5, 2025

1. What were the major topics presented in the School?

The "CECAM/ALC/CCP9 Spectroscopy Masterclass", held 1-5 September 2025 at Rutherford Appleton Laboratory, UK, was a 5-day meeting intended to strengthen theory support for experiments at large scale facilities such as the UK's Diamond synchrotron, ISIS neutron and muon source and Central Laser Facility. These facilities and similar ones at laboratories across the world perform cutting-edge science across the full spectrum of current research activities, employing thousands of beam-line scientists and technical staff and producing unparalleled societal impact across the sciences. Large scale facilities have evolved over the last four decades to offer a wide portfolio of powerful experiments, each of which may be extremely specialised in technique and application. Over the same timeframe, theoretical spectroscopy has evolved from the first principles modelling community, largely in universities, and a variety of approaches have been developed that allow first principles descriptions of different experiments. In some respects, these methods now resemble individual beamlines: extremely specialised, requiring detailed expertise and experience, and not necessarily broadly visible or understood.

The purpose of the meeting was to present the current state of the art in modelling to the experimental communities and to show what is currently possible from the theory point of view and to provide a forum for experimentalists to voice their requirements for theory support and for discussion on the topic of how theory support for large scale experiments should be organised and prioritised.

The meeting concerned theoretical spectroscopy, concentrating on materials science but specifically in the context of the large-scale facilities. Each day started with high-level talks from Diamond, ISIS or CLF which served as motivation for the discussions on X-ray, magnetic/crystal-field or ARPES-related theory discussions that followed. These topics were addressed in terms of the theoretical method currently deemed most appropriate (density functional theory, many-body perturbation theory, time-dependent density functional theory and machine learning); these were introduced by their respective world leaders. Speakers were instructed to give a critical appraisal of the successes and failures of theory support in these different areas.

In addition to the program of talks, active hands-on sessions with a variety of different electronic structure codes, organised as three parallel sessions, allowed participants to get real experience of performing practical calculations and to have the opportunity to interact directly with theory developers and ask questions in real-time about practical calculations. The meeting closed with a panel discussion with representatives of each of the large-scale facilities as well as the theory community who responded to questions from participants about theory support, training needs and the future of materials modelling.

2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

It is not possible to provide in-depth discussion or training in advanced theoretical methods within a week; it is scarcely possible to provide a survey of this large and active field. We elected to provide hands-on sessions on some representative calculations in the categories of core-spectra (X-ray), valence spectra (ARPES) and magnetic excitations; we also taught photoelectron diffraction and ran sessions on machine learning for spectroscopy.These sessions were organised such that participants could mix and match different topics according to their interest and it would be possible to attend sessions using one approach (e.g., multiple scattering) or to attend sessions focusing on one application (e.g., magnetism) or various combinations.
The codes presented were the multiple scattering DFT codes SPR-KKR and MS-SPEC (both via their python interfaces) and the GW/QSGW code Questaal and the ML codes from the Maria Chan (Argonne). Multiplet theory was taught using Quanty. Each session was led by expert developer teams; by dividing the participants among three groups each afternoon, we were able to provide small group support for better discussion and to allow participants to "play" with the codes at their own pace. Feedback on the practical sessions was extremely positive and we felt that the lively discussion and the possibility for experimentalists to perform actual calculations at high levels of theory through to completion and see actual results, justified the significant overhead of teaching presence and organisation.
We used a cloud-based computing platform that largely avoided any issues with participants' computing devices and allowed calculations to be done on sufficiently resourced cloud machines. The organisers were able to install and test all the software (which was substantial in this case) before the start of the workshop. (Unfortunately, technical issues with the service provision meant that the service was unreliable during the first session and this caused some time to be wasted; some redundancy or fallback cloud provision is advised for future events.)
A large part of the discussion revolved around establishing a common vocabulary between theorists and experimentalists and in delineating what properties are straightforwardly attainable from theory (and what cases remain a challenge even for experts). The state of the art in theory was contrasted with the state of the art in experiment: in both cases the improvement in energy resolution capability is matched by the increasing complexity of application topics/materials. Discussion often returned to the question of how theory support should be organised and prioritised, noting that the throughput of studies in the large facilities is extremely large and well beyond the scalability of individual single-topic collaborations. There is a definite need for further follow up meetings of this kind to develop solutions to these questions.

3. What was the take-home message for the participants?

The take-home message coming from the hands-on part of the school was that advanced methods are now much more robust and much more easily used than ever before. It is possible for experimentalists to partake in theory work themselves. This understanding facilitates more effective theory-experiment collaboration and the adoption of the best suited modelling methods. The significant need for enhanced theory support at the large facilities was noted by all and discussions were initiated toward this end.

4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

The meeting was significantly intended to support networking and involvement of all participants through small group work, tours of the facilities, centrally organised accommodation and a conference dinner; the location was chosen to maximise the overlap with the facilities' beamline scientists and research staff. Accordingly, the meeting was in-person only; to promote discussion, talks and teaching sessions were not broadcast or recorded. Slides of all the talks and all teaching materials were made available to the participants.

5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

 Organised accommodation and transport were provided (ensuring that cost would not present any barrier to attendance).

 Starting and finishing at midday (such that that nobody would need to travel outside of business hours).

 We took care to invite a diverse range of genders and career stages in talks and panel discussions.

 We proactively engaged with participants such that we were aware of special individual requirements and could take steps to accommodate these.

 Broad, diverse menu choices which met all dietary requirements were arranged with catering staff prior to the meeting to ensure all participants' needs were satisfied. This was done as transparently as possible to avoid difficulty or stigma.

6. Organiser list

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Lennard-Jones Centre-CECAM Meeting 2025: From electrons to atoms to molecules and materials



Location: University of Cambridge, United Kingdom

Webpage : Event webpage

Dates: Sep 1, 2025 - Sep 5, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The Lennard-Jones Centre / CECAM Meeting 2025 showcased the breadth of current progress in electronic structure theory and its applications to complex materials. Major topics included fundamental advances in density functional theory (DFT), where speakers introduced new spectral functional approaches, exact-constraint guided approximations, and adiabatic-connection perspectives on reaction barriers. These efforts directly target long-standing deficiencies of standard functionals, pushing DFT towards more accurate treatment of strong correlation, excitations, and charge delocalization.

A second key theme was the integration of DFT with machine learning (ML). Several sessions highlighted data-driven interatomic potentials, as well as foundation models for defect energetics. This combination offers quantum-level accuracy with molecular-dynamics efficiency, enabling simulations of far larger systems and timescales than previously feasible.

Applications to real materials and phenomena were a third concentration. Talks spanned moiré materials with tunable optical properties, superhydrides for superconductivity, piezoelectric biomolecular assemblies, and energy interfaces from electrolytes to CO_2 conversion catalysts. Methodological innovations (e.g., ONETEP linear scaling, advanced hybrid DFT in FHI-aims) were consistently tied to predictive studies of technologically important systems.

Finally, the program reflected on the historical and future trajectory of the field, with contributions on the early days of theoretical chemistry in Cambridge and the rise of electronic structure methods, paired with forward-looking discussions on quantum embedding, quantum Monte Carlo, and near-term quantum computing applications.

Taken together, the meeting underscored how rigorous first principles methods coupled with ML acceleration are redefining the role of electronic structure theory. The convergence of theory, algorithms, and applications is advancing the state of the art from model problems towards quantitatively reliable predictions of complex, real-world materials and processes.

2. What were the primary outcomes of this workshop, including limitations and open questions?

The workshop's primary outcome was a sharpened view of where electronic structure theory stands and where it must go. On the positive side, new density functional

frameworks (spectral functionals, exact-constraint guided DFAs, localized orbital corrections) demonstrated real progress in reducing delocalization errors, improving excited-state predictions, and addressing strong correlation. Machine-learning interatomic potentials were highlighted as a maturing technology, now capable of treating realistic materials with near–first-principles accuracy at scale. Applications showcased – from moiré materials and spin defects to superhydrides and electrochemical interfaces – illustrated how these methods can illuminate frontier systems relevant to energy, electronics, and quantum technologies.

Yet the meeting also clarified limitations. Despite advances, no single functional or ML potential is universally reliable: transferability, treatment of excited states, and the balance of exchange vs. correlation remain open questions. Scalability, interpretability, and uncertainty quantification in ML-driven simulations are recurring challenges. Similarly, while quantum embedding and quantum computing approaches show promise, they remain exploratory and face hardware and algorithmic hurdles.

Participants highlighted the need for deeper unification of theoretical frameworks (DFT, Green's functions, quantum Monte Carlo) and for methods that can reliably capture finite-temperature, dynamical, and strongly correlated phenomena. Industry sessions reinforced the demand for robust, reproducible tools that can leave the lab and impact technology development.

In sum, the workshop consolidated methodological advances, validated ML–DFT integration, and set a research agenda centered on overcoming transferability, accuracy, and scalability bottlenecks – open questions that define the next phase of the field.

3. What was the take-home message for the participants?

The take-home message was that electronic structure theory is entering a new era where advances in density functionals, machine-learning potentials, and quantum methods are converging to tackle real, complex materials. Participants left with appreciation for historical contributions, optimism about new capabilities, and awareness of key challenges--such as transferability, accuracy for strong correlations, and scalable implementations--that remain central to future progress.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

Yes, the workshop outcomes hold clear potential for societal benefit. Improved density functional methods and hybrid quantum–machine learning approaches will enable more reliable predictions of complex materials, reducing reliance on costly trial-and-error experimentation. This has direct implications for the discovery of clean energy technologies (e.g. catalysts for CO_2 conversion, high-temperature superconductors, piezoelectric biomaterials), for semiconductors and quantum devices, and for advanced pharmaceuticals and biomolecular assemblies.

By pushing electronic structure theory towards higher accuracy and scalability, participants are laying the groundwork for faster design of materials that could address global challenges in energy, climate, and health. The discussions on industry translation underscored how robust computational tools can shorten innovation cycles, lower R&D costs, and enhance reproducibility – benefits that extend beyond academia into applied sectors.

However, societal impact depends on overcoming current limitations: lack of universal transferability of ML potentials, the difficulty of capturing strong correlation and excited states, and the need for transparent error metrics. If these challenges are addressed, the workshop's advances could accelerate the path from theoretical insight to transformative technologies.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

Tangible outcomes include new collaborations across academia and industry, spurred by the dedicated industry session and networking events. Several groups presented emerging software developments (e.g., improved hybrid DFT in FHI-aims and machine-learning potentials like MACE-OFF). The program also highlighted recent and forthcoming publications and positioned many talks as springboards for joint proposals around energy, quantum technologies, and machine learning in materials. Overall, the workshop seeded concrete projects and tools that will continue beyond the meeting.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The workshop made inclusivity a priority by assembling a diverse speaker lineup spanning continents (Europe, North America, Asia) and institutions, with balanced representation across gender and career stage. For example, invited speakers nominated junior researchers to co-present. To support this effort, CECAM funds were used exclusively for early career researcher travel subsidies. Efforts were also made to accommodate accessibility needs through the choice of modern facilities at the Ray Dolby Centre. Furthermore, we offered full remote participation for free to anyone who signed up via the CECAM page.

7. Participant list

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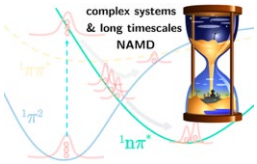
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Future directions in non-adiabatic dynamics: towards complex systems and long time scales

Location: ZCAM, Spain



Webpage : Event webpage

Dates: Sep 2, 2025 - Sep 5, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The goal of the meeting was to discuss current challenges associated with non-adiabatic dynamics simulations of complex systems, to identify the critical bottlenecks preventing the application of existing methods in these cases and to brainstorm possible solutions. Speakers were encouraged to present their work on challenging systems within the area of photochemistry, particularly highlighting problems for which they have not yet found satisfactory solutions. For example, one unsolved problem raised during the meeting was how to correctly simulate dynamics in the adiabatic basis for systems containing a dense manifold of states.

In order to provide structure to the meeting, the challenging aspects of these simulations were partitioned into four categories:

- Inclusion of environmental effects into non-adiabatic dynamics simulations.
- Description of the strong light-matter coupling regime.
- Treatment of multichromophoric systems.
- Extension of simulations to long time scales.

To aid discussion, all participants were split into 4 groups and were tasked with identifying the major problems related to their chosen topic. This involved trying to identify the limiting factors associated with current methodologies in tackling these scenarios. The groups discussed whether the issues were largely static (related to electronic structure calculations) or dynamic. On the dynamical side, discussion focused on comparison of problems faced by mixed quantum-classical and numerically-exact quantum dynamics techniques and on differentiating between difficulties in practical implementation and the need for new theories.

One theme that arose throughout the meeting was what constitutes the optimum balance between accuracy and practicality when simulating complex systems. On the topic of practicality, there was significant focus on how to improve the efficiency of numerically-exact quantum solvers for large systems, what constitutes a sufficient description of the environment, as well as the role of machine learning. We also discussed the level of accuracy to aim for in our simulations (quantitative reproduction of experiment vs qualitative trends), particularly given the lack of exact benchmark results to compare with for complex systems.

One aspect of complexity that naturally arose from the meeting which we did not preempt was the issue of complexity brought about by the experiment itself. In particular, the complexity involved in describing the correct preparation of the initial nonequilibrium state associated with photochemical experiments, as well as the correct reproduction of multiple probe-pulse signals. This arose from the conclusion that benchmarking in the field

of complex systems is perhaps best achieved via comparison with experiment (in contrast to the conclusions reached in the previous years CECAM benchmarking meeting focused on gas-phase photochemistry).

2. What were the primary outcomes of this workshop, including limitations and open questions?

The goal of this workshop was to identify limitations and open questions in the field of non-adiabatic dynamics simulations and, thus, these were the primary outcomes.

- Of the topics discussed, work on molecules in complex environments is developed furthest. Many talks at the workshop focused on the topic of molecules in various complex environments and presented successful applications of non-adiabatic dynamics simulations. While such applications are not yet routine, participants working in this field have expressed optimism that the field is reaching a more mature stage with ongoing work on refining the available workflows and method benchmarking.
- In the strong light-matter coupling regime there is considerable difficulty in modelling experiments where not all parameters are currently possible to fully control. Additionally, a better understanding of the role of triplet (and other multiplicity) states in the strong coupling regime is needed. While much work has focused on strong coupling between photons and electronic states, there remains an open avenue to explore strong coupling between photons and nuclear states.
- For the simulation of multichromophoric systems, a need for a progressive series of experiments with a controlled increase in complexity was highlighted and covalently-linked dimer systems were suggested as promising candidates. Such studies could be used as benchmarks for theorists to tackle in order to help method development.
- For simulations of processes which extend to long time-scales, the discussion centered on two problems, the problem of energy distribution across different modes in trajectory based calculations and the problem of deciding how and when to switch from the more accurate methods needed to describe the early stages of excited state processes (where non-adiabatic effects are very strong and the system is very far from equilibrium) to more approximate dynamics methods or to rate theories. While some possible solutions have been proposed for the former problem, they have not been sufficiently tested and widely adopted by the community, and this is an area where benchmarking efforts can be very helpful. Answers for the second question are less clear, a key difficulty here being the computational cost of calculations for long timescales which slow down research in this area. Hopefully, improvements to electronic structure calculations and methods to build accurate multi-dimensional model potentials will make future progress easier.

3. What was the take-home message for the participants?

One concrete take-home message that arose from the meeting was the need for experimentalists and theorists to work together in order to tackle the current challenges involving nonadiabatic effects in complex systems. In this regard, it was agreed that 'intermediate experiments' in which the complexity of the system is built up progressively in a controlled manner would be useful to help develop the required methods and fundamental theories.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

Nonadiabatic phenomena play a central role in many light-induced molecular processes with applications in molecular electronics, photovoltaics, sensing, and photopharmacology. Advancing these fields requires methods that can accurately describe photoinduced molecular dynamics well beyond the traditional focus on ultrafast small-molecule photochemistry in the gas phase. The workshop directly addressed this challenge by exploring how to incorporate key factors that are essential for real-world applications: the influence of molecular environments on light absorption, the impact of aggregation and energy transport in crystalline photoactive materials, the potential of hybrid light–matter states for functional use, and the importance of describing processes across multiple time scales. By identifying the limitations of current approaches to nonadiabatic dynamics and evaluating strategies for improvement, the workshop suggested improvements towards more realistic and predictive models. The foreseen progresses in the field will enable the rational design of advanced photoactive molecules and materials that can drive innovations in energy conversion, sustainable technologies, photobiology, and next-generation electronics.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The workshop built on the collaborative foundation laid by the Roadmap for Molecular Benchmarks in Nonadiabatic Dynamics [DOI: https://doi.org/10.1021/acs.jpca.5c02171], and helped shape ongoing efforts within the molecular benchmark's initiative. Discussions included potential extensions of the benchmark set to systems in solution and solid-state environments, with several promising candidates informally proposed. Additionally, new participants have joined the benchmarking Slack channel and are beginning to engage with different taskforces, especially the Photochem explorer one.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

We selected speakers with the aim of trying to ensure a close to 50:50 split between genders. However, due to several unforeseen cancellations by mainly female speakers close to the conference date, the gender ratio for both invited and contributed talks ended up being unfortunately 7:3 in favour of male speakers.
The conference was primarily attended by participants from a variety of European countries. We had one invited speaker from the United States and one contributed talk by a participant from Australia. Due to budget limitations, we were unable to cover travel expenses for any of the participants (although we did cover the hotel costs for two participants on request). If we had had the necessary funds to do so, this may have enabled better participation from low-income countries.
We did not receive any applications requiring accommodations for disabilities. Childcare was arranged on request for two participants.

