



Hylleraas

ANNUAL REPORT /

2025



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UiT Norges
arktiske universitet



Norwegian
Centre of
Excellence



Hylleraas Centre for Quantum Molecular Sciences

The Hylleraas Centre for Quantum Molecular Sciences is a Norwegian Centre of Excellence (CoE) shared equally between the University of Oslo (UiO) and UiT – The Arctic University of Norway (UiT), with UiO as project owner. Established on October 1, 2017, for a period of ten years, the Hylleraas Centre receives an annual funding of about 15 million NOK from the Research Council of Norway. In addition, it receives substantial financial support from UiO and UiT.

At the end of 2025, the Hylleraas Centre is one of 19 national CoEs in Norway. The goal of the CoE program

is to stimulate Norwegian research groups to establish larger units focusing on frontier research at a high international level and to raise the quality of Norwegian research.

The Hylleraas Centre aims to develop and apply computational methods to understand, interpret, and predict new chemistry, physics, and biology of molecules in complex and extreme environments. It has an extensive visitors' program for scientists from around the world, as well as for PhD candidates and postdocs from other research groups who wish to benefit from the expertise at the centre.

www.hylleraas.no

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REPORT

From the Directors

The Hylleraas Centre organized the 13th Triennial Congress of the World Association of Theoretical and Computational Chemists in June in Oslo. Chaired by Trygve Helgaker, most Hylleraas members contributed to the organization and implementation of the congress, which attracted 1098 scientists from all parts of the world. The scientific productivity of the Hylleraas Centre remained at a very high level, while Hylleraas members, adjuncts, and affiliates succeeded in securing funding for the strategically important focus areas Quantum Science and Technology and Life Science.

International conferences and meetings are crucial for the scientific community and the Hylleraas Centre has been engaged in the organization of such events from the very beginning, both small specialist workshops and large conferences covering the full breadth of theoretical and computational chemistry. Over a period of just seven years, the Hylleraas Centre has organized the three largest international congresses in the field of theoretical and computational chemistry. The 16th International Congress of Quantum Chemistry (ICQC) was held at *le Palais de l'Europe* in Menton, France, on June 18–23, 2018, chaired by then Hylleraas PI Odile Eisenstein. The 10th Triennial Congress of the International Society for Theoretical Chemical Physics (ISTCP) was held at Clarion Hotel The Edge in Tromsø on July 11–17, 2019, chaired by then Hylleraas Deputy Director Kenneth Ruud. Finally, in 2025, the 13th Triennial Congress of the World Association of Theoretical and Computational

Chemists (WATOC) was held at Oslo Congress Centre on June 22–27, chaired by former Hylleraas Director Trygve Helgaker. In addition, the new initiative Young WATOC was organized the day before the main event, on June 21, featuring invited lectures by early-career researchers, either students or with a doctoral degree obtained no earlier than 2020. Young WATOC was chaired by Ainara Nova and Abril Castro.

The organization of WATOC 2025 required intense efforts by many Hylleraas members in 2025. The Local Congress Committee comprised all PIs in Oslo – David Balcells, Michele Cascella, Abril Castro, Simen Kvaal, Ainara Nova, Thomas Bondo Pedersen, Simen Reine, and Erik Tellgren plus researcher Sigbjørn Løland Bore and affiliates Odile Eisenstein and Einar Uggerud. Simen Reine and Erik Tellgren served as congress secretaries. The committee defined the conference

program, partitioned into plenary and thematic parallel sessions and three poster sessions, with a total of 330 lectures and 627 posters. During the congress, the WATOC Crew helped the 1098 participants with any matter, including registration and assistance at all lectures. In addition, the Crew organized the social program which included morning runs, walks, and sauna sessions, as well as Wednesday-afternoon activities such as hikes, guided walking tours, and an evening networking event at Røør Bar. A detailed report on the organization and implementation of WATOC 2025 is available on the centre's website.

The Crew consisted of the following Hylleraas members: Derya Aricigil, Michael Augello, Lucas Bitencourt Theodoroviez, Marco Bortoli, Klara Elvira Haug Boström, Ning Cao, Henrique Musseli Cezar, Aurore Evelyne Francine Denjean, Mohamed Eid Ahmed Safy, Sondre Eliasson, Hanne Jeeyung

// International collaboration, combined with strong teamwork and shared vision, drives scientific progress and brings together a global community to advance innovation //

Eriksen, Håkon R. Fredheim, Miguel Ángel Gaona Fernández, Gabriel Gerez, Hanan Gharayba, Lucía Morán González, Jose Alberto Guerrero Cruz, Helena Hradiská, Catherine Hughes, Hannes Kneiding, Håkon Emil Kristiansen, Morten Ledum, Manuela Leal Nader, Oliver Macphail Bohle, Daniel Marke, Joel Ormala, Quentin Pitteloud, Mauricio Portolli Franco, Tonje Reinholdt Haugen, Jordan Rio, Inga Lena Schmidtke, and Simon Elias Schrader, and Øystein Senstad Alve.

The Crew was divided into three equally large teams, each led by one of the three team leaders: Morten Ledum, Lucía Morán González, and Henrique Musseli Cezar. Marco Bortoli acted as the official WATOC photographer, assisted by Hylleraas Communication Adviser Cathrine Strøm at the closing ceremony on June 27.

We are indebted to Trygve Helgaker for his tireless efforts in leading the organi-

zation of WATOC 2025 and we extend our sincere gratitude to all Hylleraas members for their diligent efforts in the planning and execution of the congress, which was praised as outstanding by WATOC President Prof. Peter Gill at the closing ceremony. Gill also highlighted Young WATOC as a very valuable addition that will continue at the next WATOC Congress in Merida, Mexico, in 2028.

The Annual Hylleraas Meeting is an important event for the coherence of the centre, maintaining the close ties between members working in Oslo and Tromsø. The 2025 edition of the meeting was held at Malangen Brygger Resort in Mestervik, Troms, and organized by Helena Hradiská and Inga Lena Schmidtke, the Tromsø representatives of the Young Researcher Parliament (YRP). Our sincere thanks go to them for ensuring the success of the Malangen meeting.

Several other impactful events were organized by centre members and adjuncts in 2025:

- Hylleraas School (Inga Lena Schmidtke, Tonje Reinholdt Haugen, Michal Repisky, David Balcells, Simen Reine)
- Hylleraas Hackathon (Magnus Ringholm)
- Young CAS Symposium: Can ice be described from first principles? (Sigbjørn Løland Bore)
- Quantum Science at 100 (Trygve Helgaker, Kenneth Ruud)
- Numerical Methods in Quantum Chemistry (Luca Frediani, Michal Repisky)
- Annual Meeting of the Division for Quantum Chemistry and Modelling of the Norwegian Chemical Society (Magnus Ringholm)

We extend our gratitude to all organizers for their dedicated efforts in making these events a success.

Despite the many hours invested in organizing WATOC and other events, members of the Hylleraas Centre maintained a high level of productivity, with 75 papers published in scientific journals covering a broad range of disciplines. At the end of 2025, the centre has published a total of 570 papers with more than 9000 citations and an H index of 43.

We congratulate Simen Kvaal and Hylleraas adjunct Andre Laestadius on their participation in the RCN Quantum Technology Centre grant QSTAR, which is led by Franz Fuchs (Sintef) and set to start in April 2026. We also congratulate Michele Cascella and Hylleraas affiliate Reidar Lund on their UiO:Life Science Convergence Environment grant PERMEATE, which will start in August 2026. These achievements are strategically important milestones for the Hylleraas Centre.

In February 2025, EU Horizon Europe MSCA postdoctoral fellowships were awarded to three young scientists with supervisors at the Hylleraas Centre: Josefine Hvarregaard Andersen (supervisor: Magnus Ringholm in Tromsø), Lucía Morán González (supervisors: Ainara Nova and David Balcells in Oslo) and Jordan Rio (supervisors: Michele Cascella, David Balcells, Ainara Nova, and Odile Eisenstein in Oslo). We congratulate Josefine, Lucía, and Jordan as well as their supervisors with the successful proposals and look forward to the exciting research made possible by the grants.

Three grants of computer time at the European High-Performance Computing Joint Undertaking were awarded to Hylleraas members Marco Bortoli, Henrique Musseli Cezar, and Luca Frediani. Marco and Henrique were awarded regular access grants of

about 8 million CPU and 700 thousand GPU hours, while Luca received a development access grant of 200 thousand CPU hours. Worth roughly 4.1 MNOK according to the Category A pricing model of Sigma2, these grants significantly increase the scope of computational research at the Hylleraas Centre. Congratulations to Marco, Henrique, and Luca on these important achievements.

Our congratulations and best wishes are extended to the three young centre members who defended their PhD theses in 2025: Ning Cao, Inga Lena Schmidtke, and Aurore Denjean.

Building on her foundational work in 2024, 2025 saw Communication Adviser Cathrine Strøm continue revising and improving our communication procedures and outreach activities. We are grateful to Cathrine for her efforts.

We wish to recognize the retirement of Jan Ingar Johnsen, the Head of Office in Oslo since the opening of the centre in 2017. Before that he served as Head of Office at the Centre for Theoretical and Computational Chemistry, the predecessor of the Hylleraas Centre. We are incredibly grateful for his years of dedicated service and his role in making

our daily operations run seamlessly. His contribution to our research community has been invaluable, and we wish him the very best in his retirement. We welcome his successor, Ragna Breines, as Head of Office in Oslo.

Every year, several social events are organized at the Hylleraas Centre, including the Christmas parties, Easter parties, Summer parties, and Board-game nights. We would like to thank all centre members that take the initiative and help organize these social events.

We are grateful to the Young Researcher Parliament (YRP) representatives in 2025, Quentin Pitteloud (UiT), Helena Hradiská (UiT), Inga Lene Schmidtke (UiT), Ylva Os (UiT), Manuela Leal Nader (UiO), and Oliver Macphail Bohle (UiO), for their dedicated efforts for the entire Hylleraas Centre and for the young members, in particular. In Tromsø, Quentin Pitteloud stepped down in April and Helena Hradiská in November. Inga Lene Schmidtke and Ylva Os were elected to replace them.

Finally, we would like to thank all members, adjuncts, and affiliates of the Hylleraas Centre for their excellent work in 2025, as detailed in this report.



Prof. Thomas Bondo
Pedersen
Director



Prof. Luca Frediani
Deputy Director

From the Board of Directors

The Board of Directors is pleased to note that the Hylleraas Centre continues to produce science at the highest international level, also in the final phase of the Centre's ten-year period (2017–2027). Building on last year's work, 2025 has been characterized by strategic alignment and proposal activity, particularly in areas of high national and international importance: Artificial intelligence for chemistry and computational tools for Quantum Technology developments, alongside important contributions spanning climate change, green transition and the life sciences.

A recurring theme throughout the year has been the Centre's strategy towards a possible future application for a third Centre of Excellence (CoE). The Board welcomes that this strategic ambition has now been translated into concrete action: two CoE proposals have been submitted in 2025, one centred on artificial intelligence for catalysis, led by David Balcells and anchored in Oslo, and one centred on quantum technology, also primarily Oslo-based while explicitly including the Tromsø node through the participation of Michal Repisky. The Board considers these submissions an important milestone. They demonstrate both scientific ambition and a clear alignment with priority areas where Norway and Europe are currently investing heavily.

While the CoE work has been a visible focal point, the Board notes that the overall level of additional proposal activity beyond these major initiatives

appears more limited than what the centre has achieved in some earlier years. The Board recognizes that many principal investigators already carry substantial project portfolios and leadership responsibilities. At the same time, maintaining a strong and diversified funding pipeline remains essential for sustaining momentum, enabling recruitment, and supporting high-risk, high-gain directions. The Board therefore encourages centre members to continue identifying opportunities – national and international – and to make active use of internal mentoring and collegial proposal support mechanisms that have previously contributed to notable successes.

In 2025, the Board has also been pleased to see continued progress on RTO – the Hylleraas Software Platform as a centre-wide enabling activity. Strengthening shared software foundations is increasingly important both for internal synergies and for external

collaboration with top-tier groups in Norway and abroad. The Board encourages the centre to keep investing in sustainable software practices, visibility, and community-building around key tools, as these are becoming central deliverables in modern theoretical and computational chemistry.

The availability of robust computational resources remains a prerequisite for the Hylleraas Centre's success. Following the funding-model transitions in recent years, the Board welcomes the continued attention given to securing adequate capacity for core activities. Looking ahead, the Board encourages the centre to intensify the strategic use of Euro-HPC-JU resources in addition to national infrastructure. A successful approach here can reduce vulnerability to national cost fluctuations and provide access to capability-class systems increasingly needed for research directions such as machine learning, molecular dynamics,

and large-scale quantum chemistry. The Board underlines that sustained access to computing is not merely an operational concern but a strategic asset to achieve the centre goals.

A major highlight for the centre and its community in 2025 has been the successful hosting of the WATOC 2025 congress in Oslo. The Board applauds the centre's visible leadership role in this major international event, which brought together a very large international community of theoretical and computational chemists in Norway. The Board would like to express particular thanks to Trygve Helgaker for taking the lead in organizing the congress, and to all those who contributed to its success. The Board also commends the initiative to establish a Young WATOC day in connection with the congress, and notes with satisfaction that this initiative is planned to be carried forward to the next WATOC edition.

The Board further notes as a significant recognition of scientific impact that the Trygve Helgaker Festschrift was published in 2025 as a dedicated collection in the Journal of Physical Chemistry A, with Hylleraas leadership prominently involved in the editorial work. Such contributions strengthen the

centre's international visibility and help communicate foundational advances in electronic structure theory and computational chemistry.

The Board is also pleased to see positive developments at the Tromsø node in 2025: the increased recruitment activity with strong candidates enrolled for PhD and postdoctoral positions, including the presence of an MSCA fellow, and views this as important for both scientific output and long-term capacity building. The co-organization by the Tromsø node of the NMQC2025 (Numerical Methods for Quantum Chemistry 2025) in Berlin, as a satellite workshop in connection with the WATOC falls in a now consolidated tradition. It illustrates the centre's ability to contribute to international community-building across both nodes.

In the quantum-technology direction, 2025 has also marked a strengthening of Norway's national landscape, and the Board notes with satisfaction that Hylleraas researchers contribute to the newly announced quantum-technology research centre QSTAR (Centre for Quantum Computing and Applications), led by Franz Fuchs (SINTEF), which focuses on methods for error correction,

algorithms, and software – areas where quantum chemistry is an important application and test domain. The Board welcomes this development as well aligned with the Hylleraas Centre's strategic emphasis on quantum technology and collaborations with strong national partners.

The Board also applauds Hylleraas researchers' contributions to the recently established UiO:Life Science Convergence Environment PERMEATE (Peptides for Membrane Targeting and Synergistic Drug Delivery). This grant significantly increases the visibility and impact of the Hylleraas Centre in the strategically important field of life science.

We conclude by expressing our thanks to the leadership of the Hylleraas Centre and to all members across Oslo and Tromsø for their continued efforts and achievements. The Board looks forward to supporting the centre through 2026 as the CoE proposals are followed up, as the software platform matures further as an enabler of scientific discovery, and as the centre continues to strengthen its international position in artificial intelligence for chemistry, quantum technology, and other strategically important domains.



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Aslak Tveito
Professor
Simula Research
Laboratory

From the Young Researchers

The Young Researchers Parliament (YRP) is an effort to bring together postdoctoral researchers, Ph.D. candidates, master's students and visiting students to promote a supportive and inclusive environment for early-career researchers. Representatives from each node are elected by the young researchers to sit on the Hylleraas Centre management team. Their primary role is to facilitate communication between young researchers and the management team. In addition, the YRP is responsible for planning the annual meeting, arranging alumni talks, organising events, and inviting external speakers.

Since 2019, the YRP has served as the voice of young researchers at the Hylleraas Centre. Through regular meetings, it provides a forum for exchanging ideas, raising concerns, and engaging in discussions. Subjects considered relevant for the entire Centre are communicated to the management team by elected representatives. This way, the YRP helps young researchers to play an active role in shaping the Centre and to explore their own independence as researchers. Additionally, the YRP exerts influence in the Centre by inviting external speakers and participating in the organisation of events.

To create an inclusive and enjoyable work environment, the YRP also arranges casual social events for the young researchers. During the semester, both nodes have monthly pizza meetings

that are arranged by the YRP and which provide a platform to discuss important matters. Additionally, other small social activities are being planned by the YRP. This Autumn, the YRP in Tromsø arranged a bonfire grilling in the snow. Both Tromsø and Oslo parliaments invited Angela Wilson, speaker of the Almlöf-Gropen seminar to an informal discussion, during which she talked about her career path, work-life balance and some of the challenges of being a woman in a male-dominated field.

This year's meeting was held at Malangen resort, located at the name giving Malangen fjord just outside of Tromsø. The meeting was organized by the YRP representatives of the Tromsø node. This edition of the Annual Meeting was attended by 43 participants, mainly Hylleraas members and affiliates, but

we were joined by several external speakers as well. After a brief overview on the Hylleraas Centre by Thomas Bondo Pedersen, the meeting was kicked off with a workshop covering the broad topic of visualization in scientific works given by Kess Marks and Moa Kristiansson from Visualize your Science. The workshop ended with a talk focusing on poster design and afterwards we could use that newly acquired knowledge in a poster session. During the poster session, the young researchers of the Centre presented their ongoing work. This concluded the busy scientific part, and we ended the first day enjoying a barbecue at the nearby lake.

The second day was opened by Bror-Magnus S. Strand and Gulbrand Stålet Nilsen from the UiT library with a talk on open science, data management

and the new online research information repository solution, NVA. Their talk was followed by another invited talk given by Gabriel Gerez and Jørn Dietze from the HPC group at UiT. Gabriel and Jørn gave a brief overview on slurm scripts, data handling and general best practices.

We continued the programme with the traditional 5-minute presentations, this time with reversed roles. For the first time at a Hylleraas Annual Meeting, the senior researchers of the Centre gave us an overview of their research in this format. The evening session was concluded with a talk by Odile Eisenstein who took us with her on her life journey through science with a lot of personal insight and valuable advice.

The YRP visitor programme serves as an opportunity for young researchers to broaden their perspectives on both career pathways and academic interests. Based on suggestions by fellow members of the Centre, the representatives are encouraged to invite distinguished professors and researchers from other institutions, as well as former members of the Centre, to give talks during the Friday seminar series.

On behalf of the YRP, UiO representatives invited Prof. Paul Walton for a visit to the Hylleraas Centre in Oslo on the 31st of January. During his visit, he gave a seminar on “Gender Equality in Academia” to the whole centre. Also, the YRP representatives in Oslo organised an informal discussion between Prof. Walton and the young researchers, during which he shared career advice and recounted several personal stories about the multiple times he has given this seminar on gender equality.

The alumni component of the visitor programme was particularly active in 2026. The Oslo node welcomed Audun Skau Hansen, who shared insights into his career choices and gave an overview of his latest projects. Marius Kadek was invited by the Tromsø node to share his experiences on “Life as a scientist after academia”. In Tromsø, we were also visited by former member Magnar Bjørgve, now part of the HPC group of NRIS in Tromsø, who asked and discussed the question of “Can Hylleraas achieve more science at lower cost using the national HPC resources?”. Our last invited speaker of the year was Taye B. Demissie who gave a talk titled “From Computationally-Guided Drug Design and Synthesis to Drug Delivery”.

Each node of the Hylleraas Centre elects two representatives, each serving a term of approximately one year. In Tromsø, Quentin Pitteloud stepped down in April and Helena Hradiská in November. Inga Lena Schmidtke and Ylva Os were elected as new representatives. In Oslo, there were no changes to the representatives. We, on behalf of everyone at the Hylleraas Centre, would like to thank Quentin Pitteloud and Helena Hradiská for their hard work and contributions to the YRP and the whole Hylleraas Centre.

Elected YRP representatives 2025



Oliver Macphail Bohle



Manuela Lea Nader



Quentin Pitteloud



Helena Hradiská



Inga Lena Schmidtke



Ylva Os

2025 IN BRIEF /

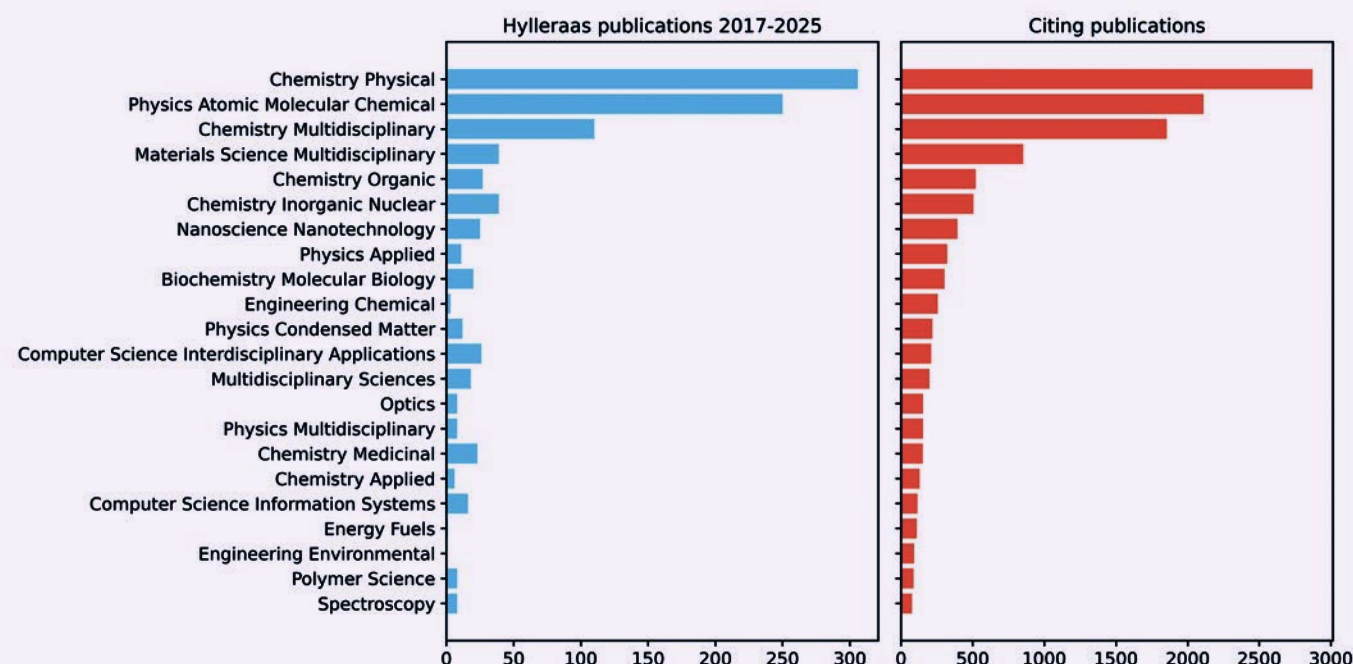


Figure 1: Categorization of the Hylleraas publications 2017-2025 and of the non-Hylleraas publications citing these. Note that the categorization is non-exclusive such that a single paper may be counted in several categories. Illustration by Thomas Bondo Pedersen using data extracted from Clarivate Web of Science.

Publications

Members of the Hylleraas Centre published 75 articles in 2025, bringing our total scientific production to 570 publications since the centre opened in October 2017. Slightly less than 10% of these were published in journals with impact factor above ten, mainly within chemistry, physics, and nanoscience. According to Clarivate Web of Science, at the end of 2025, the articles published by the Hylleraas Centre had been cited about 9000 times in 7300 publica-

tions by authors outside the centre, with an H-index of 43. In addition to the peer-reviewed research articles, Michele Cascella published the book *Theoretical Foundations of Multiscale Modelling*, together with Prof. Raffaello Potestio from University of Trento, Italy.

Most of the publications of the Hylleraas Centre can be classified as physical chemistry (53%), chemical physics (44%), or multidisciplinary chemistry

(19%). These categories also apply to most of the citing papers, as seen in Figure 1 which has been generated using data from Clarivate Web of Science, including the non-exclusive categorization. Self-citations have been excluded, i.e., papers with authors affiliated with the Hylleraas Centre are excluded in the right panel of Figure 1. The number of citing publications is an order of magnitude greater, also in research fields where the centre activities are

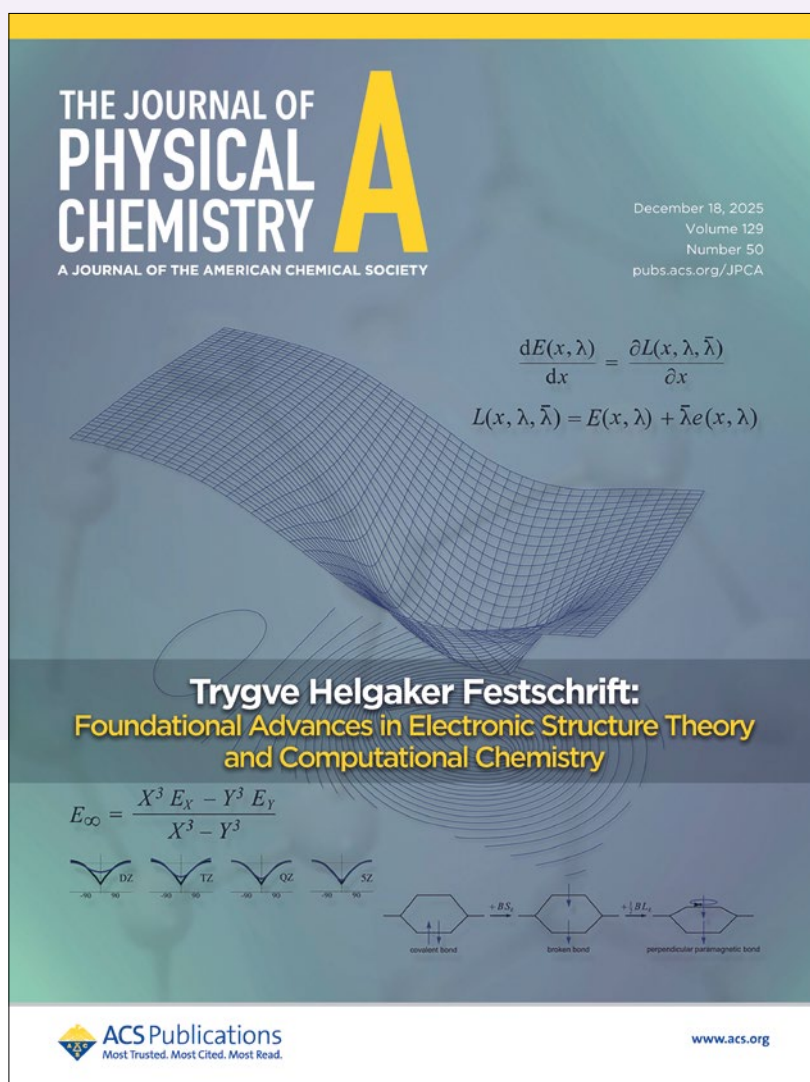


Figure 2: Front page of the Trygve Helgaker Festschrift, published on December 18 in the Journal of Physical Chemistry A.

minor, showing that the centre's research has a significant impact well beyond its core research themes.

With ongoing geopolitical changes fundamentally altering international relations, it becomes even more important to maintain international collaborations within basic science. In 2025, the Hylleraas Centre has continued international collaborations and has published papers with co-au-

thors from 24 countries across the world. Most international co-authors come from USA (118 papers in total/12 in 2025), Germany (111/19), France (62/8), England (58/6), and Denmark (52/9).

Together with Prof. Sonia Coriani from the Technical University of Denmark, Thomas Bondo Pedersen, Erik Tellgren, and Michele Cascella acted as Guest Editors of the virtual special issue *Trygve Helgaker Festschrift: Foundational*

Advances in Electronic Structure Theory and Computational Chemistry of the Journal of Physical Chemistry A (Figure 2). Published on December 18, the virtual special issue honors the career and achievements of Trygve Helgaker and contains a tribute, an intriguing autobiography, and more than 50 research papers authored by Helgaker's colleagues and collaborators around the world, including the Hylleraas Centre.



Figure 3: Prof. Seiichiro L. Ten-no, Kobe University, delivering his lecture at the Norway-Japan Seminar at the Hylleraas Centre in Oslo on February 26. *Photo: Thomas Bondo Pedersen.* **Figure 4:** Sigbjørn Løland Bore during a coffee break at the YoungCAS symposium “Can Ice be Described from First Principles”. *Photo: Camilla Kottum Elmar/CAS.* **Figure 5:** Organizers of the 2025 Hylleraas Annual Meeting Helena Hradiská (left) and Inga Lena Schmidtke (second from left) with fellow YRP representatives Manuela Leal Nader (second from right) and Oliver Macphail Bohle (right) in glorious September weather at Malangen Brygger Resort. *Photo: Marco Bortoli.* **Figure 6:** Poster session at the 2025 Hylleraas Annual Meeting. *Photo: Marco Bortoli*

Meetings and conferences

Several meetings were organized by Hylleraas members in 2025. Michiko Atsumi and Erik Tellgren organized the *Norway-Japan Seminar* on February 25–26 with participants attending physically at the Hylleraas Centre in Oslo (Figure 3) and digitally from various locations in Japan.

Sigbjørn Løland Bore (Figure 4) organized the international symposium *Can Ice be Described from First Principles* at the Norwegian Academy of Science and Letters on March 28–29, with 40

participants, including 20 invited lecturers from abroad. The symposium was organized as part of Bore’s YoungCAS project. The *Hylleraas Hackathon* was held at Skibotn near Tromsø on May 5–9, organized by Magnus Ringholm, with about 25 participants. The *Hylleraas Annual Meeting* took place at Malangen Brygger Resort near Mestervik on September 8–10 with 43 participants. It was organized by YRP representatives Helena Hradiská and Inga Lena Schmidtke (Figure 5) with support from

Stig Eide and Magnus Ringholm. The varied program included ample opportunities for scientific discussions (Figure 6) and social activities (Figure 7).

Chaired by former Hylleraas director Trygve Helgaker, nearly all members of the Hylleraas Centre in Oslo and young members from Tromsø contributed to the organization and implementation of the *13th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2025)*. The congress, which is the largest meeting



Figure 7: Barbecue at Nikkavatnet in the evening of September 8 during the Hylleraas Annual Meeting. *Photo: Marco Bortoli.* **Figure 8:** Svein Stølen, Rector of the University of Oslo, speaking at the opening ceremony of WATOC 2025 on June 22. *Photo: Marco Bortoli.* **Figure 9:** Young WATOC chairs Ainara Nova (left) and Abril Castro (right) at the podium on June 21. *Photo: Marco Bortoli.*

series on the international meeting calendar in theoretical and computational chemistry, was held at Oslo Congress Centre in central Oslo on June 22–27, with 1098 participants from across the globe. In his last official act as Rector of the University of Oslo, Svein Stølen addressed the audience at the opening ceremony on June 21 (Figure 8). A new initiative, Young WATOC, was chaired by Ainara Nova and Abril Castro (Figure 9) and held at the same venue on June 21 with 18 carefully selected lecturers with a doctoral

degree obtained no earlier than 2020. In total, 330 lectures and 627 posters were presented at WATOC 2025, making it the largest event in 2025 in the field of theoretical and computational chemistry.

Together with Dr. Florian Bischoff, Humboldt University of Berlin, Luca Frediani and Michal Repisky from the Hylleraas Centre organized the workshop *Numerical Methods in Quantum Chemistry* as a WATOC satellite meeting on June 18–20 in Berlin,

Germany. The three-day workshop gathered leading experts across theoretical chemistry, physics, and mathematics and featured 37 presentations.

The *2025 Annual Meeting of the Division for Quantum Chemistry and Modelling of the Norwegian Chemical Society* was organized by Magnus Ringholm at UiT – The Arctic University of Norway on October 20–21, gathering the Norwegian theoretical chemistry community. The program included 16 lectures



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Figure 10: Former Hylleraas member Roberto Di Remigio Eikås from Algorithmiq delivering his lecture at the annual meeting of the Division for Quantum Chemistry and Modelling of the Norwegian Chemical Society on October 20 in Tromsø. *Photo: Thomas Bondo Pedersen.* **Figure 11:** Hajime Matsumara, Deputy Head of Mission at the Embassy of Japan in Oslo, with Michiko Atsumi (left), Erik Tellgren (second from right), and Trygve Helgaker (right) in front of the Hylleraas Exhibition at the Hylleraas Centre in Oslo on October 27. *Photo: Cathrine Strøm.* **Figure 12:** Prorektor Bjørn Jamtveit of the University of Oslo opening the Japan-Norway Research Alliance Seminar at the Hylleraas Centre in Oslo on October 27. *Photo: Cathrine Strøm*

presented by early-career researchers at Norwegian universities, including 6 from the Hylleraas Centre. Former Hylleraas member Roberto Di Remigio Eikås, now at Finnish quantum computing company Algorithmiq, delivered an invited lecture on end-to-end quantum chemistry on quantum computers (Figure 10).

Celebrating 120 years of diplomatic relations between Norway and Japan, the Hylleraas Centre in Oslo hosted the *Japan-Norway Research Alliance Seminar* on October 27. Organized by Michiko Atsumi and Erik Tellgren from the Hylleraas Centre (Figure 11), the hybrid (physical and digital) event was attended by 60 people and was opened by the UiO Prorektor Bjørn Jamtveit (Figure 12).

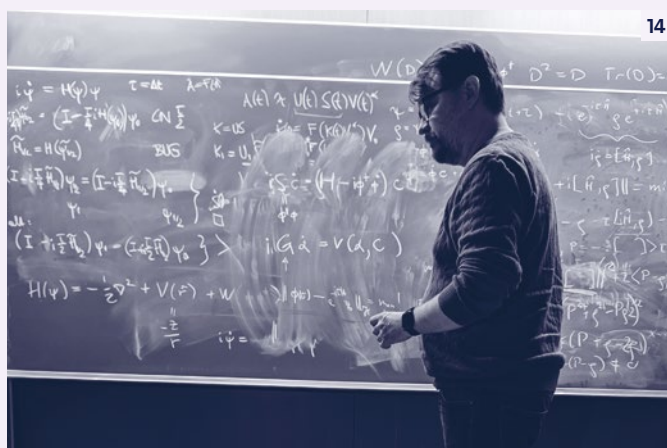
The 100th anniversary of the establishment of quantum theory was celebrated by a one-day meeting at the Norwegian Academy of Science and Letters. Supported by the Hylleraas Centre and organized by Trygve Helgaker, former Hylleraas deputy director Kenneth Ruud, Prof. Arne Brataas (Norwegian University of Science and Technology), and Prof. Susanne Viefers (University of Oslo), the event gathered a broad audience of 70 people, ranging from leading experts in the field to interested laypersons.

In 1975, Jan Almlöf was appointed professor at the University of Oslo by Royal Decree. To celebrate this anniversary, his last doctoral student, Professor Angela K. Wilson from Michigan State University, USA, delivered the 2025 Almlöf–Gropen

Lecture, *Unraveling the Periodic Table: From Thermochemistry and Excitation Pathways to Environmental Impact*, on September 23 in Oslo and September 25 in Tromsø. At both events, the Almlöf–Gropen Young Speakers were Inga Lena Schmidtke from Tromsø and Simon Elias Schrader from Oslo. The title of Inga's lecture was *Computational Insights into Methane-Benzene Dehydrogenative Coupling by a Homogeneous Iridium Catalyst* while that of Simon's lecture was *Solving the Time-Dependent Schrödinger Equation with Adaptive Gaussians*.



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Figure 13: Ainaro Nova delivering her Young Plenary Speaker lecture at the University of Bern, Switzerland, on July 17. Photo: : Swiss Chemical Society.

Figure 14: Simen Kvaal during discussions of wave-function propagation schemes at the library of the Mathematisches Forschungsinstitut Oberwolfach in the evening of March 12. Photo: Thomas Bondo Pedersen.

Figure 15: Announcement of Trygve Helgaker's XingDa Lecture at the College of Chemistry and Chemical Engineering, Peking University, China, on November 28. Photo: Trygve Helgaker

Dissemination

The members of the Hylleraas Centre gave numerous oral presentations in 2025, including 15 presentations given by young members and 11 by senior members and visitors as Friday seminars at the centre. A total of 25 Friday seminars were given at the Hylleraas Centre in 2025, one of them with two speakers. Three seminars were YRP alumni talks and two were YRP-invited speakers, Prof. Paul Walton from the University of York, UK, and Prof. Taye B. Demissie from the University of Botswana. Walton's seminar, *Gender Equality in Academia*, provided an overview of the evidence behind gender inequality in academia, and how that evidence can be used to achieve equality in academia, while Demissie's seminar discussed *From Computationally Guided Drug Design and Synthesis to Drug Delivery*.