7. Participant list

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The Dual Nature of Glycans in Protein-Protein Interactions: Bridging Computational and Experimental Insights



Location: CECAM-IT-SIMUL, Italy

Webpage : Event webpage

Dates: Sep 7, 2025 - Sep 10, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

Major topics discussed in our Cecam Event “The Dual Nature of Glycans in Protein-Protein Interactions” entailed:

- Polysaccharide Structures in Native Contexts at Various Scales. Presentations highlighted progress in deciphering the ultrastructural organization of polysaccharides in biological matrices. Integrated approaches – combining imaging, polymer physics, computation, and biosynthetic insights – demonstrated the importance of understanding spatial organization in cell walls and extracellular systems.
- Glycan Interactions and Biophysical Mechanisms. Talks focused on the determinants, energetics and potential impact of carbohydrate–carbohydrate and carbohydrate–protein interactions, using approaches such as polymer theory, atomistic simulations and machine-learning approaches.
- Quantitative and Computational Glycobiology. Exciting advances came from mass spectrometry, cryo-EM, AI-driven modeling, and molecular dynamics. In these approaches, the microheterogeneity of glycan decoration is starting to be decoded, while tools to resolve glycan ensembles and quantify their contributions to protein stability and signaling. Databases and modeling platforms such as GlycoShape and expansion of the Glycam environment exemplify the growing integration of computational resources into structural glycobiology.
- Glycans in Cancer and Immunology. Several contributions underscored the role of aberrant glycosylation in cancer progression, immune evasion, and therapeutic targeting. Described immunology approaches highlighted the clinical translation of glycobiology. Parallel studies explored sialylation and Siglec interactions in immunoregulation and pathogenic events. Core glycosylation was also linked to trafficking and function in neurotransmitters
- Post-Translational Modifications and Glycan-Mediated Regulation. Talks expanded beyond glycosylation to show how PTMs, including glycan attachment, reprogram proteins (e.g. chaperones become pathogenic scaffolds), or regulate responses to mechanic stimulations (e.g. lubricin in joint lubrication).

The event advanced the field by:

- Providing mechanistic insights into glycan-mediated recognition, signaling, and structural modulation across biological contexts.

- Introducing innovative methodologies, from single-molecule force spectroscopy and NMR to AI-enhanced modeling and Martini coarse-grained simulations.
- Demonstrating the therapeutic potential of glycans and glycan-binding molecules in antiviral, anticancer, and immunomodulatory strategies.
- Underscoring the importance of integrating different frameworks that bridge experimental precision with computational rigor, setting new standards for quantitative structural glycobiology.

Through this convergence of disciplines, the symposium underscored that glycans decorations should not be overlooked but rather considered as active regulators of biology.

2. What were the primary outcomes of this workshop, including limitations and open questions?

Primary Outcomes

- Combination and methodologies and emergence of the need for Integrative approaches: The workshop showcased the effective use of multimodal approaches (spectroscopy, imaging, polymer physics, computation, cell biology, immunological approaches) to study the role of glycoproteins and glycans in their native biological contexts. The possibility to simulate whole cells is also emerging, which would open up the possibility to study biomolecules in realistic conditions.
- Biophysical insights: Identified novel water-mediated glycan repulsion, “fuzzy” carbohydrate–carbohydrate interactions, and complex glycan–protein recognition mechanisms.
- Viral glycobiology: Clarified how SARS-CoV-2 spike glycosylation modulates dynamics and receptor binding; identified lectins and glycan mimics as promising antiviral/antibacterial strategies.
- Computational advances: Established frameworks combining glycoproteomics, AI-driven modeling, and coarse-grained simulations to resolve glycan ensembles and quantify their roles.
- Biomedical relevance: Presented evidence of aberrant glycosylation in cancer progression and immune modulation, with novel immunology-based strategies as possible therapies.
- Functional regulation: Showed glycans as active regulators of chaperone networks, mechano-responsive proteins, and synaptic receptor trafficking, expanding their recognized biological significance.
- Limitations
- Persistent challenges in capturing glycan (micro)heterogeneity and dynamics at physiological timescales.
- Data integration across experimental and computational modalities remains technically demanding.
- Model generalizability of biophysical interaction frameworks across different glycan families is limited.
- Translation of from molecular studies to novel drug design approaches poses problems of specificity, safety, and scalability.
- Computational methods constrained by force field accuracy, solvent representation, and validation against experimental benchmarks.

Open Questions

- How can multimodal data be systematically integrated to achieve confidence in models of glycan structure and function?
- To what extent are newly identified interaction principles conserved across species and glycan classes?
- What are the mechanistic links between glycan microheterogeneity and large-scale (realistic) biological outcomes?
- How can glycan-based therapeutic strategies be optimized to address viral evolution and tumor heterogeneity?
- What computational and experimental innovations are needed to bridge molecular-level insights with systems-level biology and clinical applications?
- How can improved computational power be efficaciously leveraged in the analysis of the complexity and diversity of glyco-systems?

3. What was the take-home message for the participants?

The take home message was that glycans are not merely passive decorations of proteins, but active regulators of biological function and recognition at different scales. Advances in integrative experimental and computational approaches enable novel insights into glycan structure, dynamics, and function. Significant challenges remain; to truly capture the 'Dual Nature' of glycans, the field must strengthen collaboration between experiment and theory and establish shared standards.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

The workshop outcomes have clear potential for societal benefits in medicine, biotechnology, and healthcare. Discussions generated new ideas for glycan-aware drug design, showing how glycosylation can improve predictions of drug efficacy and specificity. Insights into glycans in cancer highlighted strategies for detecting cancer types and addressing mechanisms of metastasis. Vaccine design was another focus, especially for (extensively discussed) viral glycoproteins and immune evasion.
A prominent theme was the need to unify standards in glycan modeling and data representation. Such efforts will directly support medical databases and AI models for structure prediction and drug design. The meeting also brought experimental and computational groups closer, encouraging new joint research with translational potential. It further raised the visibility of glycans as the "third pillar" of biology alongside DNA and proteins.
Long-term benefits include shared standards and better alignment of simulations with experiments, forming a foundation for precision medicine. The collaborations seeded here could enable digital twins of glycosylated systems, where accurate matching of force fields to experiments will be critical. Overall, the workshop set directions with direct relevance for diagnostics, therapeutics, and the integration of glycans into healthcare solutions.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

A round table discussion among participants highlighted the fundamental need for strong collaboration among experts in different fields. New possible collaborations between computational and experimental groups (beyond already existing ones) were established and talks are ongoing for common project submissions. The participants underlined that a follow-up of this meeting would be ideal (in 2/3 years). Round table discussion revealed several topics of broad interest:

- need to unify glycan data standards and to coordinate force-field/simulation development;
- accelerate analysis tools;
- enhance force-field interoperability and benchmarking (e.g., GLYCAM–CHARMM)*;
- define best practices for simulation design and for comparing models to sparse experiments;
- build ML-ready, metadata-rich PTM/glycan databases;
- create a parameter-sharing coalition (e.g., Martini 3).

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

We ensured inclusivity through broad geographical representation, with speakers from the US, Asia (Taiwan, Japan), and across Europe, including both Western (Portugal, Spain, France, UK, Ireland, Denmark, Germany, Italy) and Eastern Europe (Poland, Czech Republic). Outreach was conducted via LinkedIn, Twitter, Bluesky, and conference presentations to maximize reach. To avoid financial barriers, we provided travel and lodging support, which enabled at least four PIs to attend who otherwise could not. The venue was fully accessible, with taxis arranged for participants with mobility needs. We balanced career stages by inviting senior and junior PIs, as well as postdocs, and dedicated a poster session to postdocs and PhDs. Gender balance was also considered, with 14 women among 44 participants.

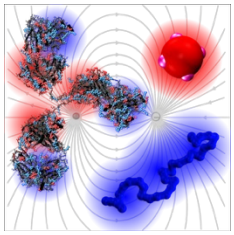
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Charged Soft Matter: Bridging Theory and Experiments



Location: CECAM-AT, Austria

Webpage : Event webpage

Dates: Sep 8, 2025 - Sep 12, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

Charged soft matter entails a broad variety of systems, sharing one common feature: they contain charged macromolecules or colloidal particles, typically few nanometers in size, accompanied by salt ions, other charged small molecules, and polar solvents. The relevant systems range from cellular membraneless organelles to protein solutions, bio-inspired or synthetic polymers, inverse patchy colloids or polymer-electrolytes found in modern battery systems. Although very different in nature, these systems share the same physics, predominantly controlled by interplay of electrostatic interactions and thermal fluctuations.
Unfortunately, most of the research in the field of charged soft matter is carried out in communities centered mainly around the target systems named above, allowing only limited exchange across these communities. This leads not only to differences in nomenclatures and concepts, but also to reinventions and rediscoveries of phenomena. The aim of this workshop was to provide an interdisciplinary platform for scientific exchange between these different communities investigating charged soft matter, underlining the shared aspects of the involved physics. The scientific contributions at the workshop presented the state of the art in various classes of materials, facilitating the transfer of knowledge between, establishing parallels between them and identifying shared aspects.
The main topics discussed were centered around the phenomena and mechanisms involved in charged soft matter:
(a) Liquid-liquid phase separation and coacervation
(b) Self-assembly, structure formation, supramolecular phenomena
(c) Dynamics, rheology, charge transport and non-equilibrium phenomena
(d) Structure and function of soft matter in nature and technology
(e) Interactions, charge regulation, responsive and programmable matter

2. What were the primary outcomes of this workshop, including limitations and open questions?

The primary outcome of the workshop was the establishment of new contacts between researchers from distinct fields, such as polymer science, biophysics, physical chemistry or molecular biology, and the transfer of knowledge between those fields.
Together, the community identified the main limitations as:
(a) different language used by various communities to describe the same phenomena
(b) focus on different details when interpreting the same observations, and attributing the same observations to different sources

The way to address these limitations is to cultivate the contact between the individual fields, and to enhance the overlap between them, which can be achieved, for example, by organizing more workshops or conferences.
More specific open questions formulated during the workshop include:
(a) Can we use liquid-state theories to describe the phase separation in protein solutions? Do the mean-field theories have quantitative or predictive power?
(b) How to experimentally characterize gels or condensates with rheology or microscopy across all of the relevant length scales and time scales?
(c) Is pH inside the gels and condensates the same as outside? Under what conditions?
(d) Is the notion of a phase and phase separation applicable for biomolecular aggregates, clusters or structures such as centrosomes?
(e) What level or resolution is needed to model condensates and polyelectrolytes computationally? Do we need explicit small ions or explicit solvent? Is the assumption of a uniform ionic strength and permittivity across the whole condensate phase a valid one?
(f) Can we use theoretical models and simulations to rationalize kinetics of polymerization of charged monomers?

3. What was the take-home message for the participants?

Communities from different backgrounds should communicate closely to exploit the existing complementary knowledge. Many recent experimental observations can be rationalized by existing theories. For other observations, the appropriate theories still need to be developed. Such communication can be successful and fruitful but requires initial effort and thinking out of the box from all participating parties. Bridging some of the above knowledge gaps should be feasible in the near future.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

One of the main goals of our workshop was to bridge theory with experiment and basic research with applied one. Many of the contributions have a direct industrial, medicinal or technological relevance. Interactions between the participants could improve the application capabilities, provide deeper fundamental understanding and potentially result in novel directions in materials research, with a couple of specific examples given below.
(a) Monoclonal antibodies are being used as a diagnostic sensor and also a therapeutic in cancer treatment. Our workshops helped to connect the experimental characterization platforms (Stradner, Schurtenberger) with the computational design (Pineda, Camerin, Blanco) of the antibodies, and also to establish parallels between antibodies and patchy colloids (Lund, Dhont, Sacana, van Oostrum).
(b) Misfolding and aggregation of charged proteins in condensates has been proposed as one of the key mechanisms in development of Alzheimer's disease or Parkinson's disease. Recent progress in experimental microfluidic characterization of relevant protein condensates (Ausserwöger) in connection with new rheological (Naghilou, Parisi) and calorimetric (Ballauff) methods could deepen our fundamental understanding of condensate aging and protein aggregation.
(c) Complex coacervation emerges as one of motifs in encapsulation of cells (Lacík), biocompatible hydrogels (Sedlačík) or generation of artificial tissues (Nader), all of them already being employed in the medical practice. Dedicated sessions of our workshops

proposed a theoretical framework for design of coacervates (Mittal, Motezakker) or electroadhesive gels (Nejedlá).
(d) Smart biomaterials based on DNA nanotechnology (Elezgaray), self-assembly (Voets) or on external driving by stimuli (Walther) all present a new paradigm in the material engineering, which could be guided by computer modelling (Larson, Schneider).

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

Most of the participants consented to recording of their talks and publishing them on the YouTube channel of the Erwin Schrödinger Institute [https://www.youtube.com/channel/UCUHyfvOFOuaUumnWaVrtfaQ] where they can be accessed by the scientific public. The workshop also provided ample opportunities for networking, and we are expecting several joint proposals and new collaborations emerging. As of now, one preprint https://doi.org/10.26434/chemrxiv-2025-dh46q has been published as a direct consequence of the discussions at the workshop.

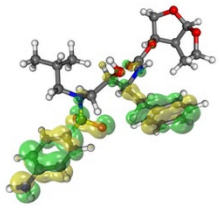
6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

We committed to promote inclusivity in career stage, geography and gender in the selection of the invitees and of the participants from the registration for the open scientific public. The preferences were continuously adjusted on the fly to balance the representation in all of the above categories. In the end, the workshop hosted 19 professors or senior scientists, 10 assistant professors or junior group leaders, 13 postdoctoral researchers, 16 doctoral candidates and 2 undergraduate students. We estimate the gender composition as 20 female and 40 male participants, with female participation of more than 33%, thereby exceeding the threshold of 20% requested by the Erwin Schrödinger Institute. The participants' institutions collectively reside over 19 countries across 3 continents (AT: 7, CY: 1, CZ: 7, FI: 3, FR: 3, DE: 9, GR: 1, IL: 2, IT: 2, NL: 3, NO: 1, PL: 3, RS: 1, SK: 1, SI: 3, SE: 5, CH: 1, GB: 3, US: 4).

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Quantum Chemistry for Drug Design: From Theory to Applications



Location: Prague, Czech Republic

Webpage : Event webpage

Dates: Sep 8, 2025 - Sep 10, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop covered a broad spectrum of topics at the forefront of quantum chemistry and its applications in drug design. In particular, significant attention was devoted to methodological advances that push the limits of current computational approaches. These included developments in semi-empirical quantum mechanical methods, empirical and Δ-machine learning (Δ-ML) corrections for them, and treatment of solvation. These efforts aim to increase the accuracy and transferability of semi-empirical approaches while retaining their computational efficiency, thus enabling their use in increasingly complex biomolecular systems.

Recent applications to protein–ligand scoring demonstrated the potential of such methods to outperform classical scoring functions and force-field and machine-learning approaches in well-defined benchmark datasets. However, their performance across free-energy perturbation (FEP) datasets remains more variable. Moreover, new studies have showcased how quantum chemical energy decomposition analyses can provide a detailed understanding of the electronic nature of protein–ligand interactions, offering mechanistic insights that complement traditional structure–activity relationship analyses. Semi-empirical quantum methods have also shown growing promise in refinement of experimental structures, particularly in X-ray crystallography and cryo-EM, where they help to improve local accuracy in electron density fitting.

In the area of machine-learning potentials (MLPs), work presented by R. Bryce and G. De Fabritiis demonstrated how these data-driven models can significantly accelerate free-energy simulations while maintaining near-quantum accuracy. K. Merz provided a perspective of future developments and current progress in the use of quantum computing for quantum chemistry, showing that one of the world's most powerful quantum computers can already be used for realistic electronic structure calculations.

Together, these developments illustrate the rapid convergence of physics-based, data-driven, and quantum-enabled methodologies, marking a tangible step forward in bringing quantum chemistry closer to practical drug discovery applications.

2. What were the primary outcomes of this workshop, including limitations and open questions?

The workshop demonstrated that quantum chemistry (QC), particularly semiempirical (SQM) methods, is becoming a practical tool for computer-aided drug design (CADD). Further developments, such as empirical and machine-learning corrections and improved implicit solvent models, can increase both accuracy and robustness while keeping computational costs low. Applications showed that SQM-based scoring can reproduce

binding affinity trends and assist in X-ray and cryo-EM structure refinement, offering a balance between speed and accuracy. Still, participants emphasized the need for broader benchmarking on diverse and high-quality datasets, as performance can vary across targets and conditions. Discussions highlighted the remaining limitations of SQM approaches, including treatment of solvation, sampling, and transferability to flexible or unconventional systems. Addressing these challenges will be key to their wider adoption in drug discovery workflows.

Another major topic concerned machine-learning potentials (MLPs), which bridge classical and quantum approaches. MLPs can significantly accelerate free-energy and energy decomposition calculations, but their transferability and dependence on training data remain open issues. More systematic validation and standardized benchmarks are needed to assess their impact in realistic pharmaceutical contexts.

The workshop also explored quantum computing as a rapidly developing frontier for electronic-structure calculations. Although practical drug-design applications are still years away, hybrid classical–quantum workflows were seen as promising first steps. Continued testing and community training will be crucial to leverage quantum hardware as it matures.

In summary, the meeting emphasized the convergence of quantum chemistry, ML, and quantum computing toward practical, data-driven molecular modeling. Key outcomes include recognition of the maturity of SQM methods for real-world problems, the need for continued benchmarking and collaboration, and shared optimism about the transformative potential of next-generation QC technologies in drug discovery.

3. What was the take-home message for the participants?

The workshop highlighted the readiness of QM, mainly modern semiempirical (SQM) methods, for real-world drug design and the growing maturity of machine-learning potentials bridging QM and MM accuracy. Participants agreed that combining data-driven models with QM will define the next phase of predictive modeling. A key takeaway was also that progress depends on understanding the limitations of experimental data and models to set realistic expectations for binding affinity predictions.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

Computer-aided drug design (CADD) accelerates the discovery of new medicines and reduces costs by prioritizing compounds with higher chances of success. Its societal impact has been demonstrated in global health crises, such as HIV and COVID-19, where computational approaches guided the identification of promising therapeutics.

Recent advances in semiempirical quantum scoring (SQM), machine-learning (ML) potentials, and AI-based structure generation are enhancing the reliability and efficiency of rational drug design. These methods can guide compound selection, predict binding to protein targets, and refine molecular interactions, shortening the iterative cycle of design, synthesis, and testing. Validated SQM scoring functions already deliver reliable results for protein–ligand interactions and structural refinement, while ML approaches increasingly approach quantum-level accuracy at near-classical speed, enabling larger and more complex screening campaigns. Discussions on quantum computing highlighted its potential for long-term societal benefits. Hybrid classical–quantum workflows may tackle

computationally demanding steps in electronic-structure calculations, supporting the design of novel drugs and therapies that are currently intractable.
The workshop also fostered collaborations between academia and industry, encouraged early-career researchers, and engaged a wider scientific community. These interactions strengthen the talent pipeline and accelerate the translation of computational discoveries into real-world applications.
Overall, integrating QM, SQM, ML, and AI in CADD holds significant potential to improve healthcare by reducing the time and cost of drug development, enabling faster responses to emerging diseases, and increasing the likelihood of identifying effective therapeutics.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The workshop produced tangible outcomes by encouraging participants to present their research openly and engage in follow-up discussions, thereby fostering knowledge exchange. It strengthened connections between academic and industrial experts in quantum chemistry, machine learning (ML), and molecular dynamics (MD), creating high potential for new collaborations. Several tools, including SQM/ML scoring methods and machine learning potentials, are being tested and validated by multiple groups, which enables the rapid cross-fertilization of methods. Discussions also explored possibilities of joint publications, collaborative benchmarking, and future proposals. Attendees widely appreciated the CECAM workshop format, which combined lectures, discussions, and networking to stimulate active exchange and provide a clear roadmap for advancing computational drug design.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The workshop promoted inclusivity across gender, career stage, and geography. Of the five organizers, one was a woman. Of the 21 invited speakers, several were women. However, five female speakers later canceled, leaving 16 invited speakers. Of the participants who applied, all six women were accepted, though two later declined. Most attendees were from Europe, and four were from the U.S. There were no valid applications from Asia and Africa. The speakers and participants represented a balanced mix of academia and industry. To highlight early-career researchers, the poster session was replaced with short contributed talks, which allowed all Ph.D. and master's students to present their work. Other students joined as attendees.