Thomas Bondo Pedersen, Simen Kvaal, and adjunct associate professor Andre Laestadius delivered invited lectures on *Quantum Dynamics Without the Born-Oppenheimer Approximation*, *A Mathematical Approach to Coupled-Cluster Theory*, and *Using Moreau-Yosida Regularization in Density-Functional Theory*, respectively, at the workshop *Mathematical Methods in Quantum Chemistry* at the famous Mathematisches Forschungsinstitut Oberwolfach in the Black Forest in Germany (Figure 13).

As Young Plenary Speaker at the XXVI European Conference on Organometallic Chemistry in Bern, Switzerland, Ainaro Nova presented an overview on *The Design of Homogeneous and Heterogeneous Catalysts for Hydrogenation Reactions Using Computational Methods and Microkinetic*

Modelling (Figure 14). Almost simultaneously, David Balcells gave an invited lecture on *Evolutionary and Deep Machine Learning for Transition Metal Chemistry* at the Telluride Science and Innovation Center workshop on *Machine Learning Advances for Molecular and Materials Property Prediction* in Telluride, Colorado, USA.

Luca Frediani and Michal Repisky both gave invited talks at WATOC 2025 in Oslo. Frediani's talk had the title *Quantum Chemistry with Multiwavelets: from Exotic Niche to Widespread Applicability*, and Repisky's title was *Relativistic Real-Time Dynamics: Ultrafast Chirality in Molecules*. Trygve Helgaker delivered the XingDa Lecture *The Exotic Chemistry of Ultrastrong Magnetic Fields* at the College of Chemistry and Chemical Engineering, Peking University, China (Figure 15).



Figure 16: Well-visited poster session at *Hvorfor Det?* on March 29 at the Department of Chemistry, University of Oslo.
Photo: Cathrine Strøm.

Outreach

On March 29, the Hylleraas Centre in Oslo hosted *Hvorfor Det?* (Figure 16), a science poster competition for school children aged 7 to 13. The event was organized by the parents' board at *Ila Skole*, a primary school in Oslo, with support from the centre. About 100 children participated together with their siblings, parents, and grandparents. Hylleraas members Audun Uglenes Bergan, Trygve Helgaker, and Thomas Bondo Pedersen along with former members Audun Skau Hansen and Benedicte Sverdrup Ofstad participated as referees.

David Balcells participated in a roundtable discussion organized by the Spanish Royal Society of Chemistry on the use of artificial intelligence in chemistry research. The transcript of the discussion is published in *Anales de Química de la Real Sociedad Española de Química*, volume 121, pages 6–10 (2025).

On September 24, Aina Nova gave an inspirational lecture to students at the event *From Student to a Career* at the Department of Chemistry, University of Oslo. Organized by the Department of Chemistry, these lectures are aimed at informing students about career opportunities in chemistry.

The open academy meeting *Kvantemekanikken 100 år: Fra usikkerhetsrelasjonen til høyteknologi* was held at the Norwegian Academy of Science and Letters on October 30, marking the UN International Year of Quantum Science and Technology. Trygve Helgaker chaired the event and Thomas Bondo Pedersen delivered a lecture on the transformative role quantum mechanics has had in the understanding of chemistry and how it remains a central component of research at the Hylleraas Centre.

An interview with Hylleraas members Michele Cascella and Manuela Leal Nader, Hylleraas affiliate Reidar Lund, and researcher Vladimir Rosenov

Koynarev appeared in the UiO web magazine *Titan* on October 30. Here they describe how their discovery of the mechanism by which antimicrobial peptides combat resistant bacteria not only requires rewriting of textbooks but may also open new pathways in the development of efficient new therapeutic strategies.

In December, Erik Tellgren was invited to a panel discussion at *Ullern videregående skole* (Ullern senior high school) in Oslo. Besides the ordinary study program for natural science, *Ullern videregående skole* has a researcher program with more focus on research. In the panel, researchers from the University of Oslo, Oslo University Hospital, and industry talked about their experiences in research and answered questions from students in their first and second year on the research program.

Following his mentoring of Piotr Ul from *Ullern videregående skole* in 2024–2025, Erik Tellgren also visited *Ullern videregående skole* on June 6 where

// 33 PhD candidates have completed their doctoral degrees at the Hylleraas Centre //

Piotr and other students presented their research projects. A jury selected Piotr's poster to be among those awarded with a Best Poster prize. Furthermore, Piotr's written report titled *Modelling Magnetic Bonds for Di- and Triatomic Molecules in the Atmospheres of White Dwarfs* was accepted for publication in the journal SPISS (Vol. 17, No. 1, 2025), and he was awarded the second prize in the competition for young researchers organized by the Young Academy of Norway.

Training and career support

Three members of the Hylleraas Centre – one male, two female – defended their PhD thesis in 2025: Ning Cao (UiO), Inga Lena Schmidtke (UiO) and Aurore Denjean (UiO). At the end of the year, a total of 33 PhD candidates had completed their doctoral degrees at the Hylleraas Centre.

The 2025 edition of the *Hylleraas School* was organized by a committee composed of Inga Lena Schmidtke, Tonje Reinholdt Haugen, Michal Repisky, David Balcells, and Simen Reine, and held at Hotell Hadeland north of Oslo on January 7–10 with about 50 participants. A course on Python programming by Radovan Bast, Group Lead High-Performance Computing and Research Software Engineering at UiT, was offered on January 6. Taught by Michele Cascella and Sigbjørn Løland Bore, the scientific theme of the 2025 edition of the Hylleraas School was molecular dynamics and molecular modelling.

Authored by Trygve Helgaker and Olaug Kristine Bringager and partly based on feedback from the participants, a report from the third career-development workshop KUPP3 was published on the centre web pages on April 30. The report is openly available and may serve as an inspiration for research groups as well as the participating Centres of Excellence at UiO.

Young Researcher Parliament

Prof. Paul Walton from the University of York was invited by the YRP for a visit at the Hylleraas Centre in Oslo on January 31 to present a seminar on gender equality in academia, a field in which he is an international leader. Former CTCC member Prof. Taye B. Demissie from the University of Botswana was invited by the YRP for a visit in Tromsø, where he gave a seminar on drug design and drug delivery with guidance from computational studies.

The alumni component of the visitor programme was particularly active in 2025. The Oslo node welcomed Audun Skau Hansen, who shared insights into his career choices and gave an overview of his latest projects. Marius Kadek was invited by the Tromsø node to share his experiences on *Life as a scientist after academia*. The Tromsø node was visited by former member Magnar Bjørgve, now part of the HPC group of NRIS in Tromsø.



Figure 17: Prof. Mats Tilset (right), newly elected honorary member of the Norwegian Chemical Society, with the President of the Norwegian Chemical Society Jørn H. Hansen at the Norwegian Academy of Science and Letters in Oslo on April 30. Photo: Stian Svelle.

The *Hylleraas Annual Meeting* in September 2025 was organized by the YRP representatives Inga Lena Schmidtke and Helena Hradiská at Malangen Resort in Malangen outside of Tromsø.

Inga Lena Schmidtke and Ylva Os succeeded Quentin Pitteloud and Helena Hradiská as YRP representatives in Tromsø. In Oslo, the YRP representatives remained unchanged.

Visitors

In 2025, a total of 10 researchers visited the Hylleraas Centre, with 7 visits in Oslo and 5 in Tromsø. This count includes the Almlöf–Gropen speaker who visited both places but excludes inter-node visits and visits by affiliate members.

External projects and funding

In December 2025, the RCN Quantum Technology Centre *QSTAR: Centre for Quantum Computing and Applications* was awarded to a consortium led by Dr. Franz Fuchs at SINTEF, with Simen Kvaal and Hylleraas adjunct Andre Laestadius as PIs. This is an important milestone for the strategic focus of the Hylleraas Centre on quantum science and technology.

Life science is another area with strategic importance to the Hylleraas Centre. In 2025, The UiO:Life Science Convergence Environment *PERMEATE: Peptides for Membrane Targeting and Synergistic Drug Delivery* was awarded to a multidisciplinary consortium of UiO-based researchers led by Hylleraas affiliate Reidar Lund, with Michele Cascella as PI.

Three Marie Skłodowska Curie Action (MSCA) postdoctoral fellowships were awarded to young scientists with the main supervisor at the Hylleraas Centre. Josefine Hvarregaard Andersen received funding for the project *HOOD: High-order geometric derivatives with multilevel coupled cluster theory*, which will be carried out at UiT under the supervision of Magnus Ringholm. Lucía Morán González and Jordan Rio received funding for the projects *BIFUCCO2: Machine Learning-Enhanced Design of Homogeneous Bifunctional Catalysts for CO₂ Hydrogenation* and *DEEP-CAT: Controlling the Structure of Transition-Metal Catalysts by Tuning their Chemical Environment*, respectively, which will be carried out at UiO under the supervision of Ainara Nova and David Balcells (Lucía) and Michele Cascella, David Balcells, Ainara Nova, and Odile Eisenstein (Jordan).



Figure 18: Left: Daniel Marke in front of his award-winning poster in Hannover, Germany. Right: Daniel Marke with German Society for Biochemistry and Molecular Biology (GBM) spokesperson Lydia Bosse (left), PhD student Khadija Aichane-Simon (Hannover Medical School; second from right), and GBM contact person Dr. Manuel Taft (right). Photos: Prof. Dr. Christoph Garbers, Daniel Marke.



Figure 19: Jose Alberto Guerrero (right) with fellow poster-prize winners Elena Betti (University of Pisa, Italy; middle) and Hande Abes (University of Girona, Spain; left) at the award ceremony at WATOC 2025 in Oslo on June 27. Photo: Marco Bortoli.

Marco Bortoli, Henrique Musseli Cezar, and Luca Frediani received grants of high-performance computing time from the European High-Performance Computing Joint Undertaking (Euro-HPC-JU). Bortoli's project, *ML-DES: Developing Efficient Machine Learned Potentials for Deep Eutectic Solvents*, received 260 thousand GPU hours and Cezar's project, *Ionic Conductivity in Metal-Organic Frameworks from First Principles*, received 7.9 million CPU hours and 410 thousand GPU hours. While these projects are regular access grants, Frediani and the MRChem team received 200 thousand CPU hours in a development access grant, which is aimed at improving the parallel processing capabilities of the MRChem program. Together, the three projects provide HPC resources equivalent to roughly 4.1 MNOK at Sigma2 (Category A pricing model).

Awards and elected memberships

Hylleraas affiliate Prof. Mats Tilset was elected honorary member of the Norwegian Chemical Society at its council meeting on April 30 (Figure 17).

Based on work done in collaboration with Michele Cascella and Marco Bortoli while a visitor of the Hylleraas Centre in Oslo, Daniel Marke won an award for his poster *Multiscale Modeling of Ebselen Binding to Inositol Monophosphatase* at the celebration of 55 years of biochemistry education in Hannover, Germany (Figure 18).

Jose Alberto Guerrero won a poster prize at the WATOC 2025 congress in Oslo for his poster *Analyzing the*

Electronic Structure of Pt(II) Complexes via ^{195}Pt NMR (Figure 19). The work was done under the supervision of Abril Castro at the Hylleraas Centre in Oslo.

Management

The Management Team met 10 times in 2025 (all months except July and August), while the Board of Directors met once (February 25).

RESEARCH HIGH- LIGHTS /

The Hylleraas Centre carries out research on a broad range of topics in theoretical chemistry, with relevance not only to chemistry but also to physics, biology, and other related fields of science. In this section of the Annual Report, we highlight recent and ongoing work at the centre.

David Balcells

Generative AI for Transition Metal Chemistry

The inverse design of transition metal complexes is one of the “holy grails” of chemistry. Together with data scarcity, the complexity of the electronic structure hampers the development of generative AI for these compounds. Our work has advanced this research frontier through the development of evolutionary and deep learning methods, including genetic algorithms for multiobjective optimization and variational autoencoders for conditional generation. Further, we have shown that these methods can be integrated into synergistic schemes enabling the generation of metal complexes that are both novel and optimal.

The interest in the chemistry of transition metals originates from different fields of technology that are critical to society. From the perspective of sustainability, most chemical industry products are made in catalytic processes, including both bulk and fine materials like polymers and medicines. In these processes, transition metal complexes (TMCs) act as the catalysts that reduce energy consumption and waste generation. More recently, in the field of quantum computing, TMC properties are being studied and tuned for the sake of using these compounds as molecular qubits. To enable these applications, one needs to find TMCs

that satisfy multiple target properties, including reactivity, stability, and selectivity, among others. Merging organic and inorganic chemistries, the TMC combinatorial space provides us with a virtually infinite number of combinations to choose from ($>10^{60}$), which poses the big challenge of finding the best candidates for a given target application. A needle-in-a-haystack riddle in which even ultra-fast machine learning (ML) predictions often fail, since the chemical spaces are simply too large for being screened explicitly. In contrast, generative artificial intelligence (AI) can tackle this challenge by formulating these same spaces implic-

itly. However, the lack of large and complex data for TMCs, and the difficulty of encoding their complex geometric and electronic structures, make generative AI for TMCs the frontier research problem that we are advancing at the Hylleraas Center.

It all started with the data.

After developing the first ML model for predicting the oxidative addition energy barrier, a key parameter in many TMC-catalyzed processes [1], we aimed for generalizing our ML research towards the TMC space. This goal required the computation and curation of a large body of data. David Balcells

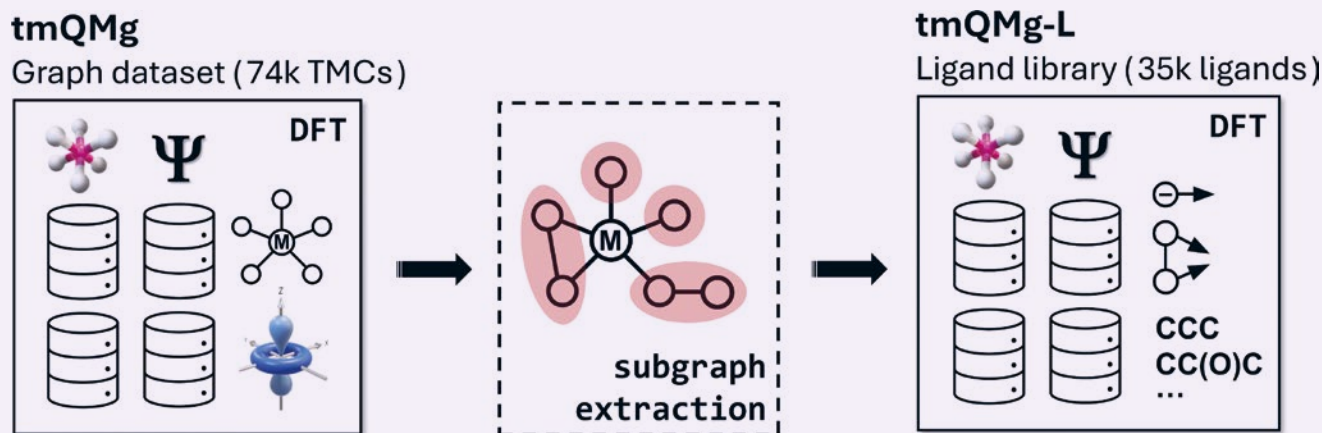


Fig. 1: ItmQMg and tmQMg-L in the tmQM dataset series. Illustration: David Balcells

and Bastian Skjelstad (Hylleraas MSc, now MSCA postdoc in Duarte's group at the University of Oxford) curated the transition metal Quantum Mechanics (tmQM) dataset [2], which contained 86k (later extended to 108k) TMCs extracted from the Cambridge Structural Database (CSD), and for which several quantum properties, including geometries, polarizabilities, and frontier orbital energies, were computed using semiempirical and DFT methods. Noteworthy, the CSD origin of the tmQM dataset implies that all TMCs in it are synthesizable, since they have been made and characterized in experimental labs through procedures reported in the literature. Later, tmQM became a

dataset series with the contributions made by Hannes Kneiding (Hylleraas PhD student and researcher), adding tmQMg [3], a graph dataset, and tmQMg-L [4], the ligand library underlying the whole tmQM series (Figure 1). In 2025, the series kept growing with tmQMg* [5], adding electron excitation data from TD-DFT calculations, and tmQMg-D [6], providing multi-level property values for D-ML. Critically, the tmQM datasets enabled the development and training of all our AI models for TMCs. Further, this series has become a popular resource in the field, collecting already 230+ citations and being used both in academic and industrial labs.

Graphs are almost all you need.

As for predictive ML, generative AI requires expressing molecules in machine-readable formats. In the context of chemistry and materials sciences, graphs are a natural format since their nodes and edges intuitively represent atoms and bonds. Further, when graph-based models are made interpretable, prediction and generation tasks can be readily explained with the language used by chemists. This data format also gives access to one of the most powerful algorithms in AI: graph neural networks. However, while expressing organic molecules as graphs is trivial, TMCs are difficult due to the complex bonding patterns that originate →

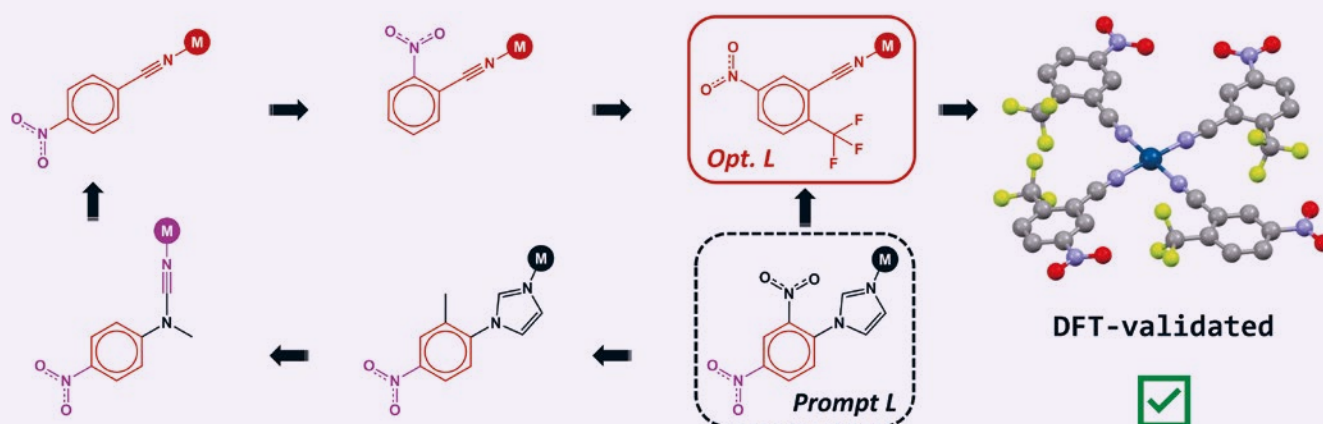


Fig. 2: Stepwise gradient-descent generation of a ligand maximizing the HOMO-LUMO gap in the latent space of the JT-VAE model for TMCs. Illustration: David Balcells

→ from the metal center d orbitals. We solved this problem by leveraging natural bond orbital (NBO) theory in the derivation of TMC graphs [3]. The resulting natural quantum graph representation connects the atomic nodes using orbital and bond order data from NBO analysis. This data, collected in the 75k tmQMg graph dataset, facilitated the deconstruction of the TMCs into metal centers and ligands, which were collected in the 35k tmQMg-L library (Figure 1), allowing also for determining ligand charge, denticity, and hapticity with high fidelity [4].

The data curated in tmQMg and tmQMg-L was used to develop a generative AI model for the inverse design of TMCs. In contrast with property prediction, inverse design reverses the X-to-y task to y-to-X, where X is a representation, here a graph, and

y a property of interest, for example, the metal center charge. In this framework, the user sets a target property value and the model returns (a distribution of) molecules having that property value. Our generative AI model [7] was based on the variational autoencoder (VAE) method. VAEs learn to encode input molecules into a reduced-dimensionality representation (the latent space) that is subsequently decoded into the same input. Once trained to reconstruct the input data through a regularized probability distribution, a VAE can be used to generate thousands of novel molecules by sampling and decoding the latent space. By adding an auxiliary model predicting a target property from latent space, one can condition the generative task by such property using differentiation and gradient-descent algorithms, in this way realizing the inverse design, y-to-X task (Figure 2).

The constraints needed to enforce chemical validity in graph generation were introduced by using junction trees, which are a coarse-grained graph representation. Another challenge was the encoding of the TMCs as strings, since the overall VAE data transformation is string → graph → junction tree → latent space, followed by the reverse process. We tackled this issue by developing a novel string encoding for TMCs, in which a notation combining dummy atoms with directed dative bonds allowed for expressing metal anchors and metallacycles, in this way supporting both dentate and haptic ligands [7]. More recently, we collaborated in the development of SMILES strings based on extended Hückel calculations to support TMCs [8]. In a case study focused on mono- and bi-dentate ligands, we showed that our VAE model can augment the training

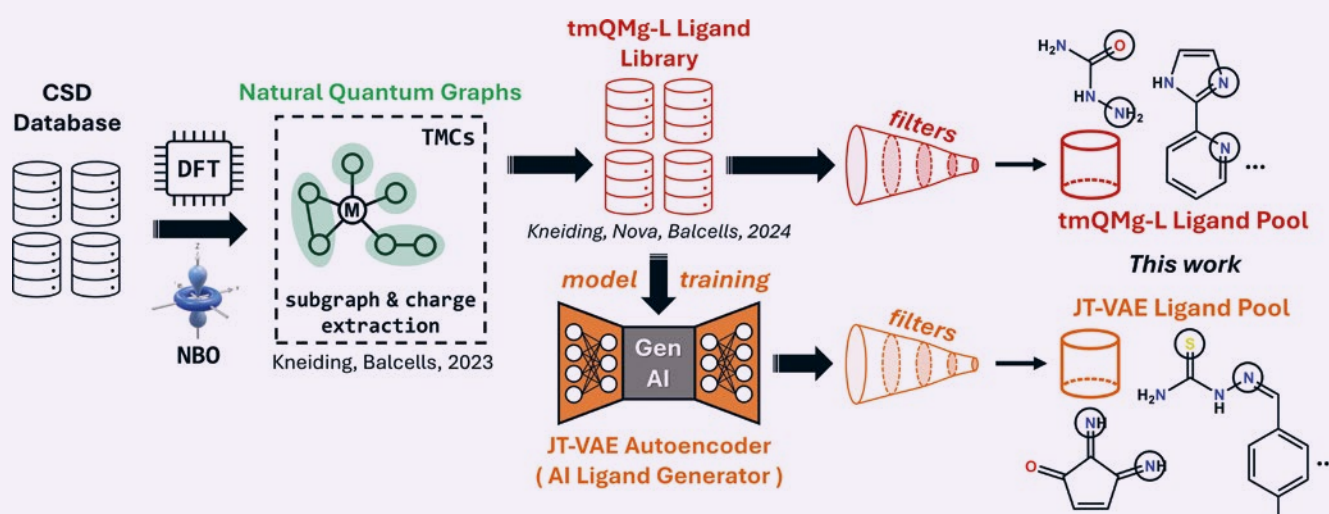


Fig. 3: Derivation of the ligand pools for the evolutionary deep learning de novo design of ruthenium chromophores. Illustration: David Balcells

dataset (tmQMg-L) with novel and valid ligands, achieving augmentation factors between 6 and 7, with chemical validation rates >95%. We also implemented inverse design tasks in which generation was conditioned by multiple target properties, including the TMC metal center charge and HOMO-LUMO gap (Figure 2), and the ligand solubility and coordination bulkiness. This work was initiated in 2024 by Magnus Strandgaard, a visitor from Jensen's group in Copenhagen, in collaboration with Trond Linjordet (Hylleraas postdoc, now at ICRDD, in Hokkaido University, Japan), Hannes Kneiding, Arron Burnage (Hylleraas postdoc), and Ainara Nova (Hylleraas PI in RT5). The research was peer-reviewed this year and published open-access in *JACS Au* [7], where it was highlighted among the most-read articles of this journal.

Evolution with AI-made genes.

Genetic algorithms (GAs) are an efficient alternative to generative AI with deep learning methods. GAs are indeed a strong benchmark that is difficult to beat with deep learning, even when the latter is supported by large data and complex models. For example, our JT-VAE generator could make extensive sets of novel ligands and TMCs but its use in inverse design was limited by validation rates decreasing from >95% to 50–70% when generation was property-conditioned [7]. In contrast, our research had previously shown that PL-MOGA, a GA algorithm using a pool of genes consisting of ligands from the tmQMg-L library, can do multi-objective TMC optimization in chemical spaces containing up to billions of possible formulations [4]. However, this approach also had its limitations; in particular, the novelty of

the TMCs evolved by the GA was limited to combinations of known ligands.

Aiming at breaking this opposing high-novelty / low-optimality (JT-VAE) versus low-novelty / high-optimality (PL-MOGA) scenario with a generative AI method that can make TMCs both novel and optimal, we explored synergies between evolutionary and deep learning methods [9]. In principle, one can either embed the PL-MOGA within the JT-VAE, to decode TMCs evolved in latent space, or the opposite, to evolve TMCs with AI-generated ligands. We explored the latter approach in the multi-objective optimization of ruthenium chromophores [10]. Three properties were maximized, namely water solubility and the intensity and broadness of visible light absorption, using a pool of ligands generated by the JT-VAE and selected based on

their synthesizability (Figure 3). Pushing both novelty and optimality, our method evolved several, diverse TMCs maximizing all these three properties, and we are currently investigating their experimental synthesis. This work was done by Alejandra Pita-Milleiro, a visitor from Campos' group in Sevilla, in collaboration with Magnus Strandgaard and Trond Linjordet, and under the supervision of Hannes Kneiding and David Balcells.

Pulling the future from noise.

We remain interested in evolutionary deep learning [9], which still requires developing complex methods like, for example, quantitative and accurate measures of synthesizability for TMCs. Besides, we are also collaborating with Trond Linjordet in the development of diffusion models (DMs) for TMCs. DMs transform molecular inputs into noisy representations and then learn their denoising back to the same, original inputs. Once the noise/denoise process is optimized, one can use a DM similarly to a VAE – random noise is sampled and decoded into generated output molecules. DMs are computationally much heavier than VAEs though offering a fundamental advantage: they support point clouds and can thus generate 3D geometries in a way that can also be conditioned for the purpose of inverse design. Since this approach is challenged by composition and structure-complexity, DMs for TMCs remain scarce and limited. This year we have started doing research on this problem, with the aim of enabling TMC DMs with physics-informed architectures.

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David Balcells
Senior Researcher

Luca Frediani

Making quantum-chemistry results less dependent on “basis choices” – and more reliable when electrons move together

Modern chemistry relies heavily on computer simulations to predict molecular structures, reaction energies, and spectra. Two long-standing challenges often limit how reliable such predictions are. The first is the basis problem: electrons are represented using a finite set of mathematical building blocks (“basis functions”), and any finite choice introduces basis-set error. The second is electron correlation: electrons repel each other, so their motions are linked. A simple “independent-electron” picture can miss important effects because electrons do not move one-by-one; they avoid each other in a coordinated way, and that coordination can become essential in bond breaking, excited states, and many transition-metal problems. Our recent work addresses *both* issues in a single workflow by combining multiwavelets to control basis-set error systematically with DMRG to treat strong correlation efficiently [1].



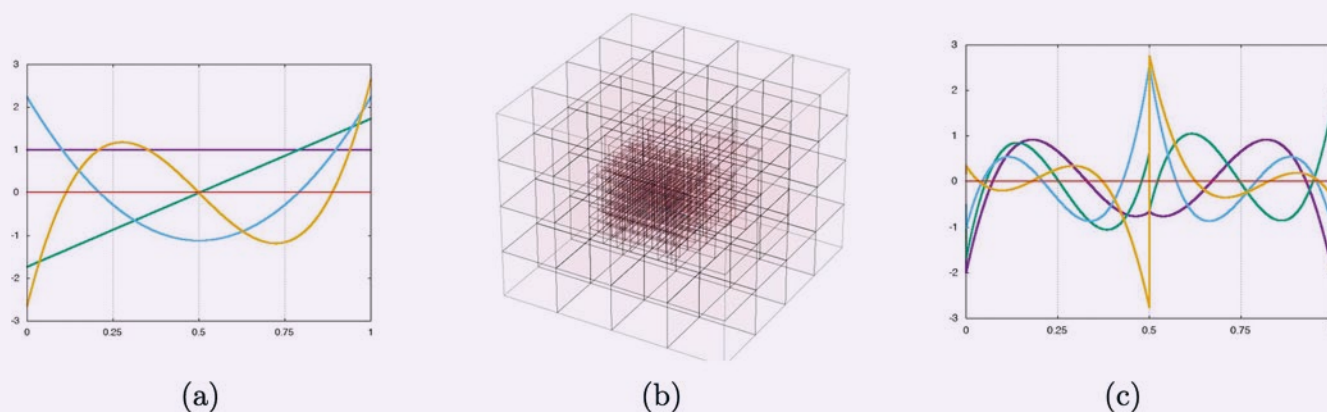


Figure 1: A basis of polynomials (a) is used to represent functions on an adaptive grid (b), whereas the multiwavelets (c) are the tool which allows us to gauge the precision of the calculation and decide how much to refine the grid. Reproduced from G. A. Gerez S. et al., J. Chem. Theory Comput. 2023, 19, 1986–1997, under CC-BY 4.0 license.

Multiwavelets: a basis with an “accuracy dial” that can also scale well.

In conventional quantum chemistry, orbitals are expanded in atom-centered functions (often Gaussian-type orbitals). Increasing the basis typically improves results but can be expensive, and it is not always obvious how close you are to the “true” (complete-basis) answer.

Multiwavelets implement a different idea called multiresolution analysis. Instead of using a fixed set of functions attached to each atom, the method represents orbitals in real space on a *hierarchy of scales*—coarse where the orbitals are smooth, finer only where more detail is needed (for instance near nuclei and in bonding regions). The key advantage for

users is that the representation error can be controlled directly by tightening a precision threshold, providing a systematic path toward the complete basis set (CBS) limit. This multiresolution approach has been pioneered by the MADNESS [2] code and later by our own MRChem code [3].

In the beginning, multiwavelets provided results of unmatched accuracy, but their computational cost prevented widespread adoption. Recently, high-performance implementations have demonstrated that, for high precision and large systems, multiwavelet-based methods can be not only more systematically accurate but also *computationally competitive* through careful parallel design. This has been shown in the

performance amost behind MRChem, our multiwavelet-based electronic-structure code [3].

DMRG: an efficient route to strong correlation (with clear trade-offs).

Even with an excellent basis, correlation can be the dominant challenge. When a single dominant electron configuration is insufficient, many “electron arrangements” must be considered simultaneously—this is what chemists mean by strong correlation. In such regimes, methods that work extremely well for weakly correlated molecules can become unreliable.

The density matrix renormalization group (DMRG) is one of the most successful approaches for strong

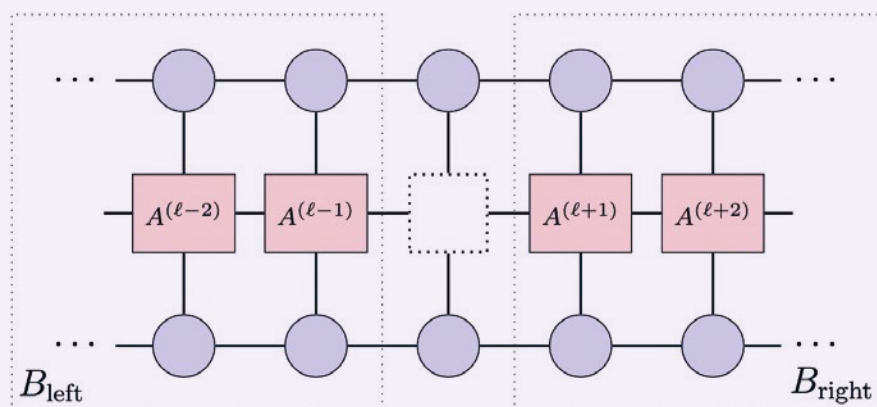


Figure 2: A schematic representation of the DMRG structure. It generates the parameters required by the MW optimization algorithm to optimize the orbitals. Reproduced from ref. [1] under CC-BY 4.0 license.

correlation in molecules. Its main idea is to represent the many-electron wavefunction in a compact structured form (often explained in terms of matrix-product states) and to improve it iteratively. DMRG is particularly effective for large active spaces, where traditional multireference approaches can become prohibitively expensive. The advantages and limitations are well summarized in reviews by Garnet K.-L. Chan and co-workers: DMRG is systematic and robust in strongly correlated regimes, but its efficiency depends on orbital choices/orderings, and it is commonly paired with additional treatments to capture remaining “background” (dynamic) correlation outside the active space when needed [4].

Our contribution: orbital optimization at the CBS limit with multiwavelets + DMRG.

In our paper, we combine these two complementary strengths: multiwavelets provide a controllable, adaptive representation of orbitals approaching CBS quality, while DMRG supplies a scalable solver for strongly correlated electrons. We integrate DMRG into a multiwavelet-based orbital-optimization framework and streamline the optimization loop by extracting the information needed to update orbitals directly from the DMRG representation. We demonstrate the approach on representative small systems (including H_2 , He, HeH_2 , BeH_2 , and N_2), establishing a clear algorithmic pathway for

multireference wavefunction optimization with systematic control of basis-set error [3].

For development and rapid iteration, we used VAMPyR as a versatile Python interface to multiwavelet functionality, enabling fast prototyping of new algorithms on top of the underlying multiwavelet infrastructure [5].

In Figure 4, we show an intuitive “before/after” view of what this combination buys you. For both H_2 (left) and N_2 (right), Hartree–Fock results (HF, blue curves) are affected by the limitations in the STO-6G basis and the lack of correlation, causing both an inaccurate energy minimum and an unphysical dissociation towards the



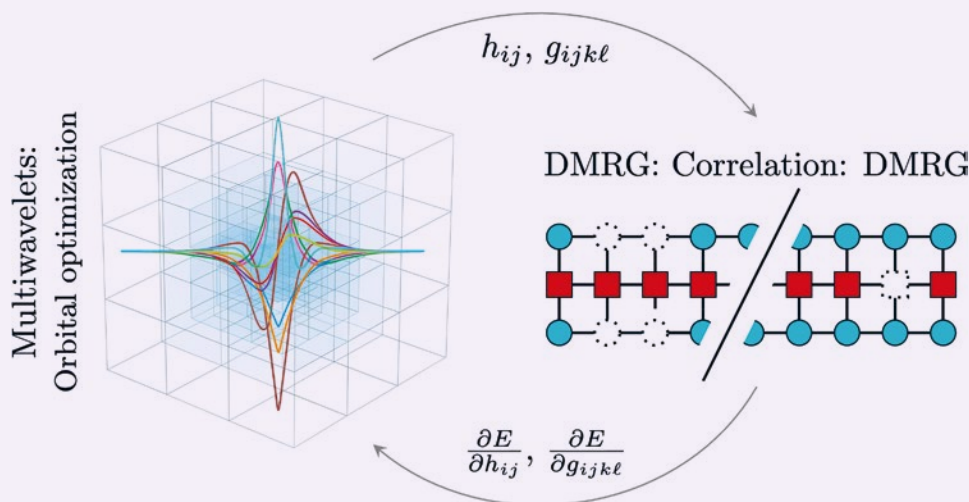


Figure 3: Coupled MW-DMRG workflow: the MW engine optimizes the orbitals using adaptive grids (left) and sends one- and two-electron integrals to the DMRG code. The DMRG code uses the integrals obtained with Multiwavelets and generates the one- and two-electron gradients, which are sent to the MW code for a new round of orbital optimization. In this way the MW orbitals are generated for a correlated wave function and the correlation in the framework of a practically complete basis. Reproduced from ref. [1] under CC-BY 4.0 license.

so-called ionic state. The Full Configuration Interaction (FCI, orange curves) includes correlation, but only within a very limited basis in the present case; it improves over Hartree–Fock, yielding the correct qualitative behavior but it remains constrained by basis-set limitations. Our MRA+DMRG results (blue curves) combine a systematically improvable spatial representation with a correlation method designed for multireference situations. The result is a consistently lower (more precise) potential-energy curve across bond lengths—including the dissociation region where strong correlation becomes important—while using a compact orbital description (2 orbitals for H_2 and 10 orbitals for N_2 , as indicated).