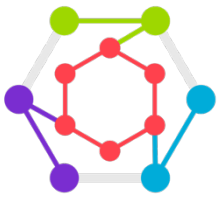
7. Participant list

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Open Databases Integration for Materials Design



Location: Vilnius University, Lithuania

Webpage : Event webpage

Dates: Sep 15, 2025 - Sep 19, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

Current OPTIMADE standard state

OPTIMADE (https://optimade.org) is a standard for data exchange between computational and experimental materials science databases (Andersen et al., 2021, https://doi.org/10.1038/s41597-021-00974-z; Evans et al., 2024, https://doi.org/10.1039/d4dd00039k). Prior to the workshop, OPTIMADE described endpoints for structures and standardised a mechanism to describe both standard-wide and database-specific properties in a uniform machine-readable way.

Outstanding problems

The most promising new design was the means to represent trajectories, which describe full outcomes of biomolecule and materials science simulations. Since trajectories usually contain orders of magnitude more data than a single structure solution of computation would yield and thus delivering the whole trajectory in a single server response would be impractical or even impossible, new challenges arose to provide mechanisms for efficient partial data requests and partial data downloads.

In crystallography, the challenge was to faithfully describe the data that a crystallographic experiment typically provides – fractional atom site coordinates and crystal symmetry description. Such additional information would allow databases to return crystallographic data as it is determined by crystallographic software and stored in such databases, without converting them (in a potentially lossy way) to the OPTIMADE 1.2 standard.

When it comes to crystallographic data of small organic molecules, molecular connectivity becomes important for both search and data presentation. Thus, chemical descriptors, such as SMILES of InChI, had to be standardised as OPTIMADE data types.

We also have a need to present material physical and chemical properties, whether computed or measured in an experiment. In the version of OPTIMADE up to 1.2, such computation or measurement outcomes would be presented as additional JSON response (OPTIMADE) properties in the '/structures' endpoint. This approach would become cumbersome when multiple properties from unrelated experiments or computations would need to be presented and would result in a constant update of the '/structures' endpoint entries. Thus, a new approach had to be discussed and standardised, where a dedicated endpoint would be standardised for such materials property results.

Looking into the future, a discussion on how to represent computations and workflows appeared to be necessary.

2. What were the primary outcomes of this workshop, including limitations and open questions?

The most prominent outcome of the current workshop was that finalisation of the trajectory definitions and the '/trajectories' endpoint. Two pull requests: #481 'JPBergsma/property_ranges' and #377 'JPBergsma_add_Trajectories' were incorporated into the OPTIMADE standard. First of all, a flexible possibility was described that allows clients to request only a part of large property (e.g. only atomic coordinates from specific frames in a trajectory). The second feature is a partial data transfer protocol, a mechanism that allows an OPTIMADE server to transfer large amounts of data by dividing the response into small fragments and informing the client where and how these fragments can be downloaded, in a standard format.
Definitions of new properties required the ability to define new, custom data types. Such a mechanism was introduced in PR #560. This mechanism opened up the possibility of defining new properties, such as chemical SMILES, that cannot be usefully expressed using the pre-existing standard OPTIMADE types.
The new extension of the OPTIMADE introduced standard properties to describe fractional coordinates and crystal symmetry. To make new definitions fully compatible with the previous OPTIMADE data presentation (versions 1.0 – 1.2), a new data item 'site_coordinate_span' was introduced that would explicitly state what extent of a crystal structure is provided in the response. Such a specification is deemed to be an improvement over both previous OPTIMADE versions (up to 1.2) where only one (the full unit cell) representation was possible and over the CIF framework (Bernstein, 2016) where the coordinate span is not specified formally and is left as an application-level agreement, thus limiting interoperability. The human-readable description of these specifications was merged during the pre-workshop preparation activities (PR #539), and the machine-readable property definitions were elaborated during the workshop (PRs #557, #569).
The PR #465 addresses the needs for 'bonds' property that is applicable for all organic molecules, and the PRs #400 and #396 are suggesting data representation for biomolecules. The custom data types enabled in full by the PR #560 will allow chemistry-specific data types to be defined, for example, chemical line representation like SMILES or InChI.

3. What was the take-home message for the participants?

New features of OPTIMADE were standardised in both human-readable and formal computer readable presentation, extending OPTIMADE applicability to fields of science like bioinformatics, chemoinformatics and chemical crystallography. Preparations for the release of the new OPTIMADE standard minor version were made, and the new version will be released shortly after the workshop (withing two-tree months).

4. Does the outcome(s) of the workshop hold potential for societal benefits?

OPTIMADE served well the needs of materials science community, as exemplified by the growing number of citations of the seminal OPTIMADE paper and growing number of

database implementations. By providing means to combine data from different sources through standardised queries, OPTIMADE contributes to the development of energy materials, hydrogen storage and carbon-capture frameworks, the development of new semiconductors and catalysts. Large amount of data available through OPTIMADE makes it especially useful for modern methods in machine learning.
Additions made in this workshop – ability of OPTIMADE to express data on biomolecule trajectories, organic molecules and, in the future, biomolecules – will make OPTIMADE applications areas even wider, enabling discoveries in biomedical and life science research through the aggregation of large amounts of standardised data. We thus expect a further increase of OPTIMADE's positive influence on our society.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

Standard development
During the OPTIMADE 2025 workshop in Vilnius several problems, such as trajectory or fractional coordinate definitions, were finalised to the point of merging their definitions into the standard draft. During the preparation for the workshop, the workshop itself and immediately after 131 commits to the 'develop' branch were made [1]; 61 were performed during the meeting time in Vilnius [2]. 13 outstanding pull requests merged into the 'develop' branch during that period.
Publication
During the workshop, the participants agreed to summarise the new features of the OPTIMADE standard in an upcoming publication. The manuscript draft was prepared and hosted on the Overleaf platform. Manuscript text should be finished and submitted for publication in the months following the OPTIMADE 2025 workshop.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The workshop organisers put explicit efforts to treat all candidates fairly, on an equal footing, to avoid any explicit or implicit discrimination based of traits not relevant to the subject matter. In fact, discrimination based on these factors is prohibited by Lithuanian law: Article 29(2) of Lithuanian Constitution enumerates prohibited grounds of discrimination: sex, race, nationality, language, origin, social status, belief, convictions, or views; these constitutional provisions are implemented in the national EOAWM and EOA laws (Davulis 2023, https://doi.org/10.2838/995901). To ensure fair treatment of all candidates, the organisers discussed and agreed upon the selection criteria for the workshop, based on the requirements of efficient event. Candidates were expected to provide concise but informative motivation and background letter. All candidates were informed about possible reimbursement. The ones who could not participate on site were admitted as online participants.

7. Participant list

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Dynamics of Non-Equilibrium Variables: Multiscale-multiphysics applications of fluctuating hydrodynamics



Location: Universidad de Zaragoza, Spain

Webpage : Event webpage

Dates: Sep 15, 2025 - Sep 19, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The main goal of the first DoNEV meeting has been gathering and feeding the scientific seeds of Aleksandar Donev on a variety of problems collected in the acronym “Dynamics of Non-Equilibrium Variables: Multiscale–Multiphysics Applications of Fluctuating Hydrodynamics”. In order to set a common route to the many students present in the workshop, we structured it in two parts, starting with tutorials and hands-on sessions (Days 1-2) followed by research talks (Days 3-5). Foundational courses established the theoretical framework of coarse-graining, stochastic PDEs, and hydrodynamics, ensuring a common understanding among all participants. Numerical methods and software were also addressed, introducing immersed boundary and Brownian hydrodynamics methods, emphasizing good software engineering practices, and providing hands-on training with LAMMPS and UAMMD-structured. These contributions helped disseminate open computational tools across the community. A complementary theoretical track focused on statistical frameworks for non-equilibrium systems. Discussing the Doi-Peliti formalism, the generalized Langevin equations via projection operators, and the Green-Kubo plateau problem.

The research talks (Days 3–5) connected theories to current applications. The bulk of these presentations applied the frameworks to soft matter, colloids, biological systems, and multiphysics couplings. Highlights included studies of Brownian motion near soft interfaces, hydrodynamic fluctuations in sedimenting colloids, phoretic suspensions, and oscillating soft structures; explorations of semi-flexible membranes, vesicle mechanics, cilia dynamics, and collective micro-swimmer flows; and multiphysics extensions covering diffusiophoresis, fluctuating electromagnetic fields, boiling and cavitation, and optical trapping and assembly. Beyond soft matter, El Niño dynamics were discussed, underlining the broad impact of fluctuating hydrodynamics.

Finally, poster sessions, flash talks, and informal discussions enhanced the participation of early-career researchers and fostered interdisciplinary connections. Overall, the workshop clarified the conceptual foundations of fluctuating hydrodynamics, promoted new computational strategies for handling noise in multiphysics systems, highlighted open questions in memory effects and non-Markovian dynamics, and provided training that strengthened reproducible research practices across the community.

2. What were the primary outcomes of this workshop, including limitations and open questions?

The primary outcome of the First DoNEV meeting was to consolidate and (importantly) enlarge a very active community which has been working and developing a series of compatible techniques for complex fluids at the mesoscale. These techniques include fluctuating hydrodynamics and immersed boundary methods but extend to many different physical systems: non-equilibrium thermodynamics, active matter, colloidal rheology, interfaces, immiscible fluids, magnetic and dielectric nanoparticles, light-matter interaction, and more. The mesoscopic domain formally connects with atomistic descriptions and importantly, we provided a connection with MD (Simon Gravelle, LAMMPS). This meso-micro connection is indeed another foundational pillar of the workshop (projection operators, Green Kubo relations, etc). In summary, the common main topics treated in the DoNEV meeting were:
Advancement of theoretical frameworks: reinforced understanding of coarse-graining, fluctuating hydrodynamics, stochastic PDEs, and projection-operator techniques → provided participants with unified frameworks for modeling non-equilibrium systems across scales
Dissemination of high performance, open-source computational tools.
Connection with experiments.
Overall, the main project outcome has been to build a scientific community by fostering discussions and collaborations across theory, computation, and applications, will potentially inspire new project ideas.

3. What was the take-home message for the participants?

The 1st DoNEV workshop united three generations of scientists around theories by Stokes, Onsager, Landau, and others. It built a global network linking senior and early-career researchers, promoting open-source tools, hands-on training, and reproducible research. The community integrates advanced math into fast computational frameworks, emphasizing that multiscale methods must fit each problem and connect closely with experiments and atomistic effects.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

The community that these workshops intend to gather has also a strong applied vector. In particular, it connects fundamental theories, with high-performance computational schemes which can quantitatively reproduce experiments at the mesoscale (nanometer scales up). Many research lines of the community are targeting applied problems on rheology, biomolecules, combustion, biosensing, climate, and science education, to name a few. In this sense, the workshop community truly connects with societal benefits. Indeed, the expertise of this community is being used in many applied international projects with direct connection with societal problems. Yet, the forum created by the DoNEV meetings focuses on the hard-core of the scientific research, going into finely tuned details. Details are essential to connect with first principles, which are essential to generate accurate models connecting with experiments. Some of the details tackled by the works concerned,

- Improved fluctuating hydrodynamics: extension to the microscale.
- Improving micro- and nano-fluidic devices for medical and laboratory applications.

- Enhancing design of materials, polymers, and responsive industrial processes.
- Advances in targeted therapies, micro-robotics, and biomedical engineering solutions.
- Better understanding and prediction of climate and environmental phenomena.
- Good software practices to encourage the dissemination of open-source tools. This approach promotes reproducibility, collaboration, and wider adoption across the scientific community.

Finally, we would like to stress the strong commitment of DoNEV workshops on connecting humans by science, beyond races, continents and any other type of affiliation. We believe this simple goal has a fundamental societal root which needs to be highlighted in these times.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

We have established several links to gather the community on the web (from email list to a stalk page and even a WhatsApp group). There have been many connections established among different experimental and theoretical groups which we expect to flourish in a recent future, leading to collaborations in the form of publications, open-source software developments and probably joint projects. Moreover, a special issue will be published in the Journal of Chemical Physics, in memory of Aleks Donev. Most of the talks of the present workshop will be published in that forthcoming issue

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

We ensured participants came from diverse geographical regions and research institutions worldwide, spanning 11 countries across 4 continents. We ensured gender equality amongst the invited speakers, women represented about half of the participants. However, it should be stated that gender equality arose naturally and did not compromise the scientific quality of the workshop. On the contrary, female scientists are thriving in our research community, both in experiments and in theory/simulation. Early-career researchers were encouraged to present through flash talks, posters, and hands-on seminars. New generations of scientists should lead the connection between the good-old theories and the novel computational paradigms. Feedback between generations is nowadays essential.

As any other collective human activity, science resonates with friendship. We hope this principle will guide future DoNEV meetings, which are already being discussed.

7. Participant list

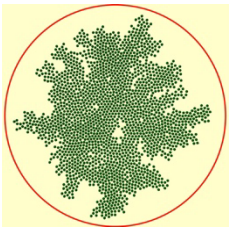
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Statistical physics of living systems



Location: CECAM-HQ-EPFL, Switzerland

Webpage : Event webpage

Dates: Sep 16, 2025 - Sep 19, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop "Statistical physics of living systems" convened experts to discuss the complex non-equilibrium dynamics of living materials, such as confluent monolayers and bacterial colonies. A major focal point was the exploration of collective behaviors emerging from local interactions (mechanical, biochemical, and social) and self-propulsion, which lead to non-equilibrium phase transitions like unjamming, flocking, and directed motion. Discussions significantly advanced the state of the art by integrating new paradigms on collective motion, such as traveling waves driven by non-reciprocal interactions, and applying the machinery of disordered systems to dense active matter. Another critical topic was the application of sophisticated statistical thermodynamics tools, i.e., specifically entropy production and thermodynamic uncertainty relations, to living organisms. Participants explored how these tools can measure the breaking of time-reversal symmetry across different length scales and quantify irreversibility in stochastic Langevin systems. Additionally, the event addressed the manipulation of active materials using external fields to control density fluctuations, and how optimal control techniques can parse the competition between thermal and non-equilibrium fluctuations. Presentations also covered topological defects in active and living matter, exploring their role in tissue organization and active nematic elastomers. By bringing together theoretical, computational, and experimental physicists, the workshop consolidated our understanding of non-equilibrium collective behavior and fostered a collaborative environment to tackle the next generation of challenges in soft living matter.

2. What were the primary outcomes of this workshop, including limitations and open questions?

A primary outcome of the workshop was the successful cross-pollination of ideas between theoretical, computational, and experimental researchers studying non-equilibrium statistical mechanics. The event established new collaborative frameworks for understanding collective behavior in living systems, particularly concerning the thermodynamics of active matter and the mechanics of dense cellular assemblies. For instance, participants presented novel model-free estimates for quantifying irreversibility and entropy production from single-molecule displacements, bridging abstract thermodynamic concepts with concrete biophysical experiments. However, several limitations and open questions were prominently identified. A significant open challenge discussed was the calculation of entropy production rates in systems where certain degrees of freedom remain hidden or unobservable, complicating the distinction between forward and backward trajectories in active particles. Furthermore, the workshop

highlighted limitations in current universal theories; for example, evidence was presented demonstrating the non-universality of jamming transitions in cellular monolayers. Studies combining Particle Image Velocimetry and Differential Dynamic Microscopy revealed that different cell lines evolve toward arrest through distinct dynamical pathways, challenging the assumption that jamming is a universal process governed by a single set of physical principles and underscoring the need for cell-type-specific frameworks. Additionally, the mechanistic description of mechano-chemical couplings in active solids remains an open frontier, as current phenomenological models cannot fully resolve the cross-talk between mechanical response and dissipation. Resolving these discrepancies and extending kinetic theories to generalized dynamics with non-reciprocal interactions remain key objectives for the community moving forward.

3. What was the take-home message for the participants?

The take-home message is that understanding living materials requires a highly interdisciplinary approach, integrating advanced statistical thermodynamics, active matter physics, and experimental biophysics. Moving beyond universal models, researchers must rigorously address cell-specific dynamics, non-reciprocal interactions, and hidden degrees of freedom to accurately capture the structural and dynamical properties of non-equilibrium biological systems.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

Yes, the outcomes of the workshop hold substantial potential for broader societal and technological benefits. By advancing our understanding of collective cell movements and tissue dynamics, the research discussed has direct implications for developmental biology and medicine, particularly in understanding wound healing, embryonic development, and the progression of diseases such as cancer metastasis. For instance, computational models of active living matter can generate testable predictions for how tissues undergo rigidity transitions during these critical biological processes. In addition to medical applications, the theoretical insights into active systems offer pathways for developing innovative bio-inspired materials and robotic swarm technologies. By understanding how confinement and social cohesion shape collective motion in animal groups, engineers can design better bio-inspired coordination strategies for distributed systems and robotics. Finally, the study of non-equilibrium forces and information engines can optimize work extraction at the microscopic level, potentially leading to the development of highly efficient, autonomous micro-scale devices and synthetic active materials.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The workshop facilitated a collaborative environment designed to define new challenges and spark joint efforts among theoretical, computational, and experimental physicists. Tangible outcomes include the dissemination and rigorous discussion of several recent preprints and ongoing research manuscripts (e.g., works on thermodynamically consistent

active solids, optimal work extraction, and self-sustained frictional cooling), which are currently being prepared for high-impact publications. The interdisciplinary nature of the event naturally laid the groundwork for new cross-border collaborations, particularly linking phenomenological modeling with experimental data from single-molecule tracking and microfluidic tissue models.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

To promote inclusivity, the organizing committee was diverse, and we actively ensured a balanced representation of speakers and participants across genders, geographical locations, and career stages. The program featured numerous female invited speakers and researchers, including both prominent experts and early-career scientists. Geographically, the event hosted participants from institutions across Europe, the Americas, and Asia. Crucially, we implemented a hybrid format, allowing researchers from countries like India, Iran, Turkey, and Jordan to participate online, effectively breaking down financial and geographical barriers. Furthermore, we blended senior keynote speakers with early-career researchers (PhD students and postdocs) who were given platforms to present their work through dedicated poster sessions, fostering mentorship and equal scientific exchange.