This is the key message of the plot: treating correlation well is necessary, but doing so in a representation that can be driven toward CBS quality is what makes the approach both reliable and systematically improvable. FCI could achieve the same result, but it would require a much larger AO basis, and consequently a much heavier computation.

Outlook.

This work moves toward “precision-controlled multireference quantum chemistry,” where one can reduce basis-set uncertainty transparently (via a numerical threshold) while maintaining a practical route to strong correlation (via DMRG). With the demonstrated perfor-

mance and scaling of modern multi-wavelet codes, the longer-term goal is not just better benchmarks, but routine high-precision calculations that are both reliable and computationally viable for increasingly large and chemically relevant systems [3].



Prof. Luca Frediani
Deputy Director

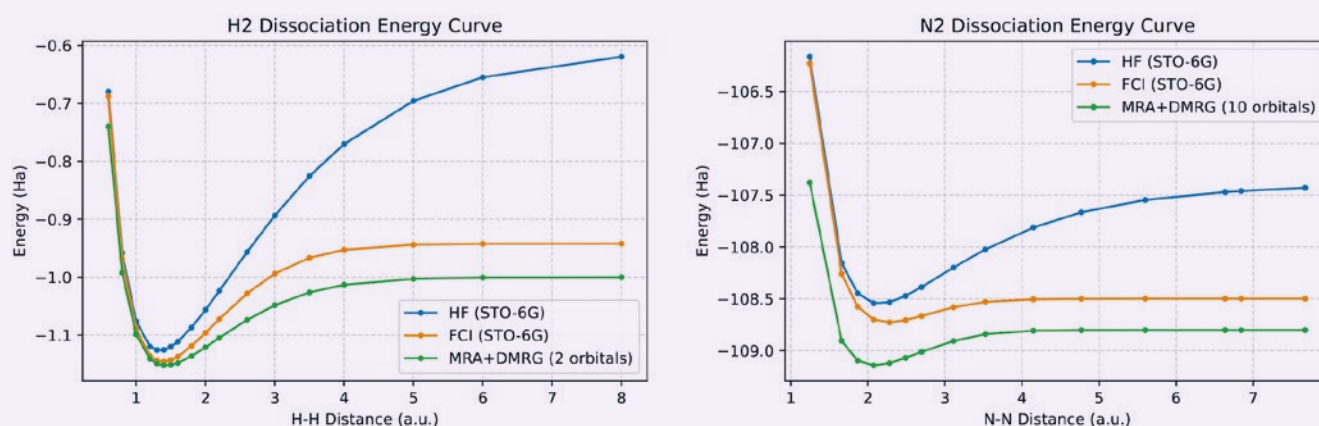


Figure 4: Dissociation energies are one of the hardest things to model: they require both a very large basis set and the inclusion of static correlation. The dissociation curves of H₂ and N₂ are pictured above. Hartree-Fock (HF, blue) produces very wrong results due to lack of correlation and a limited basis. Full Configuration Interaction (FCI, yellow) corrects the large HF anomaly when the molecule dissociates but it is still affected by the limitation in the basis set. Our MW-DMRG results (green) are both qualitatively correct and quantitatively precise. Reproduced from ref. [1] under CC-BY 4.0 license.

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Bjørn Olav Brandsdal

Computer simulations of temperature dependence of enzymatic reactions

Understanding how enzyme activity changes with temperature is essential for explaining both catalysis and biological adaptation yet has been notoriously difficult to capture in molecular detail. Both hardware and software developments have allowed us to use computer simulations to unravel and control the temperature dependence of enzyme-catalyzed reactions. With carefully designed simulation framework we can reproduce experimental activation parameters and even capture enzyme temperature optima, providing a powerful route from microscopic mechanism to macroscopic function.

Simulating temperature dependence with MD/EVB.

The central methodological advance is a protocol that combines molecular dynamics (MD) with the empirical valence bond (EVB) method to compute activation free energies as a function of temperature [1]. By evaluating the activation free energy $\Delta G^\ddagger$ at a series of well-defined temperatures, one can construct computational Arrhenius or Eyring plots and extract the corresponding activation enthalpy $\Delta H^\ddagger$ and activation entropy $\Delta S^\ddagger$, exactly as in experiment but fully resolved at atomic detail.

In this framework, the reactive potential energy surface is described by an EVB Hamiltonian that interpolates between

valence-bond-like diabatic states for reactant and product. The EVB parameters are calibrated against high-level quantum chemical data or experimental benchmarks for a reference reaction, typically in water. Once calibrated, the same EVB model is embedded into a solvated enzyme environment and combined with classical force fields for the protein and solvent. Because EVB has simple force-field character, it supports massive configurational sampling: hundreds of independent MD/free energy perturbation or umbrella sampling simulations can be performed per temperature, reducing the statistical uncertainty in $\Delta G^\ddagger$ to about 0.1–0.2 kcal/mol, which is crucial for reliable linear regressions of $\Delta G^\ddagger(T)$.

A key validation example is the pericyclic rearrangement of chorismate to prephenate, both in water and in chorismate mutase [2]. The simulations reproduce not only the experimental free energy barrier, but also the enthalpic and entropic components of activation with striking accuracy (Figure 1). The analysis reveals that chorismate mutase operates primarily by lowering the activation enthalpy through a more compact, preorganized transition state, with entropy playing a comparatively minor role. This establishes MD/EVB as a quantitatively reliable approach for computing thermodynamic activation parameters in enzymes.

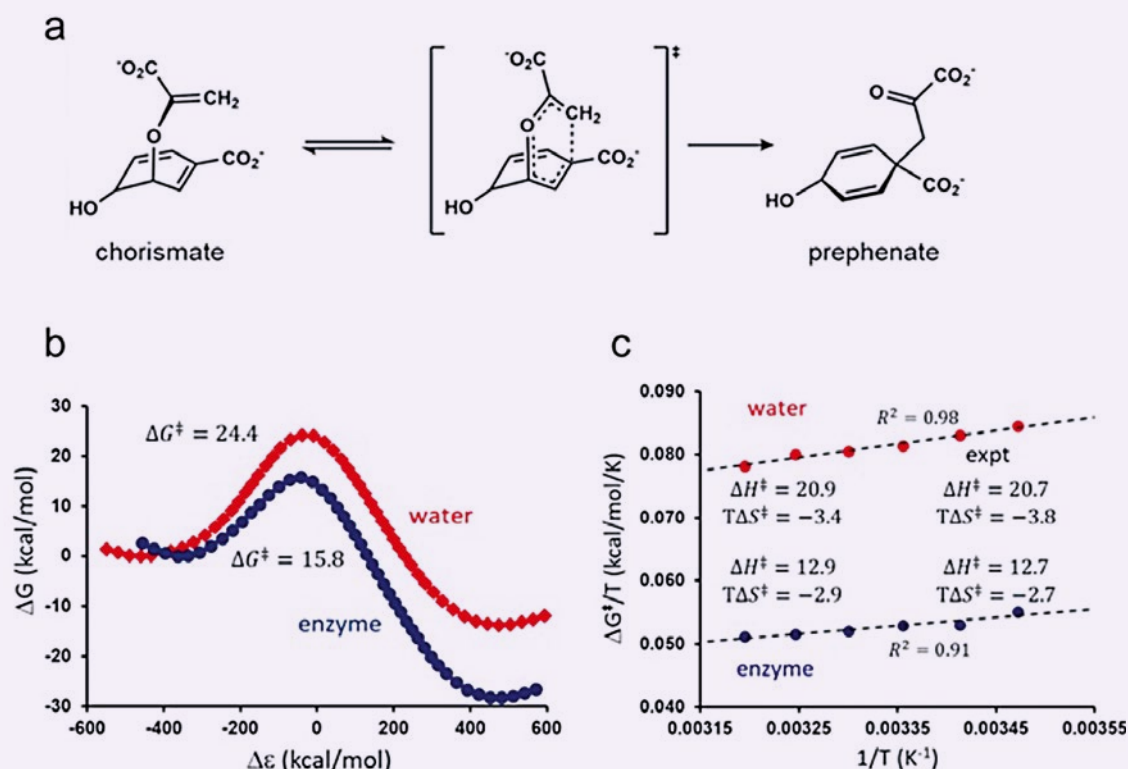


Figure 1: (a) The rearrangement of chorismate to prephenate catalyzed by the chorismate mutase. (b) Calculated reaction free energy profiles for uncatalyzed reaction in water (red) and for the *B. subtilis* chorismate mutase catalyzed reaction (blue) at 25 °C. The generalized reaction coordinate $\Delta\epsilon$ is the energy gap between the two diabatic potentials for reactant and product. (c) Computed Arrhenius plots for the two reactions from MD/EVB simulations at six temperatures. Adapted from ref. [2] under CC-BY 4.0 license.

From reference reactions to complex enzyme mechanisms.

For relatively simple reactions, the EVB model can be parametrized directly against experimental activation and equilibrium data for the corresponding uncatalyzed reaction in water. When no suitable solution reaction exists that follows the same mechanism as the enzyme, the calibration instead relies on quantum mechanical cluster models or QM/MM minimum-energy paths that include key active-site residues and water molecules. EVB parameters are then fitted to these enzyme-specific quantum data, and MD/EVB simulations are used to compute Arrhenius plots for the full solvated enzyme. Beyond reproducing numbers, this combination of quantum calibration and extensive

MD sampling allows mechanistic questions to be addressed directly.

Enthalpy, entropy, and cold adaptation: a softer protein surface.

A particularly important application of the MD/EVB methodology is to enzyme temperature adaptation. Classic biochemical work established that cold-adapted (psychrophilic) enzymes typically display lower activation enthalpies and more negative activation entropies than their mesophilic counterparts and are significantly faster at low temperatures. However, structural comparisons have struggled to explain this phenomenon, because the active sites of cold and warm enzymes are often nearly superimposable. By

computing full Arrhenius plots for pairs of cold- and warm-adapted enzymes, such as citrate synthases, trypsins and elastases, the simulations recover the hallmark shift in $\Delta H^\ddagger$ and $\Delta S^\ddagger$ observed experimentally. Psychrophilic enzymes have markedly lower activation enthalpies, partially compensated by larger entropic penalties. Decomposition of the activation enthalpy into contributions from the reacting groups and from the surrounding protein and solvent reveals a somewhat surprising result: the dominant difference lies in the protein-solvent component. In other words, the response of the enzyme environment itself to the chemical event is more favorable in cold-adapted enzymes.

This can be interpreted as a “softer” effective potential for displacing the protein coordinates from the reactant minimum to the transition state in cold-adapted enzymes. A shallower potential leads directly to a smaller enthalpic cost for reaching the transition state. At the same time, the associated change in configurational space results in a more negative activation entropy, in line with the observed enthalpy–entropy compensation. Importantly, MD analyses show that this enhanced softness is not localized in the active site, but predominantly in surface loops. Psychrophilic enzymes exhibit increased backbone fluctuations in specific surface regions, while residues directly in the catalytic center often show similar mobility across temperature-adapted homologues.

The functional role of this surface softness is supported by targeted computational “mutations” and restraint simulations. Introducing warm-adapted loop residues into cold enzymes consistently increases $\Delta H^\ddagger$ and decreases flexibility; inserting cold loop motifs into warm enzymes has the opposite effect. Furthermore, progressively restraining the surface of a cold-adapted trypsin leads the simulated activation parameters to converge toward those of a mesophilic trypsin [3], without altering the catalytic residues. Together, these results link the macroscopic signature of cold adaptation – a reduced activation enthalpy with more negative activation entropy – to subtle, distributed changes in protein surface flexibility.

Hidden equilibria and temperature optima.

In many enzymes, the catalytic rate exhibits a well-defined temperature optimum. For thermophilic enzymes, this is often close to the melting temperature and can be rationalized by thermal unfolding. However, cold-adapted enzymes frequently show temperature

optima far below their melting temperatures, implying other inactivation mechanisms.

A paradigmatic case is the psychrophilic α -amylase from *Pseudomonas haloplanktis* (AHA), which acts on α -1,4-glycosidic bonds in starch. Experimentally, AHA has a temperature optimum near room temperature, roughly 15 °C below its melting temperature, whereas a closely related porcine pancreatic α -amylase (PPA) has its optimum near 50 °C. MD/EVB simulations of the rate-limiting glycosylation step in both enzymes not only reproduce the expected lower $\Delta H^\ddagger$ and more negative $\Delta S^\ddagger$ for AHA at low temperature, but also capture a clear break in the Arrhenius plot that translates into a computed rate maximum around room temperature [4].

Detailed inspection of substrate-bound MD trajectories reveals the underlying microscopic mechanism. In AHA, a specific hydrogen-bonding interaction between Asp264, located in a $\beta 7$ – $\alpha 7$ loop, and the substrate is stable only at lower temperatures. Around room temperature this contact becomes increasingly unstable, leading to the population of an alternative, catalytically incompetent enzyme–substrate state ES' with a higher effective activation free energy. In PPA, the analogous interaction persists to substantially higher temperatures; the ES' state only becomes dominant above about 320 K, consistent with its higher temperature optimum.

This behavior can be captured by a simple equilibrium scheme $ES \rightleftharpoons ES' \rightarrow P$, in which k_{cat} depends both on the intrinsic barrier for the chemical step and on the temperature-dependent equilibrium between active and inactive bound states. From the simulated rates, one can derive effective temperature-dependent activation enthalpies, entropies

and heat capacities that match the experimentally observed non-Arrhenius behavior, while being directly traceable to a specific structural switch in the active-site loop region.

Designing enzyme temperature profiles.

Perhaps the most forward-looking implication of this work is that the same simulation machinery can be used not only to interpret, but also to design, the temperature dependence of enzyme reactions. In the AHA/PPA system, the simulations identify $\beta 7$ – $\alpha 7$ loop dynamics and the Asp264–substrate interaction as key determinants of the $ES \rightleftharpoons ES'$ equilibrium and thus of the temperature optimum [5]. This insight was used to construct a series of chimeric α -amylases in which successive sets of residues from the mesophilic PPA were introduced into the corresponding region of AHA (Figure 2). MD simulations show that even a minimal chimera, in which only the loop motif is exchanged, begins to stabilize the active ES state relative to ES'. A more extensive chimera with 16 substitutions around the loop produces a pronounced shift in the ES/ES' balance and is predicted to raise the temperature optimum by more than 10 °C. Subsequent experimental characterization confirms these trends: the simpler chimera shifts the optimum upward by about 2 °C, while the larger chimera shifts it by about 6 °C and outperforms both wild-type AHA and PPA at moderately elevated temperatures. Crystallography shows that the engineered loop adopts a conformation closer to that in PPA, corroborating the simulation-based design.

These results provide a concrete demonstration that detailed, thermodynamically grounded simulations can guide redesign of enzyme temperature profiles through targeted mutations in dynamic surface regions, rather than through trial-and-error in the catalytic

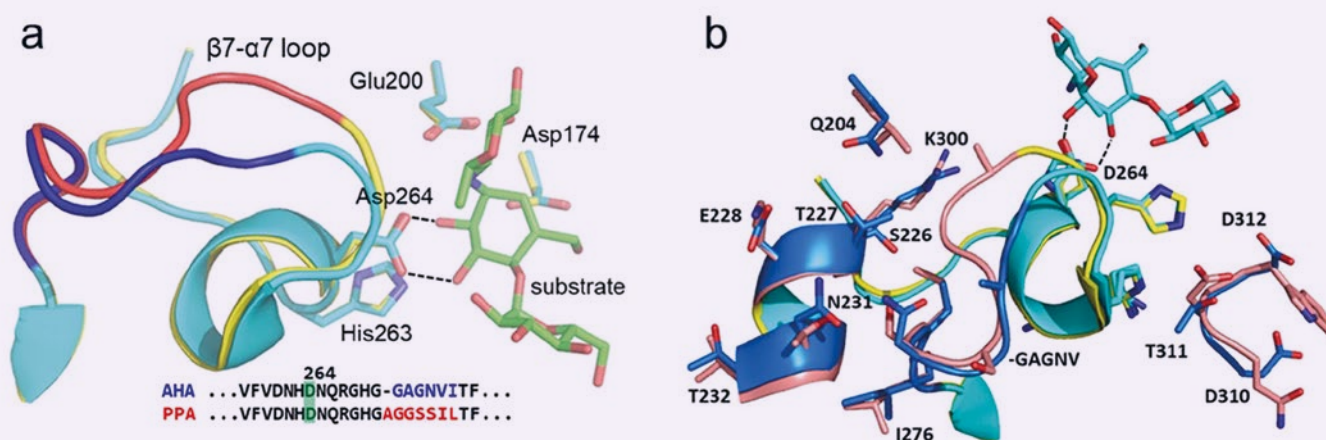


Figure 2: (a) View of the loop region following the universally conserved His-Asp motif in AHA (cyan/blue) and PPA (yellow/red). The catalytic residues Asp174 and Glu200 are also shown. (b) Mutated residues in the chimeric variants that interact with the $\beta 7$ - $\alpha 7$ loop. Adapted from ref. [5] under CC-BY 4.0 license.

center. For industrial and biotechnological applications where activity at non-native temperatures is crucial, this offers a promising route to rational enzyme engineering.

Impact and outlook.

The work highlighted here exemplifies how quantum-inspired models, classical force fields and extensive sampling can be integrated to connect quantum chemistry, statistical mechanics and enzymology in a single, predictive framework. By delivering accurate activation free energies, enthalpies and entropies across temperature, the MD/EVB methodology allows long-standing questions about enthalpic versus entropic contributions to catalysis to be revisited with unprecedented microscopic resolution. At the same time, it opens a window onto evolutionary adaptation, revealing how subtle changes in protein softness and hidden conformational equilibria tune enzyme function to specific thermal environments.

Furthermore, this line of research showcases the potential of advanced quantum molecular simulations to move beyond static structures and single-temperature observables, and to tackle genuinely thermodynamic properties of biomolecular reactions. In the longer term, such approaches may become central tools for both understanding natural enzyme evolution and designing catalysts with temperature dependencies for applications ranging from cold-wash detergents to high-temperature biorefineries.