7. Participant list

Organisers
Garcia Millan, Rosalba
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Fahmawi, Safa - Jawaharlal Nehru University, Jordan
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Komura, Shigeyuki - University of Chinese Academy of Sciences, China
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Yadav, Pradeep Kumar - University of Barcelona, Spain
Zheng, Mingyuan - HKUST(GZ), China

Atomistic Monte Carlo Simulations of Bio-molecular Systems

Location: Jülich Supercompting Centre, Germany

Webpage : Event webpage

Dates: Sep 22, 2025 - Sep 26, 2025

1. What were the major topics presented in the School?

The school started with a beginner level introduction to the theory of modern Monte Carlo (MC) methods, given by guest lecturer Prof. Anders Irbäck from Lund University, Sweden. Through alternating theory and hands-on sessions, the participants consolidated their understanding of MC techniques and their application to biological macro-molecules. The tutorial examples included unbiased protein folding simulations starting from random initial states, using techniques ranging from plain Metropolis-Hastings Markov Chain Monte Carlo, through multi-temperature tempering techniques like simulated and parallel tempering, to modified ensemble techniques such as Multicanonical and Wang-Landau techniques. The participants learned to set up their own protein folding simulations using different MC algorithms implemented in the software package ProFASi and ran them on the JSC cluster JUSUF. ProFASi is an open-source project actively developed by the organizers from the Simulation and Data Laboratory Biology at JSC. Guest lecturer, Prof. Stefan Wallin from Memorial University, Canada, demonstrated how the modular nature of the software allows it to be extended and deployed for scientific research on MC techniques and their application, beyond the research interests of the primary developers.

2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

In addition to setting up and executing prepared exercises for the tutorial, the participants were given an opportunity to present their current research work using poster presentations or short oral presentations. The objective was to help them see MC as another tool in the repertoire. By means of intensive discussions with experienced MC researchers, the participants generated exciting new ideas regarding the application of MC techniques in their own research domains. These include concrete ideas on the analysis of experiments involving the unaggregated Alzheimer's Abeta peptide, and the creation of a possible new coarse-grained model for membrane proteins. A number of smaller questions regarding the MC techniques were also raised, such as how to estimate sampling errors, how to perform parallel computations with a technique which seems sequential at the core, and how MC and molecular dynamics techniques may be combined to examine different aspects of a molecular system.

3. What was the take-home message for the participants?

The Monte Carlo technique is extremely simple at its core, but very powerful because of its adaptability.

4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

The participants received the lecture notes and the series of prepared exercises demonstrating various Monte Carlo techniques. The organizers hope that the enthusiastic discussions and the generated ideas will be translated by the participants into concrete attempts at using MC techniques in production quality research in their own areas.

5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The tutorial was attended by participants from 8 countries, a third of which were women. Since the stated topic of the tutorial was biomolecules and stochastic sampling techniques, the organizers did not entertain any limitations based on gender or geographical provenance of probable participants, as long as they could attend this on-site event. The organizers did, however, promote the tutorial as an opportunity for early career researchers, Masters students or doctoral candidates, to learn about and try a new technique in computational research, suitable as a flexible, extensible alternative to molecular dynamics simulations.

6. Participant list

Organisers
Meinke, Jan
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Forschungszentrum Jülich, Germany
Zimmermann, Olav
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Cristea, Artur - Romanian Academy, Romania
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Gomila, Alexandre - IBEC, Spain
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Liberati, Diego - National Research Council of Italy, Italy
Natale, Federico - Forschungszentrum Jülich, Germany
Salvadori, Giacomo - Forschungszentrum Jülich, Germany
Sanchez, Jose - ENEB, Spain
Thurecht, Lion - Forschungszentrum Jülich, Germany

Torielli, Luca - Forschungszentrum Jülich and RWTH Aachen University, Germany
Wallin, Stefan - Memorial University of Newfoundland, Canada

Generative AI and large language models for protein modeling across sequence-structure-function scales : From predicting protein dynamics to programmable biology and drug design

Location: USI Lugano, Switzerland



Webpage : Event webpage

Dates: Sep 24, 2025 - Sep 26, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop focused on integrating generative AI and large language models (LLMs) with biophysics to model complex biological phenomena. A central theme was the emergence of foundational models like **ESM3**, which bridges protein sequence, structure, and function within a single framework. Discussions advanced the state of the art by highlighting the transition from traditional structure prediction to "programmable biology," where AI designs functional proteins de novo for medicine and clean energy. A significant debate centered on whether biology can be solved using sequences alone or if physics-based simulations remain essential. The consensus leaned toward a hybrid paradigm, where deep neural networks are combined with physical simulations to reach atomic-level accuracy for multi-domain targets and intrinsically disordered proteins (IDPs).

2. What were the primary outcomes of this workshop, including limitations and open questions?

Integrated AI-automation pipelines demonstrated a 10-100x speedup in exploring biosystems design space, transforming the timescales of synthetic biology.
The introduction of frameworks like Ligand-Transformer and AiPP enables the identification of modulators for previously undruggable targets, such as disordered disease proteins and the "hidden" ligandable proteome.
Tools like bAIes and D-I-TASSER successfully integrated AlphaFold predictions with molecular mechanics to generate accurate atomic-resolution ensembles for IDPs and large multi-domain proteins, outperforming standard AI models.
Despite these advances, participants identified critical limitations. Modeling highly variable regions, such as the CDR-H3 loop, remains a challenge. Most current models focus on proteins in isolation. During the round table discussion some argued that sequence-trained AI captures all essential information. However, the consensus that emerged from the discussion is that the most useful insights are obtained by combining AI with physics-based models. The latter are crucial to predict rare events and allosteric regulation.

3. What was the take-home message for the participants?

The future of biological discovery lies in the synergy between generative AI and physical simulations. While LLMs like ESM3 revolutionize sequence-to-function mapping, the most robust outcomes in drug design and programmable bioengineering are achieved by grounding deep learning in the fundamental laws of physics and the complexities of the cellular environment.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

The workshop's outcomes hold transformative potential for society:
Medicine: Accelerated drug discovery for "undruggable" targets like the Alzheimer's Aβ peptide could lead to novel treatments for neurodegenerative diseases and cancer.
Human Genetics: Frameworks like MAVISp, which annotates millions of genetic variants, will enhance our ability to interpret disease-linked variations and move toward personalized medicine.
Sustainability: Programmable biology applications, such as the de novo design of proteins for bioremediation and clean energy, provide essential tools for addressing environmental crises.
Synthetic Biology: The design of precise CRISPR enzymes and transcription factors offers new pathways for treating infertility and advanced genome editing.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

Software, databases and models, including the MAVISp database (6 million variants) ; the AiPP platform ; D-I-TASSER for hybrid structure prediction; the bAles framework for IDPs; PepMLM and PepPrCLIP for peptide design ; Ligand-Transformer for protein-ligand interactions as well as HADDOCK integration with AlphaFlow have or will benefit from the discussions and new collaborations established during the workshop.
Publications: numerous new papers from the participants (e.g., Sánchez-Marin et al. 2025; Schnapka et al. 2025; Calvanese et al. 2025) indicate tangible academic output.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The workshop took concrete steps to promote inclusivity:
Gender and Diversity: The organizers prioritized a balanced speaker list, featuring prominent female scientists like Ivet Bahar, Elena Papaleo, Zoe Cournia, Alessandra Carbone, Jana Shen, and Christine Orengo. A specific objective was to address gender inequality and promote the participation of minorities.
Geographical Provenance: Speakers were invited from institutions across the US, Singapore, UK, France, Germany, Spain, Greece, Canada, Switzerland, and the Netherlands, fostering a global strategic view.

Career Stage: Dedicated poster sessions and contributed talks provided students and early-career researchers (ECRs) with direct opportunities to engage with more experienced researchers and build professional networks.

7. Participant list

Organisers
Gervasio, Francesco Luigi
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Sgrignani, Jacopo - Institute for Research In Biomedicine, Switzerland
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Weigt, Martin - Sorbonne Université, France
Zhang, Yang - National University of Singapore, Singapore
Zou, James - Stanford University, United States

International Symposium 2025 Molecular modeling in soil science – achievements and perspectives



Location: CECAM-AT, Austria

Webpage : Event webpage

Dates: Sep 24, 2025 - Sep 26, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop gave an in-depth overview of the current state of computational modeling in soil sciences. Reports were given on the modeling and description of soil minerals, soil organic matter and related substances. An important topic was also the interaction of organic matter and contaminants with reactive mineral surfaces, a topic of paramount importance for climate change mitigation and pollutant behavior. Different levels of theory (quantum mechanical descriptions, atomistic and coarse grained force fields, mesoscopic modeling) were discussed, leading to a frequent discussion on the suitability of particular methods for particular aims. Advances with respect to similar meetings in 2005 and 2009 were commemorated, establishing a clear view on the progress that was made, but also keeping an eye on the challenges that remain to describe soils and soil components and their heterogeneity computationally. Moreover, some contributions dedicated to analysis of soils at microscopic level using spectroscopic techniques, the interactions of pollutants with soils and chronosequence perspectives at major scales set the stage of current challenges in soil science and how computational modeling can fill the existing gaps in the field.

Particularly striking was recurrent discussion on the use of model substances to describe both minerals and soil organic matter. Many models described in the literature do not reflect the expected heterogeneity of real soils, but more or less appropriate models have been described. Experimental and computational results on the interactions between minerals and organic molecules were discussed as well, leading to further insights into the best way to describe these highly complex systems.

A constructive exchange between all key players in the field of modeling in soil science took place. Critical questions were formulated and new ideas for future research and improvements of the methodologies or research questions have been formed.

2. What were the primary outcomes of this workshop, including limitations and open questions?

The workshop consisted of 5 keynote presentations, and 19 additional contributed presentations about the topics described above. Sessions focused on :

- Advances of MM methods in soil science
- Soil minerals
- Fate of contaminants in soils

- Soil organic matter
- Interactions of minerals and SOM

A key limitation that was once more identified in this workshop is ill-defined chemical composition of many soil components, the relevance of immensely different spatial scales (from nanometer to kilometer) as well as temporal scales (from picoseconds to millions of years). Agreement was achieved that model systems at nanoscopic scales can give insights that are relevant at the macroscopic scale, but an awareness of these limitations should always be included, not to oversell any computational results.
Some other limitations, which are more related to the intrinsic nature of the soil, such as the structural definition of organic matter, enzymatic activity and protection mechanisms require a joint interdisciplinary effort between modeling and soil scientific communities to come up with new strategies to answer the questions from both sides to complement each other gaps.
The community of molecular modelers in the soil sciences is relatively small, and a large portion of the relevant global players were represented at the workshop. The main outcome of the workshop could therefore be described as

- A current view on the developments in the field since previous meetings in 2005 and 2009
- A clear view on the current state-of-the-art in 2025
- An awareness of the possibilities and challenges in modeling soils
- A need to maintain strong interactions within this small community, e.g. by organizing more regular meetings, best practices publications, etc.

3. What was the take-home message for the participants?

While tremendous progress has been made in the last two decades, the molecular modeling of soils and soil components remains challenging. However, the relevance in the soil sciences is finally being recognized as the field offers insights at a level that is hardly attainable experimentally. The multidisciplinary character of the field requires an understanding at a large range of spatial and temporal scales. Collaborations between groups have proved to result in the best outcomes.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

The workshops discussed computational methods to describe soils and soil components. A better understanding of these aspects plays a role in agricultural and environmental considerations. Presentations linking models to understand e.g. the pollution levels in urban gardening projects and or the fate of nuclear waste, when in contact with soil are examples where this relevance was particularly clear. Further examples directing towards societal benefits are the investigation of binding and mobility of phosphor species relevant both for the development and the application of fertilizers as well as understanding the interaction of contaminants with soil constituents on the molecular level, which can help in the risk assessment of chemicals with regard to environmental transport processes considering source-sink phenomena and can also help in the development of functionalized materials to achieve more efficient applications, e.g. for mineral sealing of waste deposits or their use as adsorbents in (waste) water treatment. However, the

participants are mostly rooted in basic research, and no immediate concrete societal benefits are to be expected from this work.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The workshop had ample time for informal discussions between the participants. Several new collaborations, or plans for future career moves have been discussed. It is too early to determine if these plans have panned out, but the atmosphere during the conference was very constructive.
A special issue in the journal Minerals is planned as the result of this workshop. The participants have been informed and will be reminded to submit their high-quality work.
The option to write a community-wide perpetual review or best practices paper in the Living Journal of Computational Molecular Sciences (LiveCoMS) has shortly been discussed. This will require further follow-ups between the participants.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

In the selection of the participants, aspects of gender, geographical provenance and career stage were explicitly followed. Some participants have been explicitly invited to take part. The speaker list represents a wide range of career stages (from PhD student to emeritus Professor and everything in between) and a solid representation of all genders. Participants and speakers travelled from more than ten countries from three continents assuring international provenance and international exchange.

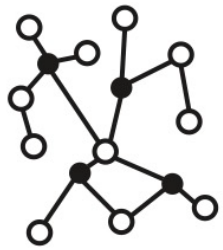
7. Participant list

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CompSysBio2025: Advanced lecture course on Computational Systems Biology



Location: CECAM-FR-RA, France

Webpage : Event webpage

Dates: Oct 5, 2025 - Oct 10, 2025

1. What were the major topics presented in the School?

Reminder of the Objectives:
This School was developed in response to the scarcity of initial training courses that prepare students for modeling approaches in biology, hence the need to take action downstream with young researchers and doctoral students. It thus aims to strengthen scientific potential in this interdisciplinary field by raising awareness among young researchers from the formal sciences of the richness and elegance of systems biology issues. It also brings them into contact with biologists who are already aware of the importance of modeling, thereby strengthening an interdisciplinary culture.
Educational and scientific assessment:
CompSysBio2025 took place in person from October 5 to 10, 2025, at the CNRS Paul Langevin Center in Aussois (Savoie). It brought together 24 invited speakers and 90 participants (including 62 students, 18 postdoctoral fellows, and 10 researchers or engineers). Twelve scholarships covering registration fees were awarded to students. CompSysBio had a truly international flavor, with 34 of the 90 participants and 14 of the 21 speakers working outside France (mostly from EU countries). The school program included two evening keynote seminars, five plenary sessions, each consisting of two guest seminars and one short presentation selected by the participants, and four practical workshop sessions. Three evenings were devoted to selected short presentations by participants, combined with poster sessions. The topics covered in the plenary sessions ranged from systems biology, biomathematics, biophysics, and automation, with parallel workshops providing an opportunity to explore a methodology or concept in greater depth.
The scientific outcome of CompSysBio was very good. The detailed program can be found here http://project.inria.fr/compsysbio2025/files/2025/10/CompSysBio2025_Program_300925.pdf. The quality of the courses was praised by all participants, with a variety of topics covered providing a good overview of the state of the art in the field. The practical sessions were also highly appreciated, allowing participants to learn or become familiar with several computational methods. Seventy-five posters were presented by participants during three poster sessions. Of these posters, ten were selected by the scientific committee for short oral presentations. Both the posters and the short presentations were of a very high standard overall. Two prizes for the best posters were awarded to reward the best presentations.

2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

The talks covered a large palette of topics: structural systems biology investigating the structure-function relationships of proteins, multi-scale and spatio-temporal modeling of cellular behaviors like microscale navigation, synthetic biology to control gene expression, machine learning and AI tools to decode the complexity of gene networks or the immune system, dynamical and stochastic modeling of gene expression and its regulation in physiopathological conditions.
The hands-on allows some practical exercises on stochastic and multi-scale modeling in various contexts (cytoskeleton, epigenomic regulation, bacterial growth, circadian clock, metabolism) as well as machine learning tools for systems biology.
A key open scientific question that was raised during the lectures and that is transversal across the many topics covered by the School is the importance of fluctuations and heterogeneities in biological systems and how cells cope with that: from the intrinsic fluctuations of molecular reactions to the heterogeneous environment faced by unicellular organisms.
Similarly, one technical challenge was raised and was transverse to many topics discussed in CompSysBio: the need for multi-scale models that allows to go from the molecular scale (protein folding, gene structure) to the phenotype (cell behavior, cell state).

3. What was the take-home message for the participants?

Attendees of the School got a broad overview of the field during the lectures and practiced standard modeling and analysis tools during the hands-on sessions. They experienced the interdisciplinarity of the field that couples computer science, mathematics, physics and biology. Invited speakers highlights the generic and specific open questions and future challenges that will be addressed, hopefully, by the future generation of scientists that were trained during the School.

4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

Lecture slides and hands-on exercises were deposited on a shared folder accessible by all participants.

5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

Gender balance was respected for invited speakers (11 females, 13 males, see https://project.inria.fr/compsysbio2025/invited-speakers/).
Scholarships (covering registration and housing fees) were systematically attributed to participants from developing or emergent countries (Cameroun, Brazil, India).

6. Organiser list

Crombach, Anton
Inria, France
Duveau, Fabien
CNRS, France
Jost, Daniel
Ecole Normale Supérieure de Lyon - CNRS, France
Richard, Magali
CNRS - University Grenoble-Alpes, France
Ropers, Delphine
INRIA - University Grenoble-Alpes, France
Thieffry, Denis
INSERM 1024 - CNRS 8187, IBENS, France
Varoquaux, Nelle
CNRS - University Grenoble-Alpes, France

Systematic coarse-graining and machine learning in soft matter physics with ESPResSo



Location: CECAM-DE-SMSM, Germany

Webpage : Event webpage

Dates: Oct 6, 2025 - Oct 10, 2025

1. What were the major topics presented in the School?

This school teaches atomistic, coarse-grained and lattice-based simulations methods suitable for modeling soft matter systems at mesoscopic length and time scales, as well as machine-learned methods to model atomistic systems with a high level of accuracy not reachable with classical forcefields, or model smart active systems that learn new behavior based on a reinforcement learning strategy. Lectures provide an introduction to the physics and model building of these systems as well as an overview of the necessary simulation algorithms. During the afternoon, students practice running their own simulations in hands-on sessions using ESPResSo, GROMACS, and machine-learned interatomic potentials. We explore topics such as parameterizing a coarse-grained forcefield for charged soft matter, hierarchical coarse-graining to speed up the exploration of chemical space, machine learning descriptors, machine-learned effective potentials, reinforcement learning, soft matter physics, curation of large molecular dynamics simulation datasets for model training, lattice-Boltzmann hydrodynamics, and polymer diffusion with and without coupling to continuum hydrodynamic fields. Time is also dedicated to research talks, which illustrate how the simulation models and software are applied, and which provide further background on soft matter at different length and time scales and machine learning.

2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

Multiscale modeling is concerned with simulations of complex physical systems with emergent properties that resolve different time- or length-scales. As a consequence, conflicting goals have to be met. On the one hand, a detailed description at the small scale is needed, but on the other hand, sufficiently long length- and timescales have to be covered to capture the problem in its entirety while keeping the computational cost limited. Understanding many soft matter systems requires such a multi-scale approach.
Systematic coarse-graining and machine-learning techniques have become an important tool for bridging the scales: data is collected on accurate but expensive quantum mechanical simulations to generate effective potentials which are suitable for molecular dynamics simulations of much larger systems. This approach helps to include quantum effects into simulations at length- and timescales that are out of reach for quantum mechanical software. Similarly, results from the atomistic scale are used to develop and

parametrize coarse-grained simulation models, enabling coarse-grained simulations at the micrometer scale.
Several aspects limit the widespread adoption of machine-learning techniques. Neural networks can be powerful tools to capture non-linear trends in quantum mechanical simulation data and interpolate it to new configurations, but they struggle to extrapolate to completely new configurations that are absent from the training data set (e.g. chemical reactions). Determining a confidence interval for predicted values remains difficult and resource intensive.
These limitations can be alleviated by providing rich and chemically diverse datasets during training. This requires data infrastructure to store curated and labeled datasets. While the field of quantum chemistry is already far ahead, chemically diverse molecular dynamics datasets are still difficult to source.

3. What was the take-home message for the participants?

Simulation data needs to be made available in open-source materials databases to help train robust neural networks and democratize AI-powered research. This requires new infrastructure to deposit large simulation artifacts. Likewise, scientists need to learn how to interact with this infrastructure. Molecular dynamics packages have an interest in providing low latency APIs to exchange data between their simulation engine and machine-learned interatomic potential libraries.

4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

- lecture slides are available in the Documents tab of the school page
- participants brought 18 posters and presented them in lightning talks
- a book of abstracts was released on Zenodo under an open source license (doi:10.5281/zenodo.17362577) and advertised on the MultiXscale Cluster of Excellence in a blog post (a EuroHPC Joint Undertaking project)
- hands-on session worksheets with solutions are available as Jupyter Notebooks in the source code of the ESPResSo project on GitHub and can be remotely executed in the web browser via the Binder platform or viewed as static pages in the online user guide
- the event format was presented in a conference proceedings paper: Grad et al., “Organizing software community workshops: Experiences from three independent simulation software projects”, Electronic Communications of the EASST, volume 85, December 2025, doi:10.14279/eceasst.v85.2700.

5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The participants’ career stages are spread out as follows: 32 PhD students, 8 post-docs, 9 professors and group leaders, 5 graduate and undergraduate students, 1 research assistant and 1 industrial researcher. To promote attendance by graduate/doctoral

students, the event was included in the science curriculum of the University of Stuttgart as an ECTS-granting module and made a pre-requisite of the advanced simulation methods module. Gender balance: 21% of participants self-identify as female. Guest speakers were invited from Germany, Sweden, Norway, Switzerland and Scotland. Most participants have their home institution in Europe, with 7 participants from Canada, India and China. Invitation letters for VISA applications were issued upon request. No conference fee was charged to make participation fair to everyone. The chosen location is barrier-free and wheelchair-accessible.

6. Participant list

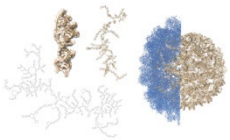
Organisers
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Bredan, Mate - HAW, Germany
Cristea, Artur - Romanian Academy, Romania
Dalla Valle, Gabriele - Universitat de Barcelona, Spain
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Zills, Fabian - University of Stuttgart, Germany

Biophysical modeling of the structure and function of viruses

Location: Cargèse, France



Webpage : Event webpage

Dates: Oct 13, 2025 - Oct 17, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

This meeting has encompassed a wide range of topics related to the function of viruses, explored through biophysical and chemical approaches. In particular, discussions covered the two- and three-dimensional structural determination of RNA viruses using computational prediction tools and experimental techniques such as SHAPE and other chemical probing methods, NMR, and cryo-electron microscopy. Other highlights included modeling virus assembly through mathematical graph-based approaches, studying the frameshifting mechanisms of viral RNA, developing coarse-grained force fields, and mapping the RNA conformational landscape along with its kinetics and thermodynamics using both experimental and simulation methods. The meeting also addressed protein/RNA and drug/RNA interactions, the mechanisms underlying viral capsid formation and cell penetration, and the evolution of viral proteins.
A crucial topic discussed at length concerned the differences between RNA conformational landscapes in vitro and in vivo. Participants highlighted the fascinating insights emerging from the growing number of in vivo structural probing experiments, which are providing increasingly important and valuable results.

2. What were the primary outcomes of this workshop, including limitations and open questions?

Participants noted the dynamism of the field, reflecting on recent major advances as well as ongoing and future challenges. A particularly important aspect was the unique blend of expertise among the participants, ranging from mathematicians to experimental molecular biologists. This workshop represented an important milestone in this highly interdisciplinary area, offering participants an overview of the state of the art across various techniques while also highlighting the challenges that lie ahead. These include :

- Improving the accuracy of atomistic force fields for molecular simulations, which have advanced significantly in recent years but remain imperfect;
- Developing more effective coarse-graining strategies, essential for studying virus-related processes that are too large or too slow to be captured by atomistic molecular dynamics;
- Enhancing simulation methods to provide a consistent and comprehensive description of the highly dynamic RNA conformational landscape, which remains a major challenge;
- Increasing the resolution of experimental techniques used for structural determination, such as cryo-electron microscopy, chemical probing methods, and NMR;

- Refining algorithms for 3D structural prediction, to improve accuracy and reliability;
- Integrating simulation and experimental approaches more effectively, for example through hybrid or integrative modeling strategies;
- Continuing to investigate the differences between in vitro and in vivo RNA structural ensembles.

3. What was the take-home message for the participants?

Modeling RNA structures, dynamics, and mechanisms involves numerous complex challenges, though steady progress continues to be made. The ongoing innovation of experimental techniques, together with advances in physics-based simulation methods, both increasingly complemented by machine-learning approaches, opens up exciting prospects for the near future.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

Because of its topic, this workshop has immense potential for societal impact. A detailed understanding of the biophysical properties of these systems remains central to developing new strategies to combat viral epidemics (such as those caused by coronaviruses, alphaviruses like Chikungunya, and retroviruses like HIV-1) through vaccines, antiviral drugs, and RNA modifications that hinder viral entry and replication. Moreover, RNA aptamers also serve as therapeutic agents for other diseases, such as macular degeneration, underscoring how advances in RNA technologies broadly influence human health conditions involving RNA.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

Several attendees have already established concrete plans for collaboration during the meeting, and we are confident that the presentations and discussions have inspired numerous new research ideas among all participants. A special issue of Biophysical Journal, a leading publication in the field, will feature a collection of articles related to the workshop's themes, contributed by participants and other virologists.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

When preparing the list of participants for this meeting, we took special care to promote diversity at several levels. We ensured a good balance of career stages, including young and promising early-career scientists as well as established leaders in the field. The participant group also reflected geographic diversity, with representation from the Americas, Europe, and Asia. Finally, we achieved a gender balance close to parity.

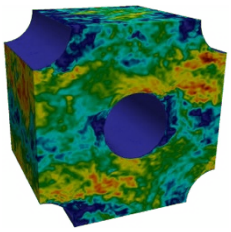
7. Participant list

Organisers
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Roeder, Konstantin
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Schlick, Tamar
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Stirnemann, Guillaume
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Amaro, Rommie - University of California, United States
Barquero Morera, Diego - École Normale Supérieure, France
Bassereau, Patricia - Institut Curie, France
Beuning, Penny - Northeastern University, United States
Božič, Anže - Jožef Stefan Institute, Slovenia
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Bussi, Giovanni - Scuola Internazionale Superiore di Studi Avanzati, Italy
Chen, Shi-Jie - University of Missouri, United States
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Valerio, Mariana - ENS de Lyon, France

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Wacker, Anna - BMRZ, Germany
Williams, Mark - Northwestern University, United States
Williamson, Jamie - Scripps, United States

Advanced CFD and Turbulence Modelling targeting HPC



Location: Barcelona Supercomputing Center, Spain

Webpage : Event webpage

Dates: Oct 14, 2025 - Oct 16, 2025

1. What were the major topics presented in the School?

On the scientific side, the School introduced Advanced Turbulence Modelling, Conjugate Heat Transfer, Massive Parallelisation and Coupling for Multi-Physics. Four lectures dealt with these topics, with Lecturers from Barcelona Supercomputing Centre-Spain, EDF-France, and UKRI-STFC-UK.
On the practical side, the School introduced the software used as a support, code_saturne, its performance on CPU and GPU machines, what domain decomposition means, how to use it in an optimal way, and finally in-situ visualisation together with ParaView.
The attendees were accessing the code using a virtual machine, and MareNostrum5 through ssh from the virtual machine, so, a large part of the School was about practically using HPC.
The highlights of the course were 2 overnight simulations, the former for a high-fidelity Large-Eddy Simulation performed in a modelised bundle of tubes, and the latter for a coupling simulation in a modelised pump, using a second-order Reynolds-averaged Navier-Stokes turbulence model.

2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

The first main open question was about turbulence modelling, and which model to be used depending on the flow. There were 2 experts in turbulence modelling (Dr Stefano Rolfo and Dr Wei Wang) that answered the questions, pushing, if the configuration was in the right range, for advanced-turbulence modelling, such as Large Eddy Simulation. Turbulence modelling is still pretty much an open topic, even if less models are developed nowadays. However, for heated flows, or flows with conjugated heat transfer, accounting for wall influence is still no resolved. The second main open question was about CPU and or GPU programming, meaning discussing the language to use, between Fortran, C and C++, and what to combined them to, between OpenMP, OpenACC, CUDA, HIP, or SYCL are used, the choice strongly depending on the way the code should look like, either portable or dedicated to a vendor because access to only 1 architecture. The answers were mainly provided by Dr Yvan Fournier, from EDF, who is the main developer of code_saturne, for pre-postprocessing and parallelisation/optimisation.

3. What was the take-home message for the participants?

The School was about Advanced Turbulence Modelling and Conjugate Heat Transfer using High Performance Computing.
The main message was about the 2 first topics, showing that it was affordable to simulate them accurately when using HPC. And the second message was about how to use a supercomputer, including on GPUs.

4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

The software we used is open source (code_saturne and ParaView). Attendees had the chance to copy all the installations if they wished to.
The lecture notes, and all the other materials were made available to them during and at the end of the School.

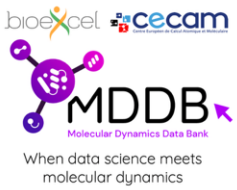
5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The Engineering community is known in Europe for not being very much gender-equal, but we managed to get 4 women out of 17 attendees (please note that in our own Group in the UK there is only 1 out of 13 people), and 1 female lecturer out of the 3 of them. People were coming from the UK, Ireland, Italy, Spain and Germany. Their career stage ranged from MSc students to senior industrial researchers.
Linking this CECAM School to the EXCELLERAT project help us to use them to more broadly advertise it, using EXCELLERAT existing channels, hence ensuring diversity.

6. Organiser list

Moulinec, Charles
UKRI - STFC Daresbury Laboratory, United Kingdom
Rolfo, Stefano
UKRI - STFC Daresbury Laboratory, United Kingdom

When data science meets molecular dynamics



Location: CECAM-HQ-EPFL, Switzerland

Webpage : Event webpage

Dates: Oct 15, 2025 - Oct 17, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop titled “When Data Science Meets Molecular Dynamics” explored how Molecular Dynamics (MD) datasets are being used in the new era of data science and Artificial Intelligence (AI). It focused on key aspects of data management, how MD data is stored, shared, and (re)used within the scientific community. Presentations by leading experts covered a wide range of topics, including:

- Generation of MD datasets using diverse methodologies, from classical MD to enhanced sampling techniques, and how they were used to tackle complex scientific challenges.
- Application of MD data in training AI models and developing new Coarse-Grained (CG) approaches, opening the door to the discovery of hidden dynamic patterns and the simulation of previously inaccessible molecular systems.
- Design and implementation of MD databases that store and expose both data and metadata, allowing the reuse of a plethora of data to the wider scientific community.

The workshop advanced the state of the art by presenting a renewed vision for MD data, as interoperable, FAIR-compliant data. It also highlighted how curated datasets are accelerating AI-driven modeling, showcasing successful integrations of MD data into machine and deep learning workflows. It encouraged cross-disciplinary collaboration between simulation scientists and new efforts centered on storing and sharing data. The workshop generated a feeling of continuity with the transformative impact of the Protein Data Bank (PDB), which revolutionized the access to static structural data, whereas the field is now committed to extend that impact by enabling the storage and dissemination of dynamic MD data.

2. What were the primary outcomes of this workshop, including limitations and open questions?

The workshop led to several clear outcomes, while also exposed limitations and open questions that remain to be addressed.

About the outcomes, the presentations offered a view on emerging MD-related methods which are generating large amounts of new data, that is mainly used in training of new AI and/or CG models. Building on these datasets, there was strong consensus within the community on the importance of storing and sharing MD data, following the work presented in the “The need to implement FAIR principles in biomolecular simulations” paper, signed by more than 100 leading scientists in the field.

Regarding limitations, post-session and coffee break discussions revealed significant concerns about the feasibility of building such an infrastructure capable of storing and

sharing the vast volumes of data generated by the MD community. Participants expressed uncertainty about optimal strategies for data transfer and raised important questions about how such heterogeneous datasets could be effectively reused, for instance, in training new AI models.
Finally, several open questions also emerged, mainly around what types of MD data should be stored. A key point of debate was whether repositories should include raw trajectory files with solvent molecules or just dehydrated trajectories to reduce file size and complexity. This decision has strong implications for the infrastructure needed behind the databases. Additionally, there was some disagreement around the minimal metadata that should be captured (if any), and how to define a metadata schema rich enough to support scientific interpretation of MD data without making the deposition process too painful.

3. What was the take-home message for the participants?

The MD field has entered the data science era, where data generated by the field start to be stored and shared for future reuse, enabling the discovery of complex patterns and the development of more accurate, data-driven AI models. Early examples such as Boltz-2 and BioEmu demonstrate the potential of dynamic MD datasets in training AI models, and these pioneering efforts mark only the beginning of a broader transformation in computational molecular science.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

The main outcomes of the workshop with regards to societal benefits appear from the possibility of storing, sharing and reusing MD data:

- Reuse of data can significantly reduce the carbon footprint associated with high-performance computing. Simulations are often computationally intensive and energy-consuming, so reusing data contributes to a greener, more sustainable science.
- Reuse of data can also lead to new scientific discoveries. A clear example was presented in the workshop, the discovery of cryptic cavities on the surface of the proteins that only emerge when analyzing the dynamic behavior of specific systems. These hidden pockets, revealed through reanalysis of existing MD trajectories, have profound implications for drug discovery, potentially enabling novel pharmaceutical strategies to target previously inaccessible regions of biomolecules.
- Reuse of large datasets in combination with new machine and deep learning methods enables the discovery of complex patterns and the development of more accurate, data-driven AI models. As an example, new AI methods for the prediction of communication pathways and binding sites in macromolecular complexes, trained with datasets of MD simulations, were presented in the workshop.
- Finally, reuse of data can lower the entry barrier for researchers and institutions with limited access to high-performance computing resources.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The workshop was a fantastic event to initiate collaborations between database developers and simulation data producers. Outcomes for these new collaborations will be demonstrated by the growth in the number of available simulations in new releases of key MD data repositories. Besides, a scientific review article is being prepared in collaboration with several invited speakers from the event, summarizing the main points discussed during the meeting and highlighting the importance of storing, sharing and reusing MD data.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

We tried to maintain a good balance. The number of non-speakers in the congress was limited by the size of the room, but the excellent remote capabilities of CECAM allowed remote access by people around the world. The co-funding of the initiative by the MDDB consortium allowed us to attract speakers from Europe, US, and Canada. A good gender balance, close to 50%, was reached with the speakers. A reduced number of short talks were selected from the on-site participants, offering early-career scientists a valuable platform to present their work and contribute to the discussions.

7. Participant list

Organisers
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MADICES 3: Machine-actionable Data Interoperability for the Chemical Sciences

Location: PSI, Villigen, Switzerland

Webpage : Event webpage

Dates: Oct 20, 2025 - Oct 24, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

Common Schemas for Workflow Exchange Participants explored the development and integration of the Python Workflow Definition as a standard for exchanging workflows between engines. Extending PWD to support cyclic graph structures and embedding import/export capabilities into community tools lays the foundation for reproducible, automated materials design pipelines. This work reduces fragmentation and accelerates discovery by enabling workflows to be portable and interoperable. **Semantic Annotation and Interoperable Data Exchange** Refining protocols and guidelines for semantic-first data exchange was a central theme. The group focused on best practices for creating machine-readable metadata and reducing technical barriers for researchers. These efforts make FAIR data production more accessible, improving transparency and reducing redundant work. **ELN Interoperability and File Format Suitability** Detailed use cases were developed to assess how Electronic Lab Notebooks can support data portability across laboratories, vendors, and research data management platforms. This work addresses vendor lock-in and strengthens long-term stewardship of publicly funded research, enabling more effective collaboration and reproducibility. **Automation of Semantic Annotations** The workshop examined strategies for integrating semantic annotation capabilities directly into commonly used scientific tools and pipelines. Automating these processes at the software level ensures metadata quality without requiring deep technical expertise, streamlining compliance. **LLM Tooling for Semantic Pipelines** Discussions on leveraging AI focused on improving semantic data pipelines, enhancing automation, and reducing human error. These approaches promise safer, more transparent laboratory workflows. **FAIR Instrument Control** Exploring how to control instruments using FAIR-compliant software highlighted opportunities for reducing complexity in experimental setups and ensuring that data generated at the source is interoperable and well-documented. **Community Engagement** Recognizing that technology alone cannot achieve interoperability, the workshop developed blueprints for mobilizing diverse research communities. Strategies include training, outreach, and demonstrating the collective benefits of FAIR practices to incentivize adoption, particularly among early-career researchers. **Common Interfaces for ORD Exchange** Finally, participants discussed implementing standardized interfaces for exchange across RDM platforms, further reducing silos and enabling seamless data sharing. These topics collectively advance the state of the art by creating practical standards, tools, and community frameworks that make interoperability achievable at scale. They strengthen reproducibility, accelerate innovation, and promote a more open and trustworthy scientific ecosystem.