Bjørn Olav Brandsdal
Professor

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ALMLÖF- GROPEN LECTURE SERIES /

The Almlöf-Gropen Lecture Series was established by the Centre for Theoretical and Computational Chemistry in 2008 to honour the memory of two pioneers of quantum chemistry in Norway: Prof. Jan Almlöf (1945–1996) at the University of Oslo and Prof. Odd Gropen (1941–2005) at UiT The Arctic University of Norway. Each year, a prominent theoretical chemist is invited to deliver the Almlöf-Gropen lecture at the Hylleraas Centre in Oslo and Tromsø, targeting a broad audience. Since 2020, the Almlöf-Gropen Lecturer has been preceded by two Almlöf-Gropen Young Speakers, selected among the young members of the Hylleraas Centre.

Almlöf–Gropen Lecture Series

Previous Almlöf–Gropen Lecturers

- | | | | |
|-------------|--|-------------|--|
| 2008 | Prof. Björn Roos
University of Lund, Sweden:
<i>Multiconfigurational quantum
chemical methods and heavy element
chemistry</i> | 2013 | Prof. Henry F. Schaefer
University of Georgia, Athens, USA:
<i>From donor–acceptor complexes to
Gallium Nitride nanorods</i> |
| 2009 | Prof. Tom Ziegler
University of Calgary, Canada:
<i>Analyzing complex electronic structure
calculations on large molecules in
simple chemical terms</i> | 2014 | Prof. Leo Radom
University of Sydney, Australia:
<i>Adventures in free radical chemistry:
a computational approach</i> |
| 2010 | Prof. Michele Parrinello
ETH Zürich, Switzerland:
<i>Through mountains and valleys with
metadynamics</i> | 2015 | Prof. Arieh Warshel
University of Southern California, USA:
<i>How to model the action of complex
biological systems on a molecular level</i> |
| 2011 | Prof. Pekka Pyykkö
University of Helsinki, Finland:
<i>Relativity and chemistry: some recent
results</i> | 2016 | Prof. Emily Carter
Princeton University, USA:
<i>Quantum solutions for a sustainable
energy future</i> |
| 2012 | Prof. Harry B. Gray
California Institute of Technology, USA:
<i>The 21st century solar army</i> | 2017 | Prof. Jack Simons
University of Utah, USA:
<i>The wonderful world of molecular
anions</i> |

2018 Prof. Walter Thiel
 Max-Planck-Institut für
 Kohlenforschung, Mülheim an der
 Ruhr, Germany:
Chemistry with the computer

2019 Prof. Sharon Hammes-Schiffer
 Yale University, Connecticut, USA:
*Proton-coupled electron transfer in
 catalysis and energy conversion*

2020 Prof. Leticia Gonzalez
 University of Vienna, Austria:
*Light and shadows on the quantum
 simulation of molecular electronic
 excited states*

2021 Prof. Alán Aspuru-Guzik,
 University of Toronto, Canada:
*There is no time for science as usual:
 materials acceleration platforms*

2022 Prof. Clémence Corminboeuf,
 École Polytechnique Fédérale de
 Lausanne (EPFL), Switzerland:
*Going further by leveraging data
 for solving quantum/computational
 chemistry problems*

2023 Prof. Frank Neese,
 Max-Planck-Institut für
 Kohlenforschung, Mülheim an der Ruhr,
 Germany:
*A perspective on large scale quantum
 chemical codes and algorithms*

2024 Prof. Fernanda Duarte
 University of Oxford, United Kingdom:
*Exploring chemical reactivity in the
 age of automation and machine
 learning*



Almlöf–Gropen Lecturer 2025

Angela K. Wilson

Michigan State University, USA

Unraveling the
Periodic Table: From
Thermochemistry and
Excitation Pathways to
Environmental Impact

September 23, 2025,
University of Oslo
September 25, 2025, UiT
– The Arctic University of
Norway

Angela K. Wilson is John A. Hannah Distinguished Professor and a University Distinguished Professor at Michigan State University, with appointments in the Department of Chemistry, Department of Physics and Astronomy, and Department of Medicine. Angela received her B.S. from Eastern Washington University and a Ph.D. from the University of Minnesota, where she completed her Ph.D. under the mentorship of Professor Jan Almlöf. She was a postdoctoral fellow at Pacific Northwest National Laboratory, a U.S. Department of Energy facility, with Dr. Thom H. Dunning, Jr. In 2000, she joined the faculty at the University of North Texas (UNT), where she founded and directed the Center for Advanced Scientific Computing and Modeling (CASCaM). At

UNT, she achieved the rank of Regents Professor and served as Vice Provost for Faculty before transitioning to Michigan State University and the U.S. National Science Foundation (NSF) in 2016. At NSF, she led the Division of Chemistry and was responsible for nearly \$1 billion in national research investments. In this role, she introduced and set strategic research priorities—including the national focus on data-driven discovery and had oversight of ten national research centers and components of two of the nation's largest research facilities. At Michigan State University, she established the MSU Center for Quantum Computing, Science, and Engineering and co-founded the MSU Center for PFAS Research.



Prof. Angela Wilson delivering the 2025 Almlöf-Gropen Lecture in Oslo on September 23. Photo: Thomas Bondo Pedersen.



Almlöf-Gropen Lecturer Angela Wilson with Almlöf-Gropen Young Speakers Simon Elias Schrader and Inga Lena Schmidtke on her right and left, respectively, in Auditorium 2 at the Department of Chemistry in Oslo on September 23. Photo: Thomas Bondo Pedersen.

In her Almlöf–Gropen lecture, Wilson discussed two very different themes: (1) electronic structure approaches across the Periodic Table for thermochemical descriptions and control of excitation pathways; and (2) environmental chemistry.

Transition metal and heavy element species are among the most complex molecular species, with many possible electronic configurations, partially filled higher-angular momentum states, often resulting in strong electron correlation effects and multi-reference wavefunction character. Strategies for addressing this complex chemistry were

discussed, including a family of *ab initio* composite approaches, with examples of recent applications across the transition metal and heavy element spectrum, and comparisons to commonly used but less reliable density-functional approaches. For transition metals, Wilson's work in time-independent quantum mechanical methodologies were discussed, as well as her real-time quantum electron dynamics developments, including developments towards polaritonic chemistry.

In terms of environmental chemistry, an overview of Wilson's work on per- and polyfluoroalkyl substances (PFAS) was

provided. The use of PFAS in industrial and commercial applications for over six decades has resulted in their pervasive presence in the environment, as these species can move through soils and contaminate water sources, become airborne, and bioaccumulate in animals such as fish and cattle, as well as humans. PFAS have been linked to a multitude of health issues including thyroid disease and cancers. Wilson presented a multi-faceted computational chemistry strategy to address several key molecular-level concerns about PFAS, considering their presence in soils, water, air, plants, fish and other animals, and humans.

Almlöf–Gropen Young Speakers 2025



Inga Lena Schmidtke

*Hylleraas Centre,
UiT – The Arctic University
of Norway*

Computational insights
into methane–benzene
dehydrogenative coupling
by a homogeneous iridium
catalyst

Inga obtained her BSc. and MSc. in Chemistry at the University of Hamburg, Germany. Initially trained as an experimental organometallic chemist, she was introduced to the fascinating world of computational chemistry during an exchange to the University of Oslo as part of her master's degree. She fully shifted her research interests toward computational chemistry and entered the PhD program at UiO where her work focused on mechanistic studies of small molecule activation by homogeneous transition metal catalysts. After fulfilling her PhD degree, she moved to Tromsø to start a PostDoc at the Hylleraas Centre at UiT.



Simon Elias Schrader

*Hylleraas Centre,
University of Oslo*

Rothe's method:
Solving the time-dependent
Schrödinger equation with
adaptive Gaussians

Simon Elias Schrader is a PhD candidate at the Hylleraas Centre at the University of Oslo. He received his master's degree in computational science from the same institution in 2022, where he worked on eigenvector continuation and quantum computing. His PhD research focuses on developing new numerical methods to solve the time-dependent Schrödinger equation for strong-field dynamics using time-dependent Gaussian functions.

Egil A. Hylleraas



CHR. MICHELSENS INSTITUTT

for Videnskap og Åndsfrihet

Beretninger III, 3

EGIL A. HYLLERAAS

Bølgemekanikkens betydning for forståelsen av den kjemiske binding

(Foredrag holdt 18. januar 1933)

BERGEN 1933

A.S. JOHN GRIEGS BOKTRYKKERI

Egil A. Hylleraas

The Norwegian physicist Egil A. Hylleraas (1898–1965) helped usher in the era of scientific computing by carrying out accurate calculations on helium, thereby confirming the validity of quantum mechanics for more than one particle (1929), by predicting the stability of the hydrogen anion, later detected in the Sun's atmosphere (1930), and by performing the first calculation of the cohesive energy of a molecular crystal (1930). In 1933, he introduced the term “kvantekjemi” into the Norwegian language:

“Idet jeg avslutter den utredning håper jeg at tilhørerne vil ha fått et inntrykk av at der nå foreligger ganske vidtrekkende muligheter for å bygge opp en teoretisk kjemi, en kvantekjemi, på samme grunnlag som den fysikalske kvanteteori.”

English translation:

“In closing my presentation, I hope to have convinced the audience of the far-reaching opportunities that now exist for establishing a theoretical chemistry, a quantum chemistry, on the same footing as the physical quantum theory.”

“Importance of wave mechanics for understanding the chemical bond.” (1933)

MEETINGS AND EVENTS /



Participants at the 2025 Hylleraas School.
Photo: Marco Bortoli.

Hylleraas School

Hotel Hadeland, Gran
January 7-10, 2025

The 2025 Hylleraas School melded scientific education with social interaction, fostering new collaborations at Hotel Hadeland, with 50 participants. The scientific theme was Molecular Dynamics.

The fourth edition of the Hylleraas School was held at Hotel Hadeland on January 7-10, 2025, with an additional add-on day starting January 6. The school series aims to introduce central research topics within the Hylleraas Centre to our interdisciplinary student community, which includes chemists, physicists, biologists, mathematicians, and computer scientists. The school also dedicates a generous amount of free time to promote social activities, fostering new research projects, and facilitating interaction between junior and senior members.

The 2025 edition of the Hylleraas School was organized by Inga Schmidtke, Tonje Reinholdt Haugen, Michal Repisky, David Balcells, and Simen Reine. The first day of the school started was an optional day for those who wanted a Python course lead by

Radovan Bast, with Gabriel Gerez and Morten Ledum assisting, for an optimal outcome of the week. The following days, Michele Cascella and Sigbjørn Løland Bore covered different aspects through lectures and tutorials.

The traditional Thursday night festive banquet was well received and on the final day, Thomas Bondo Pedersen provided an overview of the activities of the Hylleraas Centre, followed by “state-of-the-RT” presentations by the PIs.

At the conclusion of the Hylleraas School, a survey was distributed to collect feedback from participants. In general, the students were very satisfied with the contents and organization, providing suggestions for further improvements for the next 2026 edition.



Participants at the Norway-Japan Seminar at the Hylleraas Centre in Oslo on February 26. Photo: Michiko Atsumi.



Organizer Michiko Atsumi with Roland Lindh (left) and Trygve Helgaker (right) on February 26. Photo: Michiko Atsumi.

Norway-Japan Academic Network and Activity Seminar

The Hylleraas Centre,
University of Oslo
February 26-27, 2025

Aimed at stimulating academic, industrial, and educational exchange between Norway and Japan, the two-day hybrid physical-digital seminar was organized by Michiko Atsumi and Erik Tellgren with support from the Hylleraas Centre, the Research Council of Norway, Innovation Norway (Tokyo), the Norwegian Directorate of higher education, and Japan Society for the Promotion of Science.

The seminar presented the activities and exchanges developed between Norway and Japan within scientific research, education, and industry. The objectives of the research exchange were presented by Nordic and Japanese representatives, and mutual understanding and the direction of future project development were confirmed.

With more than 100 participants, roughly half of them attending via zoom, the seminar featured lectures within natural sciences and medicine related to Norway and Japan, providing new stimulation to basic science in both countries. The Rector of the University of Oslo and the Deputy Head of Mission in Embassy of Japan were among the speakers. The Embassy of Japan, Japan

Society for the Promotion of Science (JSPS) Stockholm Office and Team Norway (Research Council of Norway, Innovation Norway (Tokyo), Directorate of higher education) presented their funding opportunities.

Invited speakers included Prof. Pekka Pyykkö (University of Helsinki, Finland), Prof. Roland Lindh (Uppsala University, Sweden), and Prof. Seiichiro Ten-no (Kobe University, Japan).



Participants at the symposium *Can Ice be Described from First Principles?* at the Norwegian Academy of Science and Letters on March 28. Photo: Camilla Kottum Elmar/CAS.

Young CAS workshop: Can ice be described from first principles?

The Norwegian Academy of Science and Letters in Oslo
March 27-28, 2025

As part of his Young CAS project *Can ice be described from first principles?*, Sigbjørn Løland Bore, together with Pablo Piaggi from CIC nanoGUNE, San Sebastian, Spain, organized a two-day symposium at the Norwegian Academy of Science and Letters in Oslo.

The symposium focused on the latest advances and challenges in modelling ice and water from first principles, providing a diverse range of perspectives in this crucial field of study. The event included a poster session and lectures organized into six thematic sessions:

- Beyond density-functional theory
- Density-functional theory for water and ice
- New trends in ice experiments
- Machine learning potentials
- Nuclear quantum effects
- Complex ice phenomena

Each session featured international invited speakers and each session ended with a panel debate where the audience could raise questions for discussion.



Veronica Killi from the Department of Chemistry, UiO, introduces the school children from Ila Skole in Oslo to the fascinating world of chemistry at Hvorfor Det? on March 29. Photo: Cathrine Strøm.



While all participating kids received a prize for their research posters, special prizes were awarded for the funniest, excellent, and impactful research projects and posters by Ruth Aga, founder of the non-profit organization Hvorfor Det?. In addition, the audience elected their favorite poster. Photo: Cathrine Strøm.

“Hvorfor Det?” – Science fair for school children

Hylleraas Centre, Department of
Chemistry, University of Oslo
March 29, 2025

“Hvorfor det?” is a science fair for school children aged 7 to 13 (third to seventh grade) where they get to formulate, plan, execute, and present research projects of their own choosing.

Solely based on curiosity, there are no requirements regarding the type of project – the kids decide entirely on their own, but receive training regarding planning, execution, and presentation at several workshops in the weeks leading up to the event.

At the main event held at the Department of Chemistry, University of Oslo, the young researchers presented posters to a referee panel consisting of professional researchers, including several present and former members of the Hylleraas Centre in Oslo. Prizes were given for the most excellent, funniest, and impactful research projects and posters.

Accompanied by their parents and siblings, about 100 children presented 38 posters on subjects ranging from the taste of grilled candy to battery

recycling and the primary education system’s ability to teach pupils with invisible impairments.

While the referees discussed the research projects and presentations, the children and their families enjoyed a spectacular demonstration of chemistry in action by senior engineer Veronica Killi from the Department of Chemistry, and an engaging performance by Norway’s first candidate to become an astronaut, Nima J. Shahinian, and program host, author, and science communicator, Dennis Siva Lie.

The event was organized by Anne Pedersen, Sook Berge Buer, Kevin Geers, and Kristine Eknes from the parents’ board at Ila Skole in Oslo in collaboration with the Hylleraas Centre. The training workshops were conducted by Mikkel Bugge.



Participants at the Skibotn Hackathon 2025. Photo: Marco Bortoli.

Skibotn Hackathon

Skibotn field station
May 5–9, 2025

The 2025 Skibotn Hackathon took place May 5th to 9th at the Skibotn field station of UiT – The Arctic University of Norway.

The Skibotn Hackathon is an annual event organized by the Tromsø node of the Hylleraas Centre. Participation is open to Hylleraas members and current or upcoming affiliates and is an opportunity to get away from the everyday workday environment and spend a week working on topics of their own choosing, on their own or together. It is also encouraged to give or participate in informal presentations or workshops and enjoy social activities together.

This year, there were 24 participants spanning all levels of seniority, and we saw presentations of Clifford algebras for quantum chemistry (Jacopo Masotti), a demonstration of molecular vibrational functionality in the VeloxChem program (Josefine H. Andersen), and an introduction to quantum chemistry for quantum computers (Roberto Di Remigio Eikås). We also enjoyed a barbecue in the field station's barbecue hut, and were treated to excellent home-style cooking by the field station staff.



Poster session at NMQC 2025. Photo: Luca Frediani.



NMQC 2025 logo by Quentin Pitteloud.

Numerical Methods in Quantum Chemistry 2025

Humboldt University of Berlin,
Germany 18–20 June 2025

The international workshop Numerical Methods in Quantum Chemistry 2025 (NMQC 2025) was held on 18–20 June 2025 at the Adlershof Campus of Humboldt University of Berlin, Germany. The meeting was co-organized by Luca Frediani and Michal Repisky together with Florian Bischoff. The workshop continued the traditional NMQC conference series and was organized as a satellite event of the WATOC 2025 Congress.

Alongside the traditional presentation of foundational and applied advances in numerical methods for quantum chemistry and chemical physics, the 2025 edition of the workshop placed particular emphasis on topics related to light–matter interactions and relativistic effects. The scientific program thus reflected both the core methodological focus of the NMQC series and emerging research directions, including advanced spectroscopic simulations based on time-dependent approaches.

The workshop featured 16 invited lectures by internationally recognized experts, complemented by 20 contributed talks and 15 poster presentations from senior researchers, postdoctoral fellows, and PhD students. In addition to the scientific sessions, the program included a social gathering, which further encouraged informal discussions

and networking. The diversity of topics and participants fostered lively scientific discussions and facilitated the exchange of ideas across different subfields of theoretical and computational chemistry.

The topics discussed at NMQC 2025 were closely aligned with the core research activities of the Hylleraas Centre for Quantum Molecular Sciences, particularly in advanced numerical methods, relativistic electronic-structure theory, and time dependent simulations of molecular properties and spectroscopy. The workshop provided valuable feedback for ongoing and future methodology development and software implementation, while also strengthening collaborations within the international theoretical and computational chemistry community.