2. What were the primary outcomes of this workshop, including limitations and open questions?

A brief summary of outcomes:

- We explored integrating Semantikon into the AiiDA workflow management system, at the workflow level, to capture input/output semantics, and provide semantic validation for AiiDA's workflows. This fits with efforts in AiiDA to semantically annotate core objects internally, to provide full semantic meaning to AiiDA's provenance graphs.
- Two connected hackathon-style LLM-based projects were initiated during the MADICES3. The first, "Herbert", investigated the automation of semantic annotation from semi-structured source data in cases where a suitable ontology already exists. The second, "RDMage", made use of "Herbert" and other tools to provide an agent that reviews digital research objects and provides a report assessing compliance with FAIR principles, possible semantic integrations, and whether enough "out-of-band" data has been included for an experiment or otherwise to be reproduced. This heuristic review can suggest not just missing data values, but missing fields in the schema that should be required.
- At MADICES 3, we introduced the PREMISE-developed RO-Crate-Schema-Plus standard to the ELN community and, through a series of tests, gathered feedback regarding its usability in practice, and polled interest in future integration of the Schema Plus standard into ELNs beyond openBIS.
- Another approach to interoperability arose at MADICES 3 - FINALES-mediated workflows across ELN-WFMS covering experimental/simulation data. Here, the FINALES platform is actively being considered as a middle-layer between ELNs and WFMSs, facilitating standard communications between the platforms, thus avoiding specific platform API usage.
- A practical prototype standard and implementation was developed for automatic upload of raw data from instruments in an RDM platform-agnostic way via RO-Crate. Rather than putting the burden on each lab or instrument to write connectors to each RDM platform, instead each RDM platform simply has to announce support for this standard.
- The workflow interoperability group advanced the Python Workflow Definition (PWD) toward becoming a practical cross-platform workflow exchange standard. Participants extended the PWD specification to support cyclic workflow graphs (e.g., while loops), a critical capability for representing realistic scientific workflows that are inherently iterative or adaptive. In parallel, multiple demonstrators were produced to show how PWD can be integrated into existing community tools, including a new NOMAD parser plugin for importing PWD-defined workflows and an export prototype from the Per Queue workflow engine. These examples highlighted both the feasibility of cross-engine workflow mobility and open questions, such as how to handle dynamic, runtime-determined workflow branching or differences in execution semantics across engines.

3. What was the take-home message for the participants?

Building an open, interoperable research ecosystem is a socio-technical endeavor that requires people at its core, and as such needs education and engagement. Community-

developed tools and best practices improve the production of FAIR data and facilitate interoperable data exchange between systems (e.g. ELNs), whilst training and supporting researchers strengthens adoption. Integrating these solutions at the point of data creation strengthens reproducibility and accelerates innovation.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

The 2025 MADICES Workshop addressed major barriers that prevent scientific data, software, and workflows from being reused across disciplines and platforms. By advancing interoperability, automation, and semantic clarity in data pipelines, the workshop's outcomes contribute to a more transparent, efficient, and trustworthy research ecosystem.
More specifically:
The development of common schemas for workflow exchange lays the groundwork for reusable and reproducible materials-design pipelines, with the potential to significantly shorten discovery timelines.
The ELN Interoperability use cases support the portability of experimental data across laboratories, vendors, and RDM platforms. This reduces lock-in, strengthens long-term stewardship of publicly funded research, and enables more effective collaboration in fields where reproducibility is critical.
Advances in semantic-first data-exchange guidelines and community-driven best practices collectively lower the barrier to producing FAIR data at scale. By enabling researchers to generate high-quality metadata without deep technical expertise, these efforts democratize access to reliable scientific information, reduce redundant work, and accelerate innovation cycles.
The development of practical and reusable blueprints for mobilizing diverse research communities toward interoperability strengthens open-science culture, supports early-career researchers, and promotes broader participation in FAIR data practices.
Discussions on AI/LLM-based tooling and FAIR instrument control further point toward safer, more transparent laboratory automation with reduced human error and improved sustainability.
Taken together, these outcomes support a more open, interoperable, and efficient scientific infrastructure that benefits society through faster discovery, improved verification of scientific claims, and better transfer of research results into industry, policy, and education.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

MADICES 3 enabled a vast level of knowledge exchange, which in turn has fostered new collaborations, insightful discussions and technical examples committed to the GitHub Repository. As a consequence of these a number of reports were generated, which provide valuable information to the community, and can provide the basis for some further research and scientific papers.

- PWD Extension to while loops; NOMAD parser plugin for PWD; PWD export prototype from the Per Queue workflow engine.

- ORD exchange in the context of simulation workflows initiated by an ELN, executed by a WFMS, and mediated by FINALES, with two-way ORD exchange resulting in new research data deposited in the ELN.
- FAIR control of instruments: An implementation and standard for automatic upload from instruments in a platform-agnostic way.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The organisers utilised their networks to invite a diverse range of participants, in addition to using GitHub, social media, and conferences to identify relevant individuals in the field. There was a strong focus on supporting early career researchers, and funds were made available to support those who were otherwise unable attend. In total 82 individuals (15 female, 67 male) were offered the ability to attend, through a combination of invitations, and requests to attend after hearing about the event. In total 48 individuals (7 female, 41 male) were able to attend, spanning 23 institutions and 7 countries. We organised several pre-workshop meetings for participants to present their work and open up initial dialogues to identify areas of interests. This fostered a community spirit and engaged the attendees in the months leading up to the meeting. After the workshop we also sent out our own feedback form to help us plan for the next MADICES event.

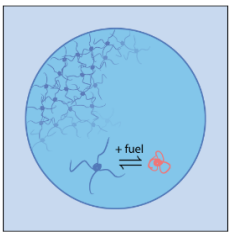
7. Participant list

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Multiscale modeling of chemically active mixtures



Location: CECAM-HQ-EPFL, Switzerland

Webpage : Event webpage

Dates: Oct 27, 2025 - Oct 30, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The 2025 CECAM workshop addressed chemically active mixtures by bringing together theory, simulation, and experiment to understand how chemical reactions drive self-organisation across scales. A central theme was pattern formation in mass-conserving reaction–diffusion systems, including biological examples such as the Min and PomXYZ systems. The concept of a mass redistribution potential enabled geometric interpretations of instabilities, interface dynamics, and arrested coarsening, providing a unifying perspective on pattern selection.

Size control and droplet dynamics were extensively discussed. Experiments on chemically fueled emulsions demonstrated how periodic driving induces pulsations and shell formation, while theoretical and computational studies showed that nonequilibrium fluxes shift coexistence conditions and can stabilise finite droplet sizes beyond equilibrium constraints. These results clarify the mechanisms underlying size regulation in active phase separation.

Active droplet motility and oscillations emerged as another key topic. Models of self-propelled and oscillatory droplets highlighted how reaction-driven gradients and internal feedback generate motion, waves, and complex dynamics. In particular, reaction-driven diffusiophoresis was identified as a robust mechanism for transport in the absence of surfactants, with potential relevance for intracellular organisation.

The workshop also emphasised multiscale modelling. Stochastic simulations revealed the role of fluctuations, crowding, and finite-size effects in shaping droplet properties, often beyond the reach of continuum descriptions. At the same time, recent efforts to derive active and non-reciprocal field theories from microscopic models provide a promising route toward systematic coarse-graining. The role of cyclic reaction networks in sustaining fluxes and enabling interfacial phenomena was also discussed.

Finally, non-equilibrium thermodynamics provided a common framework to interpret these phenomena, in particular through entropy production and stability criteria. Overall, the workshop contributed to consolidating a more unified and physically grounded description of chemically active mixtures, while highlighting the need to bridge microscopic detail and macroscopic behaviour.

2. What were the primary outcomes of this workshop, including limitations and open questions?

The workshop led to several important outcomes. First, there is increasing convergence toward a common language for pattern formation in chemically active systems, based on conserved reaction–diffusion dynamics and mass redistribution mechanisms. Second, the

role of nonequilibrium fluxes in controlling droplet size and stability is now more clearly established, going beyond equilibrium thermodynamic arguments. Third, progress was made in identifying generic mechanisms for motility and oscillations, including diffusiophoresis and reaction-driven feedback. Fourth, there is a growing consensus on the need for multiscale approaches that consistently link microscopic dynamics, stochastic effects, and continuum descriptions. Finally, integrating reaction networks with phase separation remains a promising route toward synthetic, cell-like systems.
At the same time, several limitations remain. Quantitative discrepancies between stochastic simulations and continuum theories persist, particularly regarding fluctuations and droplet size distributions. The effects of crowding, non-ideal interactions, and complex chemical composition are still insufficiently understood. Moreover, while active and non-reciprocal field theories are advancing, their derivation from realistic microscopic models and their predictive power in complex systems remain open issues.
Key open questions include: how reaction network topology and kinetics control pattern stability and dynamics; what minimal ingredients are required for growth, division, and self-replication; and how to coarse-grain reaction–diffusion systems without losing thermodynamic consistency. Addressing these questions will require closer integration between theory, simulation, and experiment.

3. What was the take-home message for the participants?

Chemically active mixtures provide a minimal framework for life-like organisation driven by nonequilibrium reactions. Understanding their behaviour requires connecting reaction networks, transport, and phase separation across scales, using thermodynamically consistent approaches that integrate theory, simulation, and experiment.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

The outcomes of the workshop have potential long-term societal impact by advancing the foundations of systems chemistry and active matter. A better understanding of chemically driven self-organisation can inform the design of synthetic compartments, adaptive materials, and programmable chemical systems. This includes potential applications in drug delivery, where responsive droplets or vesicles could be engineered to release cargo under controlled conditions, and in biomanufacturing, where artificial cell-like systems could provide new routes for chemical production.
Insights into biomolecular phase separation are also relevant for understanding cellular organisation and dysfunction, with possible implications for diseases linked to aberrant condensates. More broadly, the development of thermodynamically consistent models contributes to safer and more predictable design principles in synthetic biology and chemical engineering.
While these applications remain long-term, the workshop contributes to establishing the conceptual and methodological basis required for future technological developments.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The workshop stimulated new interactions and collaborations among participants. In particular, follow-up discussions between the organisers led to the identification of a gap in the current description of chemical reactions in non-ideal mixtures. This has motivated a joint research effort that is expected to result in a publication and potentially further collaborative projects.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

Inclusivity was considered in the selection of speakers and participants, with attention to gender balance, career stage, and disciplinary diversity. Approximately 25% of invited speakers were women, and the program included both junior and senior researchers from different backgrounds (theory, simulation, experiment). The format of the workshop—combining talks, poster sessions, and open discussions—was designed to encourage broad participation and interaction across career stages.

7. Participant list

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SIESTA School 2025

Location: online

Webpage : Event webpage

Dates: Nov 17, 2025 - Nov 21, 2025

1. What were the major topics presented in the School?

The school was aimed at students and researchers from different disciplines who already used, or planned to use, first-principles techniques to simulate properties of matter at the atomic scale. In particular, the school focused on the SIESTA method. Participants learned its essential theoretical foundations, and how to use the SIESTA code effectively. The topics presented in the School were:

- General SIESTA Theory.
- Pseudopotentials.
- SIESTA input files, execution and output.
- Basis sets in SIESTA.
- Basis set optimization.
- Ghost atoms and basis sets on surfaces.
- Mulliken and other atomic charges.
- Convergence in SIESTA: mesh cut-off convergence, k-mesh convergence and SCF convergence.
- Analysis: DOS, bands, fatbands, PDOS.
- Geometry optimization.
- Molecular dynamics
- Phonons.
- Spin, spin-orbit couplings and magnetism.
- TranSIESTA.
- Building, deployment and execution of SIESTA.
- SIESTA solvers.

The topics were presented at the beginner/intermediate level, with lectures covering the basic theory behind the implementation and hands-on materials prepared to cover the core functionality of the program and the most common analysis options.

2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

The SIESTA School 2025 presented foundational concepts and functionalities of the SIESTA method and software. Therefore, most questions were asked by students in order to fully understand those basics, or to identify what kind of simulations they would need to employ in order to study some systems of their interest. Questions aimed at exploring open technical or scientific questions related to SIESTA were very limited.

Regarding limitations related to the school, in previous editions of the school we had deployed SIESTA on HPC facilities but we had received feedback that showed

disappointment in losing access to that installation at the end of the school, which hampered the ability of students to continue using SIESTA after the School. For this edition we changed our approach, and given the stability of the SIESTA conda distribution we decided to base the School on the students running SIESTA on their own computers via conda. We believe this proved a positive change, and while students may not have been able to access a fully performant version of SIESTA on an HPC system, they were still were presented with information on how to build and run SIESTA for such systems, and they did not lose access to the version of SIESTA they had used during the school.

3. What was the take-home message for the participants?

In this school, participants learned that SIESTA is an efficient method for first principles simulations of matter at the atomistic scale. SIESTA works under a few approximations, and enables simulations for very large systems. The quality of the calculations is controlled by users. SIESTA has lots of different functionalities (MD, NEGF, phonons, optical properties), and it is under continuous development.

4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

- School presentations (pdf files) are available from https://siesta-project.org/siesta/events/SIESTA_School-2025/Sessions.html.
- Several SIESTA tutorials (https://docs.siesta-project.org/projects/siesta/) were updated and improved for the School. They can also be accessed directly from the list of sessions on https://siesta-project.org/siesta/events/SIESTA_School-2025/Sessions.html.

5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

Regarding school "students", we had a large and diverse pool of applicants (130 persons) from all career stages (from university students to senior faculty), a wide range of countries of origin/residence, and a significant number of women. We accepted all participants, except for those that had already participated in previous editions of the School or those who were based in the usual few blacklisted countries. This resulted in participants based in 30 different countries, with 75% of the participants based outside of the EU. Also, 25% of the participants were women.
Regarding speakers and tutors, unfortunately three of the organisers (and expected speakers) left the organisation of the event in the few months before the School took place due to job changes, with little time to adapt. This resulted in a slight increase in the seniority average of speakers (in the end peaked at junior faculty) and a decrease in the percentage of women (2/3 of the leavers were women).

6. Participant list

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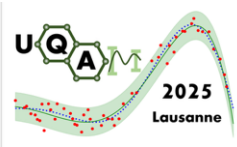
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Uncertainty quantification in atomistic modeling: From uncertainty-aware density functional theory to machine learning

Location: CECAM-HQ-EPFL, Switzerland



Webpage : Event webpage

Dates: Nov 25, 2025 - Nov 28, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The CECAM workshop "Uncertainty Quantification in Atomistic Modeling: From Uncertainty-Aware Density Functional Theory to Machine Learning", held in Lausanne from 25–28 November 2025, brought together experts from computational materials science, electronic-structure theory, and machine learning to address a central challenge in modern atomistic simulations: the rigorous quantification and propagation of uncertainty from first-principles methods to data-driven models.

The workshop focused on three main themes. The first was **uncertainty quantification (UQ) in density functional theory (DFT) and related *ab initio* methods**. While DFT is widely used to predict materials properties, systematic error estimates are rarely reported. Speakers examined how numerical settings and model approximations introduce inconsistent and often hidden errors, and discussed approaches such as error balancing, verification datasets, and standardized protocols to establish meaningful error bounds. These efforts aim to improve the reliability, reproducibility, and comparability of DFT results across codes and large-scale workflows.

The second theme addressed **UQ in atomistic machine learning (ML)**. ML potentials and neural networks dramatically expand the scope of atomistic simulations but introduce statistical uncertainty due to limited or biased training data. Presentations covered ensemble-based and Bayesian methods for estimating predictive uncertainty, enabling the detection of out-of-distribution predictions and more reliable model deployment. Practical advances, including last-layer ensembles and scalable uncertainty estimators, demonstrated how uncertainty awareness can be incorporated into ML models with minimal additional computational cost.

The third theme focused on the **practical use of UQ in ML-accelerated atomistic modeling**. Uncertainty estimates were shown to play a key role in active learning, guiding the efficient selection of new training data and improving model generalization. Participants also discussed the propagation of uncertainty from atomistic predictions to higher-level observables and multiscale models, as well as generative settings. Such approaches ensure that predicted materials properties are accompanied by meaningful confidence estimates.

Overall, the workshop advanced the state of the art by integrating rigorous UQ in electronic-structure theory with statistically grounded ML methods and their practical application. This contributes to a more transparent, reliable, and uncertainty-aware framework for atomistic modeling and materials design.

2. What were the primary outcomes of this workshop, including limitations and open questions?

The workshop led to several important outcomes that clarify both the current state of uncertainty quantification (UQ) in atomistic modeling and the directions needed for future progress. A primary outcome was the establishment of a community of researchers focused on UQ across electronic-structure theory and atomistic machine learning, and atomistic modeling in general. Participants collectively identified common sources of uncertainty and discussed how these can be consistently defined, quantified, and propagated across modeling scales. This helped consolidate best practices and highlighted the need for standardized benchmarks and validation protocols.

Another key outcome was the recognition that uncertainty-aware workflows are now technically feasible for many practical applications. Advances in scalable uncertainty estimation for ML models, coupled with improved verification strategies for DFT, demonstrated that UQ can be integrated into high-throughput and ML-accelerated simulations without prohibitive overhead. This will far more motivate the attendees and other researchers to perform UQ that accompanies their ML model development and atomistic modeling.

The workshop also identified limitations and open challenges. One major limitation is the lack of universally accepted protocol for comparing uncertainty estimates across different methods, models, and codes. While multiple UQ approaches exist, their calibration, interpretability, and transferability remain open questions that are tackled independently by different research teams. Another important open question highlighted during the workshop is how to connect computational UQ with experimental uncertainty in real laboratory settings. While computational models can increasingly provide internal confidence estimates, meaningful integration with experimental error bars, measurement noise, and systematic biases is still rare. Bridging this gap is essential for making uncertainty-aware simulations actionable in experimental design, materials screening, and model validation. Participants emphasized the need for closer collaboration with experimentalists, shared datasets, and workflows that allow computational uncertainty to directly inform experimental decision-making.

Overall, the workshop clarified that while the foundations of UQ in atomistic modeling are rapidly maturing, significant work remains to harmonize methods, validate uncertainty estimates, and connect them meaningfully to experimental reality. These open questions define a clear and impactful agenda for future research.