Figure 1: The door is open for the participants of WATOC 2025. *Photo: Cathrine Strøm.* **Figure 2:** Prof. Trygve Helgaker, Chair of WATOC 2025, welcomed participants to the 13th Triennial Congress of the World Association of Theoretical and Computational Chemists. *Photo: Marco Bortoli.* **Figure 3:** Professor Fernanda Duarte Gonzalez, Department of Chemistry, University of Oxford. *Photo: Marco Bortoli.*

WATOC 2025

Oslo Congress Centre
21-27 June, 2005

The 13th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2025) was held at the Oslo Congress Centre from 21 to 27 June 2025. Hosted by the Hylleraas Centre at the University of Oslo, the congress brought together 1,098 participants and was among the largest and longest meetings ever organized in the field of theoretical and computational chemistry.

The scientific programme extended over all seven days of the week and comprised a total of 330 oral presentations and 627 posters. It included six plenary sessions, each featuring two speakers, for a total of 12 plenary lectures delivered in the main congress hall. In addition, the programme featured 75 thematic parallel sessions, each comprising four speakers, resulting in 300 presentations across five parallel streams. The sessions covered the full breadth of contemporary theoretical chemistry, from electronic-structure theory and spectroscopy to catalysis, materials, biosystems, machine learning, and quantum computing. Three evening poster sessions, each with more than 200 contributions, were lively and well attended.

Half of the speakers in the parallel sessions were invited directly by the organizers, while the remaining speakers were selected on the basis of a competitive evaluation of more than 400 submitted abstracts. In total, 30% of all speakers at the congress were female, reflecting a conscious effort to achieve a balanced and inclusive scientific programme.

A major new feature of WATOC 2025 was Young WATOC, a pre-congress held on Saturday 21 June and dedicated to PhD students and early-career researchers who defended their theses in 2020 or later. From 102 submitted abstracts, 18 speakers were selected for the programme. The event attracted

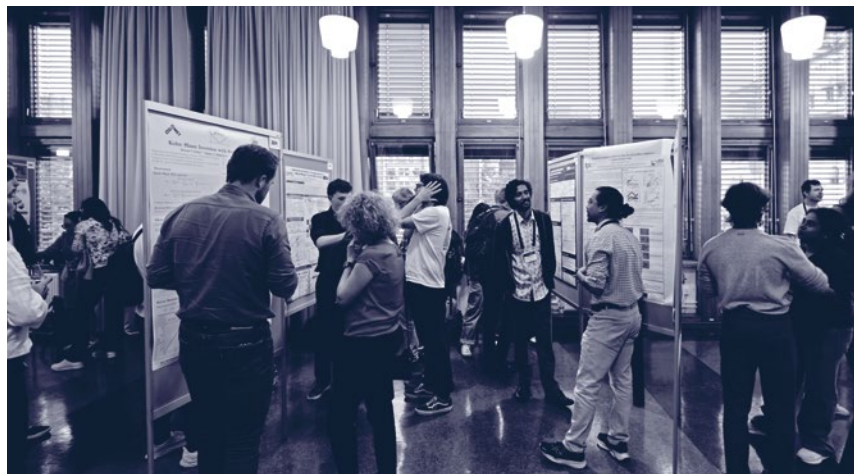


Figure 4: Barbecue at Skullerudstua on the outskirts of Oslo. *Photo: Marco Bortoli.* **Figure 5:** Hylleraas member Prof. Einar Uggerud. *Photo: Marco Bortoli.*

around 300 participants and concluded with a barbecue at Skullerudstua on the outskirts of Oslo.

Young WATOC, which was chaired by Hylleraas Pls Abril Castro and Ainara Nova, was highlighted by the WATOC president as a great success and will be continued at the WATOC 2028 in Mérida, Mexico.

WATOC 2025 attracted participants from 37 countries and about 230 institutions worldwide. Europe accounted for the largest share of attendees, followed by North America and Asia, with additional representation from Latin America, Oceania, the Middle East, and Africa. Students made



A moment from one of the poster sessions at WATOC 2025. *Photo: Marco Bortoli.*



7



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Figure 7: Prof. Michele Parinello during the discussions following his plenary lecture. Photo: Marco Bortoli. **Figure 8:** The Hylleraas Crew, consisting of 33 younger members of the Hylleraas Centre, ensured smooth daily operations and a warm, welcoming atmosphere. Photo: Marco Bortoli. **Figure 9:** Morning run outside the Oslo Opera House. Photo: Marco Bortoli.

up about one third of the participants, underlining the congress's important role in education and early-career development within the field.

The congress was chaired by Trygve Helgaker and organized by the Hylleraas Centre in collaboration with the professional congress organizer Gyro Conference. The smooth daily operation of the meeting was strongly supported by the 33-member Hylleraas Crew, whose members provided

technical and logistical assistance and helped create a welcoming atmosphere throughout the week.

A varied social programme complemented the scientific activities. Wednesday afternoon was reserved for excursions, offering participants guided tours of the National Museum, hiking trips in the surrounding hills, ferry excursions in the Oslo fjord, and guided historical walks in the city centre. The conference banquet, attended by

nearly 700 participants and guests, featured Norwegian cuisine including moose as the main course along with speeches and musical entertainment, providing a memorable highlight of the congress week.

The congress concluded on Friday with the presentation of poster prizes, acknowledgements to organizers and the crew, and the formal introduction of WATOC 2028, to be held in Mérida, Mexico.



Figure 10: About 1,100 theoretical and computational chemists participated in WATOC 2025. *Photo: Marco Bortoli.* **Figure 11:** The Hylleraas Crew, consisting of 33 younger members of the Hylleraas Centre, ensured smooth daily operations and a warm, welcoming atmosphere. *Photo: Cathrine Strøm*

// WATOC President Peter Gill praised the congress as “outstanding” and singled out Young WATOC as a particularly valuable addition that will shape future WATOC congresses //



Participants at the 2025 Hylleraas Annual Meeting. Photo: Marco Bortoli.



Thomas Bondo Pedersen, winner of the best 5-minute presentation for PIs

Hylleraas Annual Meeting

Malangen Resort, Malangen
September 8–10, 2025

This year's meeting was held at Malangen resort, located at the name giving Malangen fjord just outside of Tromsø. The meeting was organized by the YRP representatives Helena Hradiska and Inga Lena Schmidtke with assistance from Magnus Ringholm and Stig Eide of the Tromsø node.

This edition of the Annual Meeting was attended by 43 participants, mainly Hylleraas members and affiliates but we were joined by several external speakers as well. After a brief overview on the Hylleraas Centre by Thomas Bondo Pedersen, the meeting was kicked off with a workshop covering the broad topic of visualization in scientific works given by Kess Marks and Moa Kristiansson from Visualize your Science. The workshop ended with a talk focusing on poster design and afterwards we could use that newly acquired knowledge in a poster session.

During the poster session the young researchers of the center presented their ongoing work. This concluded the busy scientific part, and we ended the first day enjoying a barbecue at the nearby lake.

The second day was opened by Bror-Magnus S. Strand and Gulbrand Stålet Nilsen from the UiT library with a talk on open science, data management and the new online research information

repository solution, NVA. Their talk was followed by another invited talk given by Gabriel Gerez and Jørn Dietze from the HPC group at UiT. Gabriel and Jørn gave a brief overview on slurm scripts, data handling and general best practices.

After a well-deserved break with outstandingly good weather, we continued with the traditional 5-minute presentations, this time with reversed roles. For the first time at a Hylleraas Annual Meeting, the senior researchers of the center gave us an overview on their research in this format.

The evening session was concluded with a talk by Odile Eisenstein who took us with her on her life journey through science with a lot of personal insight and valuable advice.

To end the meeting with a real highlight, most of us could enjoy the Northern Lights dancing over the Malangen fjord after the banquet dinner.

// The annual meetings provide an opportunity for the researchers in theoretical chemistry from all parts of Norway to meet and share their results //



Magnus Ringholm (UiT)

Annual Meeting of the Division for Quantum Chemistry and Modelling of the Norwegian Chemical Society

UiT – The Arctic University of Norway,
Tromsø
October 20–21, 2025

Organized by Magnus Ringholm with support from Stig Eide, the 2025 annual meeting of the Division for Quantum Chemistry and Modelling of the Norwegian Chemical Society took place at UiT – The Arctic University of Norway in Tromsø on October 20–21.

The annual meetings provide an opportunity for the researchers in our field from all parts of Norway to meet and share their research, and this time, there were 46 registered participants, and all four major Norwegian universities (UiB, UiO, UiT, NTNU) were represented. There were 13 contributed presentations covering several different areas, ranging from quantum chemistry topics such as coupled-cluster methods to machine learning research and computational catalysis. We also had an invited speaker, Roberto di Remigio Eikås, previously a Hylleraas Centre member in Tromsø, now working for the Finnish quantum computing company Algorithmiq. Roberto gave the interesting talk *Aurora: end-to-end quantum chemistry on quantum computers*.

The conference dinner was held at restaurant Hildr, where they aim to use local ingredients but not limit their culinary inspiration to the local region. We thank all of the participants for an enjoyable meeting and look forward to next year's event.



Bjørn Jamtveit, Pro-Rector at University of Oslo, with opening remarks. *Photo: Cathrine Strøm.*

Japan-Norway Research Alliance Seminar

The Hylleraas Centre, University of
Oslo
October 27, 2025

The seminar was part of a collaboration between Japanese research institutions, the Embassy of Japan, the Japan Society for the Promotion of Science (JSPS), and the Hylleraas Centre. The seminar was a one-day hybrid event, organized with support from the Hylleraas Centre and the Department of Chemistry. Norway and Japan have maintained diplomatic relations since 1905 and are now celebrating 120 years of friendship.

The meeting was opened by pro-rector Bjørn Jamtveit. Then the Embassy of Japan, JSPS Stockholm Office, and Team Norway – Norwegian Directorate for Higher Education and Skills, Research Council of Norway, Innovation Norway Tokyo, and Norwegian Embassy in Tokyo provided information about their different funding schemes and existing collaborations between Norway and Japan.

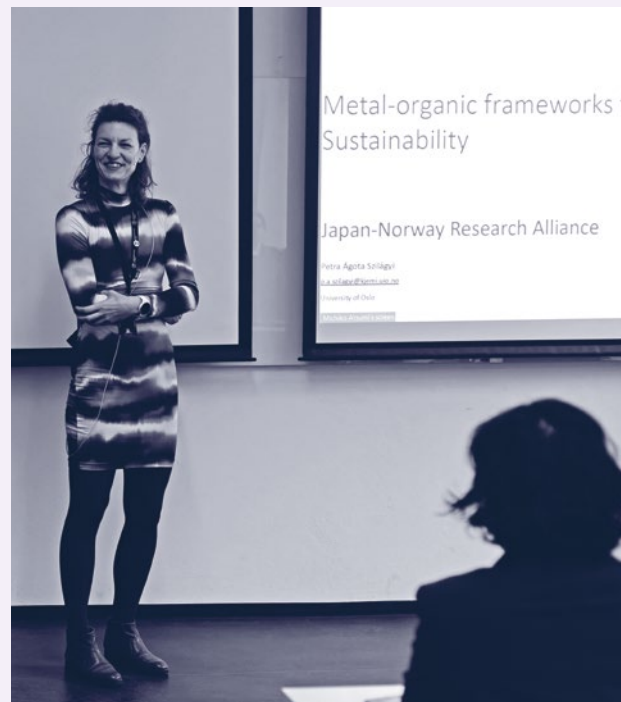
In the following sessions, the scientists from several universities in Norway talked about their research as well as their Japanese partner universities and their connections with Japan. Board members of JSPS Norway Japan Academic Network were represented among these speakers.

The lectures were aimed at a general scientific audience and covered a wide range of topics, from agricultural science to chemistry and statistics. They also provided examples of academic collaboration, practical aspects of educational and research exchange, and experiences during stays in Japan. More than 60 people attended the seminar.

In the evening, people from JSPS NJAN and the Department of Chemistry met again for dinner at the Japanese Ambassador's residence.



The Deputy Head of Mission at Embassy of Japan Hajime Matsumura.
Photo: Cathrine Strøm.



Professor Petra Agota Szilagy, University of Oslo, presented her work on metal-organic frameworks for sustainability. *Photo: Marco Bortoli.*



Ms. Mana Oshima from JSPS Stockholm Office.
Photo: Marco Bortoli.



Trygve Helgaker. Photo: Barbara Helgaker.

Quantum Science at 100

The Norwegian Academy of Science and Letters in Oslo
October 30, 2025

Interdisciplinary academy meeting marked the UN International Year of Quantum Science and Technology: The meeting featured nine invited lectures addressing the birth of quantum mechanics around 1925, its theoretical foundations, and its central role in modern science and technology.

On 30 October, the Norwegian Academy of Science and Letters (DNVA) hosted a full-day interdisciplinary meeting to mark the United Nations' International Year of Quantum Science and Technology. The meeting was held in Norwegian under the title «Kvantemekanikken 100 år: fra usikkerhetsrelasjonen til høyteknologi».

The meeting featured nine invited lectures addressing the birth of quantum mechanics around 1925, its theoretical foundations, and its central role in modern science and technology. Speakers represented a broad range of disciplines including philosophy, history, physics, chemistry, computer science, and cryptography highlighting the enduring reach and relevance of quantum science across fields.

The audience was broad, ranging from leading experts in the field to interested laypersons. The talks were designed to address this diversity, and the program offered both depth and accessibility, ensuring that all participants found material of interest and value.

The meeting was opened by Marit Westergaard, Secretary General of the Norwegian Academy of Science and Letters and a linguist by training. In her remarks, she drew on perspectives from linguistics to illuminate foundational questions in quantum mechanics, setting the stage for several of the themes explored throughout the day.

The first session, with contributions from Hans Herlof Grelland (University of Agder) and Trygve Helgaker (Hylleraas

// The program offered both depth and accessibility, ensuring that all participants found material of interest and value //

Centre, University of Oslo), revisited the early quantum revolution. The talks offered historical perspectives on the development of quantum mechanics and included a presentation on Egil Hylleraas, Norway's first quantum physicist.

The second session, featuring Asle Sudbø (NTNU) and Thomas Bondo Pedersen (Hylleraas Centre, University of Oslo), focused on the scientific significance of quantum mechanics in contemporary research, ranging from first-generation quantum technologies to quantum chemistry and advanced electronic-structure simulations.

Fundamental conceptual issues formed a central theme of the meeting. In the first session after lunch, lectures by Anders Kvalseth (University of Oslo)

and Jørn Kløvfell Mjelva (University of Oslo) addressed the interpretation of quantum mechanics and the nature of quantum correlations, engaging with long-standing questions that remain at the core of the theory.

The final session turned to second-generation quantum technologies, with presentations on quantum sensors (Marianne Etzelmüller Bathen, University of Oslo), quantum computing (Franz Fuchs, SINTEF), and the implications of quantum technologies for secure cryptography (Martin Strand, Norwegian Defence Research Establishment).

The meeting was well attended, with approximately 70 registered participants. Around 50 participants also took part in the concluding dinner at the Academy, which provided an opportu-

nity for continued discussion among speakers and attendees.

The meeting was jointly organized by the Chemistry Group and the Physics Group of the Norwegian Academy of Science and Letters. The organizing committee consisted of Arne Brataas (Physics), Trygve Helgaker (Chemistry), Kenneth Ruud (Chemistry), and Susanne Viefers (Physics), with Helgaker serving as chair.

The event received financial support from the Norwegian Academy of Science and Letters and the Hylleraas Centre. Overall, the meeting offered a timely and wide-ranging perspective on quantum mechanics as both a foundational scientific theory and a driving force behind emerging technologies in a new quantum era.

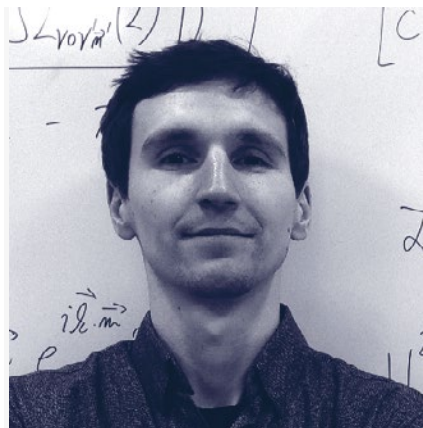
ALUMNI TALKS /

To inspire and help the young researchers at the Hylleraas Centre in planning their future career, the Young Researcher Parliament (YRP) of the centre invites previous members and collaborators to give a short seminar about their career choices and the position they hold today, whether in academia or in industry.

Dr. Marius Kadek

Life of a scientist after academia

Online seminar from the Hylleraas Centre, University of Tromsø
March 28, 2025



In the seminar, I briefly outlined my scientific journey from my PhD and postdoctoral fellowship to my current R&D role in the semiconductor industry, working on atomistic simulations in Synopsys QuantumATK. I described our work across various areas of atomistic simulation, ranging from electronic structure to dynamical properties in systems containing tens of thousands of atoms. I emphasized the importance of scientific rigor, independent thinking, and a strong focus on quality and validation as key drivers of a successful product. I concluded with my personal reflections on conducting research in both industrial and academic settings.

Dr. Magnar Bjørgve

Can Hylleraas achieve more science at lower cost using the national HPC resources?

Online seminar from the Hylleraas Centre, University of Tromsø
October 31, 2025



This presentation examines how the Hylleraas Centre can maximize scientific output while minimizing HPC costs. We discuss common inefficiencies in job configurations – misconfigured hybrid parallelism, suboptimal compilers, and memory issues – that waste computational resources. Using CPU utilization data from Betzy 2025, we present recommendations for optimizing MPI/OpenMP balance, scaling tests, and compiler selection. We also highlight available support from NRIS to help researchers achieve more science at lower cost.