3. What was the take-home message for the participants?

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(1) UQ is important to perform and should become integral to any atomistic ML and modeling workflow; (2) there exist diverse points of view on UQ, it is important to rationally choose the “right” type of uncertainty for the problem of interest; (3) there is a need for a comprehensive UQ workflow/protocol that begins with the uncertainties in the ab initio calculations, then extends to the ML models trained on them and the physical observables of the simulations conducted with the models

4. Does the outcome(s) of the workshop hold potential for societal benefits?

We believe in the importance of allowing not only the atomistic modeling community, but the wider research community and society to recognize that most, if not all, AI and ML methods inevitably suffer from their inherent, statistical nature that makes them prone to committing statistical errors in their predictions. While this workshop has facilitated a dialogue along this direction for the atomistic modeling community, it can also catalyze similar dialogues and workshops to take place in other research fields, and for the general public to realize the importance of concerning themselves with uncertainty quantification, or in general, "interpreting the AI/ML predictions and content with a grain of salt". We believe this to be an important benefit that comes out of our workshop, which will become apparent in the next years to come.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

As organizers, we have witnessed the formation of a tight-knit community of researchers focused on the complementary areas of UQ for DFT, UQ for ML, and applications of UQ in atomistic modeling. We foresee multiple collaborations which can in turn lead to publications by the parties involved. Through a survey, we also recognized the strong demand for the follow-up editions of the workshop to continue the timely, crucial dialogue in the realm of UQ for atomistic modeling, and we plan to submit workshop proposals in the future for the next editions of "UQAM" with renewed objectives.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

We would like to note that we actively strove to achieve good balance in terms of gender, career stage, and geographical provenance at all levels of organization. This includes the organization team itself, composed of 2 female and 3 male researchers (also 1 postdoc and 4 professorial level). In composing the speaker lineup, while we had been faced with the thematic constraint, we still strove for a good gender and nationality balance. We ended up inviting 1 female and 2 male keynote speakers, 12 male and 4 female speakers. We also note that we also strove for balance in the career stage by inviting 4 PhD students and 1 postdoc to deliver tutorials and talks. In selecting the participants, we took similar care in achieving good gender and geographic balance, then facilitated maximal inclusivity within our capabilities by holding the workshop in hybrid format, allowing all applicants to the workshop to at least take part remotely via Zoom.

7. Participant list

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Unveiling self-phoretic colloidal propulsion



Location: CECAM-HQ-EPFL, Switzerland

Webpage : Event webpage

Dates: Dec 3, 2025 - Dec 5, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The event *workshop* addressed the fundamental mechanisms, control strategies, and emergent phenomena of phoretic and self-phoretic transport in active colloidal systems, integrating theory, simulations, and experiments across molecular to macroscopic scales. Central topics included the physical origins of self-phoretic propulsion, encompassing diffusiophoresis, thermophoresis, electrodiffusiophoresis, magnetophoresis, and enzyme-driven motion, with particular emphasis on nonequilibrium thermodynamics, chemical potential gradients, and interfacial transport. Theoretical contributions provided unifying multiscale and conceptual frameworks clarifying how propulsion emerges from coupling between particles and chemically and thermally active environments, resolving long-standing ambiguities between equilibrium and nonequilibrium descriptions. A major advance was the recognition of chemical gradients as information-bearing fields that generate chemotaxis, non-reciprocal interactions, and collective behavior, linking molecular kinetics to large-scale organization. Simulation studies highlighted the decisive roles of hydrodynamics, particle geometry, confinement, and surface properties in shaping propulsion and collective states. Experimental contributions introduced advanced control and diagnostic tools, such as structured light fields, feedback control, refractive-index-based mapping of chemical gradients, and interferometric scattering microscopy, enabling unprecedented access to nanoscale dynamics. The workshop further expanded active-matter paradigms by addressing anisotropic swimmers, anomalous diffusion, fluctuation-induced interactions, airborne and microgravity propulsion, biohybrid microrobots, and sustainable design principles. Collectively, these contributions advanced the state of the art by moving the field beyond single-particle phenomenology toward predictive, multiscale, and programmable active systems where propulsion, sensing, communication, and collective functionality are intrinsically coupled.

2. What were the primary outcomes of this workshop, including limitations and open questions?

The workshop led to a more coherent and critical understanding of phoretic and self-phoretic mechanisms by confronting theory, simulations, and experiments across scales. A major theoretical outcome was the consolidation of multiscale, thermodynamically consistent descriptions coupling chemical reactions, transport, interfacial physics, and hydrodynamics. Discussions helped frame interpretations of diffusiophoresis, thermophoresis, electrodiffusiophoresis, and enzyme-driven motion by highlighting solute correlations, nonequilibrium chemical potentials, and differing views on interfacial slip versus alternative momentum-transfer mechanisms. Simulations highlighted the decisive

roles of hydrodynamic interactions, confinement, particle anisotropy, and crowding in shaping propulsion efficiency, collective dynamics, and slow or glass-like behavior, exposing limits of minimal models and challenges related to computational cost and model idealization. Experimentally, the workshop showcased major advances in measurement and control. Interferometric scattering microscopy enabled access to nanoscale dynamics dominated by thermal fluctuations, directly addressing whether self-phoresis at the nanoscale can exceed thermal diffusion and be reliably detected. Refractive-index-based techniques provided label-free mapping of chemical gradients around active particles, enabling correlations between local fields and motion. Structured light, optical manipulation, and feedback-based control offered strategies to activate, guide, and interrogate active particles in a controlled and reversible manner. These studies also highlighted the emergence of non-reciprocal interactions and anomalous transport in active systems. At the same time, several fundamental open questions were identified. A concern was in the definition of self-phoresis itself: whether it should be restricted to Anderson-like motion driven by tangential interfacial flows, or whether alternative mechanisms (e.g. momentum exchange, pressure waves, bubble formation, osmotic-pressure-driven propulsion) should be considered within the same physical framework. Closely related is whether chemical or thermal pumping of the surrounding fluid is equivalent to swimming. It also remains debated whether self-phoretic propulsion is meaningful at the nanoscale or overwhelmed by thermal diffusion. For enzymatic motors, the dominant motion mechanism (genuine self-diffusiophoresis versus solutal buoyancy or convection) and the appropriateness of the term chemotaxis remain unresolved. Finally, the physical origin of collective behavior in 3D systems, active swimming vs buoyancy-driven or hydrodynamic convection, remains poorly understood, as do limits of real-time feedback and autonomous control under strong noise and bandwidth constraints. Together, these outcomes reflect both the growing maturity of the field and the key conceptual and technical challenges that remain.

3. What was the take-home message for the participants?

Understanding and exploiting self-phoretic propulsion requires tight integration of theory, simulations, and experiments across scales. Progress depends on unifying thermodynamics, hydrodynamics, and chemistry with advanced experimental control, manipulation, and precise mapping and tracking techniques to clarify self-propulsion relative to coupled transport and collective effects. Such integrated approaches are essential for predictive design and functional applications of active matter.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

The outcomes of the workshop hold clear potential for societal benefit by advancing the fundamental understanding and control of self-phoretic transport, which supports emerging technologies in medicine, environmental science, and soft robotics. Experimental results demonstrated how enzyme-powered micro- and nanomotors can achieve chemotactic navigation, collective transport, and targeted delivery in biologically relevant environments, directly linking phoretic mechanisms to precision therapy and biomedical applications. Other contributions showed how active colloids and biohybrid systems can be engineered to interact with and modify their surroundings, enabling

functions such as contaminant elimination, material clearance, and enhanced transport in complex environments, with clear relevance for environmental remediation and adaptive materials. Improved mechanistic understanding and multiscale modeling enable the rational design of these systems, including sustainable and application-oriented microrobotic platforms. Advances in control, manipulation, and high-resolution mapping and tracking techniques contribute to safer and more predictable active systems. More broadly, by grounding self-phoretic propulsion in well-defined physical and chemical mechanisms and explicitly accounting for environmental interactions, the workshop highlighted how active-matter systems can be designed in a more predictable, suitable, and safer manner for real-world applications.

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The workshop generated tangible outcomes primarily by fostering new and strengthening existing research collaborations. Several scientific discussions revealed strong complementarities and synergies between theoretical, simulation, and experimental approaches, opening opportunities for joint work. These interactions are expected to potentially materialize into joint publications and coordinated project proposals, with follow-up exchanges already initiated after the workshop. In particular, participants identified overlapping interests where concepts and methods developed independently can be combined into unified studies, with follow-up exchanges already initiated after the workshop. Overall, the workshop acted as a catalyst for aligning ongoing research efforts and for shaping future collaborative activities.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

Inclusivity was an explicit consideration in the organization of the workshop. The program brought together participants and invited speakers from a broad geographical range, including Europe, the United States, China, and Japan, ensuring a diversity of scientific perspectives and research cultures. We also made a conscious effort to improve gender balance by inviting several outstanding young women researchers whose work represents some of the most innovative and rigorous contributions in a field that has historically been male dominated. Their strong scientific presence reflects a positive and ongoing shift toward greater gender diversity in the community. The workshop format, including extended discussion sessions and poster presentations, was designed to encourage participation from all attendees and to foster an inclusive and open scientific environment.

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Recent advances in first-principles modeling of electron-phonon interactions



Location: CECAM-HQ-EPFL, Switzerland

Webpage : Event webpage

Dates: Dec 8, 2025 - Dec 11, 2025

1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The field of electron-phonon coupling (EPC) in electronic structure has matured significantly in the past decades and grown quite substantially in community size and reach of applications and topics. With respect to previous workshops, the CECAM workshop in 2025 was less focused on a single important problem, and opened many doors to new physics in different directions, including:

- Exciton-phonon coupling;
- Charge transport and polarons;
- Ultrafast dynamics under laser fields;
- Coherent vs incoherent dynamics of phonons and their populations;
- Data compression techniques and algorithmic improvements to attain converged
- accuracy in reciprocal space wavevector sampling;
- Machine learning methods to predict phonons and EPC;
- Complex materials treatment, including interfaces and large 2D materials.

These topics reflect our choice of invited speakers covering the different frontiers in the state of the art, and the spectrum of codes, approaches, and workflows. The discussion sessions pointed clearly to gaps in our existing knowledge and capability.

2. What were the primary outcomes of this workshop, including limitations and open questions?

A primary outcome of the workshop was a clear and up-to-date assessment of the current state of the art in first-principles EPC theories and methods and their rapidly expanding scope. Presentations demonstrated that first-principles EPC methods are now being applied to increasingly complex phenomena, including exciton-phonon coupling, polaron formation and transport, ultrafast laser-driven dynamics, strongly-correlated systems, etc. The workshop discussions highlighted several important limitations of present-day methods. System size remains a major challenge, e.g. for interfaces, large 2D materials, and disordered or strongly correlated systems. Data-compression techniques and machine-learning approaches are starting to make an impact on the field. The treatment of multi-phonon effects, anharmonicity, and finite-temperature dynamics requires further theoretical and computational development. The consistent treatment of multiple coupled excitations, such as exciton-phonon, magnon-phonon, and plasmon-phonon interactions, within unified and predictive frameworks in realistic systems is still a major challenge.

Beyond theoretical and technical advances, an important outcome of the workshop was the strengthening of the EPC community itself. The event facilitated the exchange of ideas between developers of different codes, methodologies, and application domains, helping to build the next generation of EPC development and groups.

3. What was the take-home message for the participants?

One of the main messages was the vibrancy of the topic and community, which has expanded significantly over the past 20 years and linked to many other fields.
More specifically, a central take-home message was the ability of current theorical approaches to attack a new order of magnitude in the complexity of both methods and materials, including e.g., large interfaces and systems with strongly correlated electrons. The range of applications for EPC methods has become extremely broad.

4. Does the outcome(s) of the workshop hold potential for societal benefits?

In the short term, the workshop itself does not have societal benefits, but much potential. The quantitative prediction of materials properties is entering a new era with the advent of quantitative first-principles tools. Properties linked to EPC are crucial in many technological areas (thermal, transport, spectroscopic, electronic and mechanical properties...). The short-term integration of the methods discussed and advanced in our workshop into computational workflows, open databases, and machine learning tools for materials discovery will have societal impact in the following fields:

- Energy production and efficiency
- Batteries
- Electronics, including high power, superconducting, and optoelectronic technologies
- Sensors
- Quantum technologies

5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

- Many specific collaborations were discussed, initiated, or cemented. Publications will probably follow, as it happened quite successfully in our previous iterations, but it would be premature to make such claims only 1 month after the workshop.
- Plans were discussed for the organization of workshops, schools, and conferences by individuals or groups of participants.
- The update of the state of the art in theory and in the software implementations of algorithms presented by the different speakers will benefit the field and show all the groups the frontiers which we will have to address soon.

6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

- The organizing team made a deliberate effort to select a speaker lineup that included a strong representation of women (although, unfortunately, several canceled their participation) and early-stage researchers.
- We strive for a balanced mix of invited and contributing participants and talks, aiming to represent the full global palette of EPC codes currently in use. This is becoming a significant challenge within a manageable size (< 50 people). The workshop was also an opportunity to assess the current state of the field and EPC codes being developed and learn about further groups and initiatives in the USA, China, and elsewhere.

7. Participant list

Organisers
Poncé, Samuel
Université Catholique de Louvain, Belgium
Verdi, Carla
University of Queensland, Australia
Verstraete, Matthieu
University of Liege, Belgium

Antonius, Gabriel - Université Du Québec à Trois-Rivières, Canada
Aubry, Corto - EPFL, Switzerland
Bernardi, Marco - Caltech, United States
Bornhake, Thomas - Forschungszentrum Jülich GmbH, Germany
Carrasco Alvarez, Alvaro Adrian - UCLouvain, Belgium
Coulter, Jennifer - Flatiron Institute, United States
Draxl, Claudia - Humboldt-Universität zu Berlin, Germany
Girotto Erhardt, Nina - Université Catholique de Louvain, Belgium
Giustino, Feliciano - The University of Texas at Austin, United States
Gonze, Xavier - UCLouvain, Belgium
Hanrath, Friedrich - Forschungszentrum Jülich GmbH, Germany
Houtput, Matthew - University of Antwerp, Belgium
Hu, Jiaming - Westlake University, China
Kioupakis, Emmanouil - University of Michigan, United States
Li, Zhenglu - University of Southern California, United States
Lihm, Jae-Mo - Flatiron Institute, United States
Lin, Changpeng - EPFL, Switzerland
Luque Canete, Miguel - King's College London, United Kingdom
Mauri, Francesco - University of Rome Sapienza, Italy
Mignolet, Maxime - University of Liège, Belgium
Miranda, Henrique - VASP Software GmbH, Austria
Paleari, Fulvio - Nanoscience Institute - National Research Council, Italy
Pan, Yiming - Christian-Albrechts-Universität zu Kiel, Germany
Ping, Yuan - University of Wisconsin-Madison, United States
Poliukhin, Aleksandr - EPFL, Switzerland
Protik, Nakib - Humboldt University of Berlin, Germany
Pruneda, Miguel - Consejo Superior de Investigaciones Científicas, Spain

Rajkov, Bogdan - University of Cambridge, United Kingdom
Savic, Ivana - King's College London, United Kingdom
Stefanucci, Gianluca - University of Rome Tor Vergata, Italy
Tiwari, Rupesh Kumar - Trinity College Dublin, Ireland
Trukhan, Elena - Humboldt-Universität zu Berlin, Germany
Ustimchuk, Daria - Fritz Haber Institute of the Max Planck Society, Germany
Van De Walle, Chris - University of California, United States
Vasilchenko, Vasilii - Université Catholique de Louvain, Belgium
Wang, Huimin - University of Bremen, Germany
Zacharias, Marios - The Cyprus Institute, Cyprus
Zhumagulov, Yaroslav - EPFL, Switzerland



MARY ANN MANSIGH CONVERSATION SERIES

The *Mary Ann Mansigh Conversation series* focuses of non-strictly technical topics of cultural interest for the simulation and modelling community.

The format reflects the informative and informal nature of these sessions, with talks introducing the subject followed by a conversation between the speakers and the audience.

The lecture series "*Mary Ann Mansigh Conversation series*" is co-organized by CECAM (https://www.cecam.org) and MARVEL (http://nccr-marvel.ch/) at EPFL.

Telling scientific stories - from science journalism to comics and visual storytelling



Dates: Nov 20, 2025

View full video

Scientists are trained to communicate work through journal articles, seminars, and conferences. But reaching audiences beyond the lab requires different tools and languages - whether through news media, books, or creative formats like comics. This panel explores how researchers can broaden the impact of their work by engaging with diverse forms of science communication.

Each of the two speakers will bring a unique perspectives: an experienced science journalist from a major Swiss news outlet, who translates complex research into stories that capture the public's attention and constantly looks into the societal and ethical implications of new technologies; and an editor at a publishing house specializing in science-themed comics, who uses visual storytelling to make scientific ideas accessible and memorable. Together, they will share insights on how science can travel across different platforms, the challenges of simplifying without oversimplifying, and why clear communication is crucial for building trust between science and society.

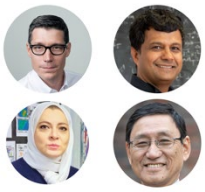
Sara Ibrahim - SWI swissinfo.ch, Switzerland

Sara Ibrahim *is a multilingual science and technology journalist born in Milan to an Italian-Egyptian family. She joined SWI swissinfo.ch in 2020, where she makes complex research and innovation topics understandable to an international audience. Previously, she worked between Milan and Paris as an editor for tech magazines. Her areas of interest include artificial intelligence, the social impact of emerging technologies, democracy, human rights, and policy issues related to innovation. Committed to making science accessible, she uses her reporting to bridge the gap between experts and the public, highlighting how new discoveries shape everyday life. She mainly writes in English and Italian and is based in Switzerland.*

Roberto Natalini – CNR, Italy

Roberto Natalini *is the Director of the Istituto per le Applicazioni del Calcolo at the National Research Council of Italy (CNR), with a research focus on partial differential equations and their applications in biology, fluid dynamics, and cultural heritage. He is deeply engaged in mathematics education and outreach, coordinating the national platform MaddMaths! and co-leading the science communication project Comics&Science. From 2015 to 2022, he chaired the Mathematics Outreach Committee of the European Mathematical Society, promoting innovative approaches to public engagement with mathematics.*

Science and diplomacy



Dates : Feb 28, 2025

View full video

In these complex times, we believe that the theme of Science and Diplomacy is of utmost relevance. We plan to address it from points of view that include education and scientific exchange in developing countries, the potential of computational science as a facilitator for diplomacy, actions of international institutions promoting peace and disarmament, and the management of cooperative research infrastructures in problematic areas.

Roland Bouffanais, University of Geneva, Switzerland

Computational diplomacy: Understanding and analyzing international relations in the digital age

As technology rapidly evolves, computational diplomacy is emerging as a transformative field, offering new insights into the analysis and understanding of international relations. This talk delves into the role of artificial intelligence, big data, and machine learning in examining multilateral governance and decision-making processes. By harnessing computational tools, we can uncover hidden patterns in global diplomatic dynamics, particularly in addressing challenges such as global health crises and climate diplomacy. Additionally, we will highlight key research initiatives from the SiDLab (Science in Diplomacy Lab), a collaborative effort between the University of Geneva and ETH Zürich.

Roland Bouffanais *is an Associate Professor at the Global Studies Institute and the Department of Computer Science (Faculty of Science) of the University of Geneva. He holds the Chair in Computational Diplomacy and is Co-Director of the SiDLab (Science Diplomacy Lab) at the University of Geneva. His research on complex systems involves a synergistic combination of computational and theoretical developments with real-life experimental validations. Specifically, he focuses on interdisciplinary research at the intersection of complexity science, the social sciences, and AI. He received his Ph.D. from EPFL (Lausanne, Switzerland) in computational science, for which he was awarded the prestigious IBM Research Prize in Computational Sciences (2008) and the ERCOFTAC Da Vinci Award Silver Medal (2007).*

Atish Dabholkar - International Center for Theoretical Physics, Italy

Uniting the world for and through science

For over six decades, Abdus Salam International Centre for Theoretical Physics (ICTP) has been a shining example of living science diplomacy. As an international hub for science, the Centre has been a model for ensuring excellence and inclusion in advanced science around the world, and for promoting international cooperation through science. Close to 200000 scientists from 188 nations have profited from various programs at ICTP

for advanced scientific exchange overcoming the barriers of gender, ethnicity, geography or economics.
Science is a universal language which makes dialogue possible to build bridges even across geopolitical differences. Ideas for new research or for new international infrastructures such as SESAME or SEEIIST have often been seeded at ICTP. As a UN organization, ICTP has the mandate and convening power to bring scientists together to address global challenges like climate response which necessarily require global participation.
The role of ICTP is of even greater importance in coming years. Recent decades have seen spectacular progress in fundamental and applied science spanning quantum science and technology to high-performance computing and machine learning. These present great opportunities and great challenges. ICTP is responding by expanding its mission with exciting new initiatives like the `International Consortium for Scientific Computing (ICOMP)' in collaboration with foundations, countries, corporations and research agencies (which include Kuwait Foundation, Arab Fund, Simons Foundation, Brazil, South Africa, IBM, and CECAM among others).

Atish Dabholkar *is the director of the Abdus Salam International Center for Theoretical Physics (ICTP) in Trieste, Italy. He is a theoretical physicist from India working in the field of string theory, black holes, and holography. Atish Dabholkar received his PhD in theoretical physics from Princeton University under the supervision of Jeffrey Harvey. He did his Masters in Physics from the Indian Institute of Technology, Kanpur. Dabholkar is the recipient of the 2006 Shanti Swarup Bhatnagar Prize, the highest Indian science prize awarded by the Prime Minister of India. He was awarded the Chaire d'Excellence of the Agence Nationale de la Recherche in France in 2007. He is an elected Fellow of Indian Academy of Sciences and The World Academy of Sciences (TWAS) for the advancement of science in developing countries. Dabholkar was the Head of ICTP's High Energy, Cosmology and Astroparticle Physics section prior to taking up the directorship. He has been Professor of Theoretical Physics at the Tata Institute of Fundamental Research, Directeur de Recherche of the Centre National de la Recherche Scientifique (CNRS) at Sorbonne Université and a Visiting Professor at Stanford University and CERN. He was a post-doctoral associate at Rutgers University and Harvard University, and a senior research fellow at California Institute of Technology.*

Gihan Kamel, SESAME Facility, Jordan

SESAME: a beacon of hope in the Middle East, shining through even in times of wars

Synchrotron-light sources are particle accelerators used across a wide range of scientific and technological fields, from basic to applied sciences like physics, chemistry, biology, and geology, to materials science, biomedicine, and environmental studies. They have also garnered significant interest in cultural heritage, archaeology, and paleontology.
Functioning democratically based on scientific merit, these sources have a well-recognized societal impact on education, advancing science and technology, and building human capacity.
The Synchrotron-light for Experimental Science and Applications in the Middle East, SESAME, is the only synchrotron light facility in the Middle East and its neighboring regions. An intergovernmental organization at the service of its members and the whole world. Its current Members are Cyprus, Egypt, Iran, Israel, Jordan, Pakistan, Palestine and Türkiye. With Brazil, Canada, China (People's Republic of), the European Organization for

Nuclear Research (CERN), the European Union (EU), France, Germany, Greece, Italy, Japan, Kuwait, Portugal, Russian Federation, Spain, Sweden, Switzerland, the United Arab Emirates, the United Kingdom, and the United States of America are observers.
SESAME aims for excellence in science and technology, human capacity building, reversing brain drain, enhancing gender balance, and fostering peace and understanding in a turbulent region. It is celebrated as a prime example of science diplomacy in action.
SESAME provides an inclusive platform for scientists worldwide to pursue their ambitions in an unbiased, supportive, and tolerant environment that upholds human rights and promotes gender equality. It represents a concerted effort to strengthen self-determination and ensure justice. The presentation highlights SESAME's role in the Middle East, showcasing its milestones, success stories, and ongoing challenges across various fronts.

Gihan Kamel *is the SESAME (Synchrotron Light for Experimental Science and Applications in the Middle East) Infrared Beamline Principal Scientist, on leave from the Physics Department, Faculty of Science, Helwan University, Cairo, Egypt. Dr Kamel obtained her Ph.D. in Physics in 2011 from the University of Rome, La Sapienza, Italy, and was beamline researcher at Daϕne-light at the Italian Institute for Nuclear Physics (LNF-INFN) before moving to SESAME in 2015. At SESAME, she focuses on using infrared light for various scientific studies, ranging from biology, medicine, archaeology, material science among many others. Her work has had a significant impact on expanding research opportunities and fostering scientific exchange across borders in a region with a complex political landscape. Through her efforts, Kamel has become an advocate for the role of science in building bridges and fostering peaceful collaboration. She is also extensively involved in the establishment of the first African Light Source. In 2015, she earned recognition for her presentation at a TEDxCERN | TED conference on the theme of "Breaking the Rules.". Dr. Kamel was honored with a recognition of the President of the Italian Republic at the International Day of Women in 2017. In 2020, she was awarded the Eureka South Shore Prize ex-aequo Laureate of Eureka Prize of the French organization amcsti (The professional network of scientific, technical and industrial cultures) for her role at SESAME that brings together scientists from the eight founding states of this unique experiment in this region. In 2021, as part of the 'Championing the Decade of Action' - an initiative being implemented by ECA and other UN agencies, Dr Kamel was selected by the United Nations Economic Commission for Africa (ECA) as one of twenty-five African Women scientists featured within the African and global research and development (R&D) communities in the publication titled "Earth, Oceans and Skies: Insights from selected, outstanding African women scientists". In 2023, she was chosen by Nature to comment on the challenges facing women scientists in the Middle East. Gihan Kamel received the John Wheatley Award from the American Physical Society (APS) in 2024.*

Tatsujiro Suzuki, Research Center for Nuclear Weapons Abolition, Nagasaki University, Japan

Role of science (scientists) in policy making - personal experiences in civilian nuclear energy and nuclear disarmament issues

"*Science without policy is science, but policy without science is gamble*" – This is a famous quote from Dr. David Grey, former Director of International Institute for Applied Analysis (IIASA). I was inspired by this statement and have been working mainly on the nexus between civilian nuclear energy and nuclear weapons and I have also been involved as a

member of Pugwash movement since late 1990s. I would like to outline my own personal experiences on the following three subjects:

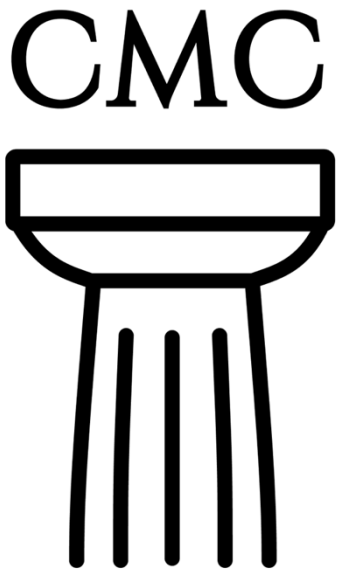
First, plutonium issue is the key nexus between civilian nuclear energy and nuclear weapons. Scientific rationale to produce plutonium (i.e. reprocess spent nuclear fuel) for civilian use has been fading away, but a few countries, including Japan, have been maintaining a policy of reprocessing. As a result, as of the end of year 2022, more than 560 tons of plutonium stockpile exists worldwide[1] It is important to provide scientific evidence to change this "unnecessary" reprocessing activities worldwide.

Second, scientific studies on humanitarian consequences of nuclear weapons use are major driving force for maintaining "nuclear taboo" and pushing nuclear disarmament. Especially, diplomatic efforts leading to conclusion of Treaty on Prohibition of Nuclear Weapons (TPNW) are noteworthy. I was personally involved in a project to assess humanitarian consequences of possible nuclear weapons use in Northeast Asia[2]. The study is intended to illustrate risk of "nuclear deterrence" and suggest alternative security policies not dependent on nuclear deterrence.

Third, Pugwash movement was originated from the famous Russell-Einstein Manifesto. The Manifesto called for abolition of nuclear weapons and war and there is a famous quote from the Manifesto; "Remember your humanity and forget the rest"[3] Based on this spirit; Pugwash scientists contributed to nuclear disarmament through diplomatic efforts through "dialogue across the divides". Pugwash movement and Dr. Rotblat won the Nobel Peace prize in 1995 for their efforts on the movements toward abolition of nuclear weapons. Social responsibility of scientist is even more important, as new disruptive technologies, such as cyber, drones and, notably, Artificial Intelligence (AI), have been extensively used for both civilian and military use.

[1] RECNA, "World's Fissile Material Data 2024", June 2024
[2] RECNA/Nautilus Institute/APLN, "Project on Reducing the risk of Nuclear Weapons Use in Northeast Asia", 2021-2024.
[3] "Statement: The Russell-Einstein Manifesto", July 9, 1955.

Tatsujiro Suzuki *is a Professor of Research Center for Nuclear Weapons Abolition at Nagasaki University (RECNA), Japan. Before joining RECNA, he was a Vice Chairman of Japan Atomic Energy Commission (JAEC) of the Cabinet office from January 2010 to March 2014. Until then, he was an Associate Vice President of the Central Research Institute of Electric Power Industry in Japan (1996-2009) and Visiting Professor at the Graduate School of Public Policy, University of Tokyo (2005-009), an Associate Director of MIT's International Program on Enhanced Nuclear Power Safety from 1988-1993 and a Research Associate at MIT's Center for International Studies (1993-95). He is now a member of Advisory Board of Parliament's Special Committee on Nuclear Energy since June 2017. He is also a Council Member of Pugwash Conferences on Science and World Affairs (2007-09 and from 2014~), co-chair of International Panel on Fissile Materials (IPFM) and an International Advisory Board member of Asia Pacific Leadership Network for Nuclear Non-Proliferation and Disarmament (APLN). Dr. Suzuki has a PhD in nuclear engineering from Tokyo University (1988).*



CLASSICS IN MOLECULAR AND MATERIALS MODELLING

In this lecture series, we take a different look at fundamental developments of simulation and modelling. Milestone conceptual steps, methods and algorithms are presented by their originators.

These technical lectures are followed by an interview in which the speakers recall for us the period, problems, people and circumstances that accompanied these developments, providing important and unusual insight in the birth and growth of tools that we now take for granted.

The lecture series “Classics in molecular and materials modelling” is co-organized at EPFL by CECAM (https://www.cecam.org/) and MARVEL (http://nccr-marvel.ch/).

Quantum Monte Carlo



Dates : Jan 25, 2025

View full video

In this series, methods that have become fundamental tools in computational physics and chemistry are presented by their originators at a level appropriate for master and graduate students. The lectures are followed by an interview: we ask our guests to recall for us the period, problems, people and circumstances that accompanied the creation of milestone methods and algorithms that we now routinely use.
Join us to share this exciting opportunity to learn first-hand from our pioneers and get to know better the genesis of work that is now recorded in books!

David Ceperley, University of Illinois Urbana-Champaign

Quantum Monte Carlo methods in the continuum

Quantum Monte Carlo (QMC) methods, including variational Monte Carlo, and diffusion Monte Carlo are now in their seventh decade. We will briefly explain these methods and illustrate their use on several simple systems that have impacted condensed matter physics: the homogeneous electron gas and dense hydrogen. QMC methods are good at calculating microscopic properties such as the energy and optical properties when the many-body system can be modeled by a supercell of fewer than a few hundred electrons. But prediction of the phase diagram can require a larger system. In the past decade, machine learning has made remarkable progress in their ability to model intermolecular potentials. Once an accurate potential is found, It can be used to quickly survey the phase diagram. But training such potentials rely on copious accurate data. We discuss why QMC might play an important role in providing this data and illustrate with dense hydrogen. We find a surprising result for the stability of the solid hydrogen and how hydrogen transforms from a molecular hydrogen to atomic hydrogen.

David Ceperley *received his BS in physics from the University of Michigan in 1971 and his Ph.D. in physics from Cornell University in 1976. After one year at the University of Paris and a second postdoc at Rutgers University, he worked as a staff scientist at both Lawrence Berkeley and Lawrence Livermore National Laboratories. In 1987, he joined the Department of Physics at Illinois. He was a staff scientist at the National Center for Supercomputing Applications from 1987 until 2012. Professor Ceperley's work can be broadly classified into technical contributions to quantum Monte Carlo methods and contributions to our physical or formal understanding of quantum many-body systems. His most important contribution is his calculation of the energy of the electron gas, providing basic input for most numerical calculations of electronic structure. He was one of the pioneers in the development and application of path integral Monte Carlo methods for quantum systems at finite temperature, such as superfluid helium and hydrogen under extreme conditions. Professor Ceperley is a Fellow of the American Physical Society and a member of the American Academy of Arts and Sciences. He was elected to the US National Academy of Sciences in 2006 and to the UIUC Center for Advanced Studies.*



CECAM WEBINARS

Webinars are a new adventure for CECAM. We hope that you will enjoy experimenting with us on the possibilities offered by this tool to share exciting science with the community.

This format offers an interesting opportunity to facilitate access to our activities for a broader community.

While our love of the informal and productive environment of face-to-face meetings is unchanged, we plan to explore its potential as a complementary tool to our workshops and schools, being an alternative format to the CECAM Flagship program.

MDDB webinar series: “DynaRepo and beyond: Computational tools to decode dynamics and interactions in macromolecular complexes”

Dates: May 27, 2025

View full video

The Molecular Dynamics Data Bank (MDDB) project is a European-scale repository for biosimulation data, which harnesses decades of cutting-edge computational resources to build a unified database that compiles and organises all data generated by molecular dynamics (MD) simulations.

MDDB is a collaborative initiative, bringing together some of Europe’s leading institutions to transform the handling of MD data and facilitate its sharing within the scientific community. The partners involved in this exciting project are IRB Barcelona, Barcelona Supercomputing Center, their joint spin-off Nostrum Biodiscovery, along with the Royal Institute of Technology (KTH), the European Molecular Biology Laboratory, the University of Oxford, and CECAM (EPFL).

If you would like to learn more about MDDB, please visit the project’s website.

With this series of webinars, MDDB aims to engage the MD community and discuss the importance of data sharing, the methodological and technological issues involved, and present how they are addressing these challenges, with examples taken from recent projects such as the Covid19-related MD simulations database.

In this fifth instalment of the MDDB webinar series, titled DynaRepo and Beyond: Computational Tools to Decode Dynamics and Interactions in Macromolecular Complexes", Yasaman Karami and Hamed Khakzad, from Inria, University of Lorraine together with Roy Gonzalez-Aleman, from LPCT, University of Lorraine, France, will present DynaRepo, a repository of macromolecular conformational dynamics for a large set of macromolecular complexes, carefully selected from PDBind and ASBench datasets. The speakers will demonstrate how this data has been used to elucidate communication networks and allosteric signaling [1] and predict binding sites across macromolecular complexes [2]. They will also explain how DynaRepo is connected to and complements MDDB.

MDDB webinar series: “The MemProtMD Database & MDDB”

Dates: Mar 27, 2025

View full video

The Molecular Dynamics Data Bank (MDDB) project is a European-scale repository for biosimulation data, which harnesses decades of cutting-edge computational resources to build a unified database that compiles and organises all data generated by molecular dynamics (MD) simulations.

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In this fourth instalment, Charlotte Lynch & Phillip Stansfeld will present the MemProtMD database, which includes more than 7000 molecular dynamics simulations of individual membrane proteins, with each protein having been embedded in a lipid bilayer.

MDDB webinar series: “The hexABC & MDDB”

Dates: Feb 27, 2025

View full video

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During this third webinar, Federica Battistini from IRB Barcelona, will present the hexABC project, a DNA conformational study involving molecular dynamic simulations of 20-mer sequences over the sub-millisecond timescale and more of 200 TB of data.

MDDB webinar series: “High throughput molecular dynamics simulations from the LIGATE project”

Dates: Jan 23, 2025

View full video

The Molecular Dynamics Data Bank (MDDB) project is a European-scale repository for biosimulation data, which harnesses decades of cutting-edge computational resources to build a unified database that compiles and organises all data generated by molecular dynamics (MD) simulations.

MDDB is a collaborative initiative, bringing together some of Europe’s leading institutions to transform the handling of MD data and facilitate its sharing within the scientific community. The partners involved in this exciting project are IRB Barcelona, Barcelona Supercomputing Center, their joint spin-off Nostrum Biodiscovery, along with the Royal Institute of Technology (KTH), the European Molecular Biology Laboratory, the University of Oxford, and CECAM (EPFL).

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With this series of webinars, MDDB aims to engage the MD community and discuss the importance of data sharing, the methodological and technological issues involved, and present how they are addressing these challenges, with examples taken from recent projects such as the Covid19-related MD simulations database.

During this second webinar, Andrew Emerson from CINECA will introduce the LIGATE project, which aims to create and validate a leading application solution for drug discovery in High Performance Computing (HPC) systems up to the exascale level.