Dr. Audun Skau Hansen

The Quantum Edge: from Gaussians to real-time graphics

Online seminar from the Hylleraas Centre, University of Oslo
December 12, 2025

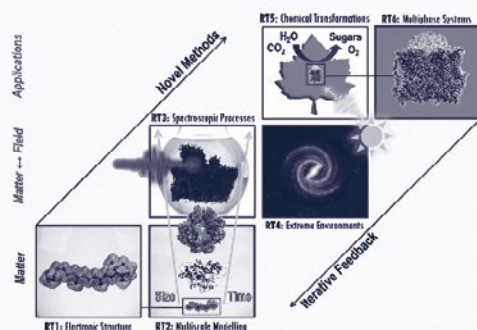


In this talk, Audun presented a surprisingly strong connection between quantum chemistry, 3D deep learning for reality capture, and real-time graphics for the entertainment industry. From Gaussian primitives used in electronic structure theory to anisotropic Gaussians driving modern radiance fields, we trace a shared mathematical lineage that connects the molecular world to buildings, the defense industry, TV-studios and beyond. Along the way, he argued that quantum chemists are uniquely positioned to fill critical workforce gaps thanks to their cross-domain intuition, mathematical (and quantum) literacy, and computational mindset.

Avslør naturens hemmeligheter med laptopen som ditt laboratorium

Hylleraas-senteret for teoretisk kjemi bringer deg til forskningsfronten

Ved Hylleraas-senteret utvikler og anvender vi simuleringstoder for å forstå, tolke og forutsi ny kjemi, fysikk og biologi for molekyler i komplekse og ekstreme miljøer.



Våre forskningstema (RT)

Gjennom et bachelor- eller masterprosjekt ved Hylleraas-senteret kan du fordype deg i tema som matematiske modelleringsmetoder, programmering og maskinlæring innen teoretisk kjemi, og du vil få en dyp innsikt i hvordan naturen frembringer molekyler struktur og dynamikk.

I tillegg vil du tilegne deg etterspurte spesialkunnskaper for en fremtidig karriere.

Finn ditt prosjekt hos oss i kolonnen til høyre.



Med Michele Cascella som veileder vil du krysse ulike størrelsesskalaer, fra kvantemekanikk til statistiske felter, for å utforske kjemiske reaksjoner, selv-aggregering og myke materialer. En tett tilknytning mellom teori og eksperiment gir også muligheter for samarbeid med eksperimentister.
Kontakt: michele.cascella@kjemi.uio.no

Sammen med Thomas Bondo Pedersen kan du blant annet utvikle helt nye beregningsmetoder for å simulere kvantedynamikken til molekyler i ultrakorte laserpulser og sterke magnetfelter i tidskalaer ned til femto- og attosekunder. Du vil utvikle *high-performance computing* algoritmer og få innsikt i avanserte spektroskopiske teknikker.
Kontakt: t.b.pedersen@kjemi.uio.no



Sammen med Ainara Nova vil du ta i bruk simuleringstoder for å utforske struktur og reaktivitet for katalysatorer nødvendig for gjenvinning verdifulle kjemikalier fra CO₂. Forskningen omfatter mange ulike systemer, blant annet homogene og single-site heterogene katalysatorer.
Kontakt: a.n.flores@kjemi.uio.no



Med David Balcells som veileder vil du ta i bruk maskinlæring og high throughput virtuell screening for å utforske katalysatorer for fornybare energiprosesser. Du vil tilegne deg ferdigheter innen dataanalyse, programmering og evaluering av prediktive modeller.
Kontakt: david.balcells@kjemi.uio.no



Sammen med Simen Kvaal kan du blant annet utvikle nye metoder for å løse den tidsavhengige Schrödingerlikningen for molekyler på datamaskinen, utforske kvantekaos og grenselandet mellom kvante- og klassisk mekanikk, og benytte maskinlæring for å gjøre kvantekjemiske beregninger kjappere.
Kontakt: simen.kvaal@kjemi.uio.no



Med Erik Tellgren som veileder kan du utforske eksotisk kjemi for molekyler i sterke magnetfelter, hvor nye kjemiske bindinger og fysiske effekter gjør seg gjeldende. Prosjekter kan fokuseres mot anvendelse, programmering av beregningsmetoder, eller matematiske/teoretiske aspekter.
Kontakt: erik.tellgren@kjemi.uio.no



Sammen med Abril Castro vil du lære hvordan du simulerer strukturelle, elektroniske og spektroskopiske egenskaper. Mulige emner er modellering av NMR-egenskaper for å forutsi og tolke eksperimenter, analyse av kjemiske bindinger i løsnings- og faststoffsystemer, og studier av molekyler som inneholder tunge atomer.
Kontakt: abril.castro@kjemi.uio.no



← Besøk vår nettside

 Hylleraas

Recruitment poster of the Hylleraas Centre at the Department of Chemistry, University of Oslo

PHD DEFENCES 2025 /

PhD Defences 2025



Candidate: Ning Cao

University: University of Oslo
Thesis: Computational Studies of Biomimetic Cu Metal Organic Systems
Trial lecture: Metal-Organic Frameworks: Definition, Key examples/systems, Applications, Problems/Challenges...
Supervisors: Senior researcher Ainara Nova Flores, University of Oslo
Prof. Unni Olsbye, University of Oslo
Senior researcher David Balcells Badia, University of Oslo
Committee: Prof. Marcel Swart, University of Girona, Spain
Assoc. Prof. Aleix Comas-Vives, Technische Universität Wien, Austria
Senior Researcher Ole Swang, SINTEF, Norway
Prof. Ute Krengel, University of Oslo, Norway
Chair: Prof. Harald Walderhaug, University of Oslo, Norway
Format: Physical



Candidate: Inga Lena Schmidtke

University: University of Oslo
Thesis: Investigations into transition metal complex reactivity – A computational perspective on C-H and C=C bond activation reactions
Trial lecture: Converging Homogeneous Organometallic Catalysis and Heterogenous Catalysis
Supervisors: Senior researcher Ainara Nova Flores, University of Oslo
Senior researcher David Balcells Badia, University of Oslo
Prof. Mats Tilset, University of Oslo
Committee: Prof. Fahmi Himo, Stockholm University, Sweden
Prof. Maria Besora Bonet, University Rovira I Virgili, Spain
Assoc. Prof. Jonathan Polfus, University of Oslo, Norway
Chair: Prof. Truls Norby, University of Oslo, Norway
Format: Physical



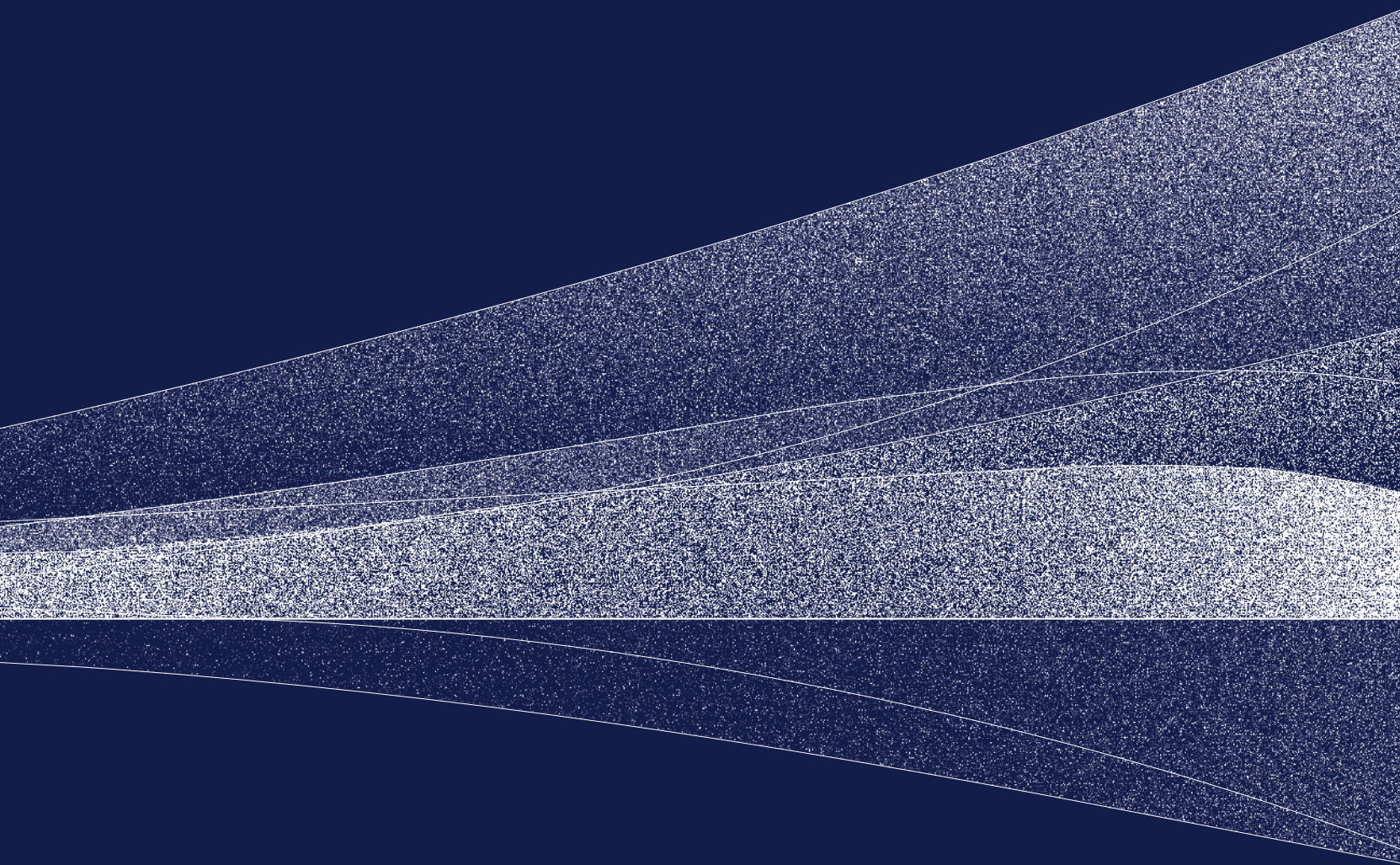
Aurore Denjean with supervisors and committee members after her successful PhD defense on September 13, 2025, in Oslo. From left: Steven Wilson, Julia Contreras, Aurore Denjean, David Balcells, Ute Krengel, and Gregori Ujaque. *Photo: Marco Bortoli. MISSING PHOTO*

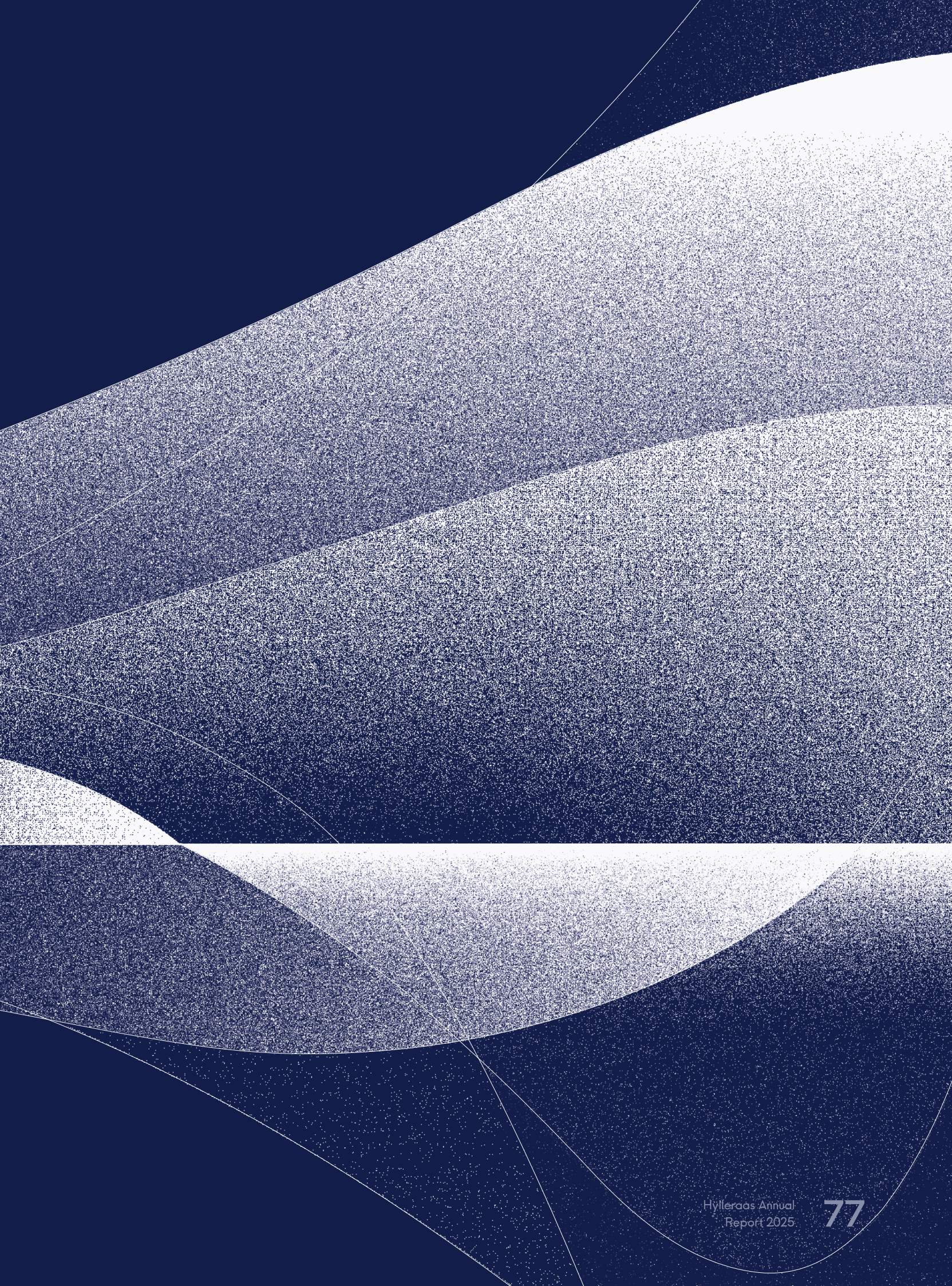


Candidate: Aurore Evelyne Francine Denjean

University:	University of Oslo
Thesis:	Structure, Reactivity, and Dynamics of Transition Metals for Catalysis Applications. A Computational Journey from Molecular to Single-Atom Systems
Trial lecture:	The Application of Machine Learning to Catalysis
Supervisors:	Senior researcher David Balcells Badia, University of Oslo Senior researcher Ainara Nova Flores, University of Oslo Prof. Michele Cascella, University of Oslo
Committee:	Prof. Gregori Ujaque Pérez, UAB University, Spain Prof. Julia Contreras-Garcia, Sorbonne University, France Prof. Steven Wilson, University of Oslo, Norway
Chair:	Prof. Ute Krengel, University of Oslo, Norway
Format:	Physical

VISITS AND MOBILITY /





*Interview
with visiting researcher:*

Jacopo Masotti

From teaching at a young age to advanced research in Tromsø, Jacopo Masotti (2001) has built an impressive academic career at the intersection of physics and chemistry. He now researches relativistic effects in quantum chemistry, while also leading an active life as both a musician and an extreme sports enthusiast.

Mr. Jacopo Masotti (San Daniele, 2001) holds a bachelor's in chemistry and a double master's degree, one in chemistry with a specialization in nano materials and one in theoretical chemistry and computational modelling, all of them attained with honors. During the studying years he has been teaching both in high school and at Trieste university as a teaching assistant. Now I am currently working as a PhD student in Tromsø, under the supervision of Luca Frediani. This forced him to advance his studies to university level during the high school years, leaving him a lot of free time during the proper chemistry university period. In his time, he followed both bachelor and master's courses in theoretical physics. Jacopo believes firmly that the best comes from the mixing of theoretical chemistry and

theoretical physics, taking the best of both worlds, using the mathematical elegance of physics, and applying it to the concrete and more common systems of chemistry. His PhD is currently focused on implementing the relativistic effects in quantum chemistry, within the multiwavelets mathematical framework.

Outside the university walls, Jacopo is a musician and has been playing French horn, oboe and piano in several orchestras for more than 15 years. Aside from this he's also an athlete, practicing many extreme and acrobatics sports like gymnastics, parkour, freerun and cliff diving. He's a great lover of nature, enjoying walks in the mountains and swims in ice water, also reason for which he eventually ended up at the Tromsø node of the Hylleraas centre.

Why did you choose to visit the Hylleraas Centre and how did you learn about the Hylleraas Centre and its visitor program?

While I was doing my Master's in *Theoretical Chemistry and Computational Modelling*, I started the slightly stressful process of figuring out where to do my thesis. So, I emailed my supervisor at the Università degli Studi di Trieste and asked if he knew any interesting research centers, adding one very important condition: **"It HAS to be COLD."** He sent me a list of universities in the Nordic countries, but he especially pointed out the Hylleraas Centre, calling it a real centre of excellence. He also mentioned that he had personally attended seminars by some of the researchers there and was genuinely impressed.





PhD candidate Jacopo Masotti from the Università degli Studi di Trieste Photo: private.

// I was already convinced by the research, but Tromsø's unique environment and inspiring academic atmosphere made the decision easy //

→ After checking out the research topics, I was already pretty sold on Tromsø. And since I'm probably the least stereotypical Italian alive, I actually *enjoy* cold and dark places, the decision became even easier. In the end, I chose to do my thesis with Luca Frediani. His group offered the chance to work on fundamental electronic structure theory using an elegant and unconventional mathematical framework. Once I got in touch and explained what I was personally interested in, he came up with a very stimulating project for me: implementing the relativistic ZORA two-component method within the multiwavelet framework.

Can you describe your visit to the centre and your stay in Tromsø?

The centre turned out to be much better than I could have expected. The atmosphere in Tromsø was very exciting, with the weekly seminars and plenty of other meeting occasions, which expanded my knowledge and horizons, also allowing me to witness the absolute beauty of the nature surrounding the city. At my arrival I was welcomed by Luca and by Stig Eide, who made sure to introduce me to everyone, so to be

included in the daily office social activities right away. Soon after Luca made sure that I was up to speed to start working on my project, while being completely open to discuss any relevant topic for my thesis. Thanks to Luca's guidance and time dedicated to me, the project was done in no time and thus I proceeded much further than expected. Outside the working hours Tromsø is full of marvellous nature, from the colors of the northern light to the uniqueness of the midnight sun. The stunning scenario of this region made coming home more difficult than expected.

In what way was the stay at the centre important for your scientific activities?

Everybody is a specialist in something, while lacking in other fields. Being together with so many people, each with a different area of expertise, really brought the best into play. Taking up strategies and thought process from every possible subject, as well as sharing mine, tackling interesting and new problems every day. In detail, the daily discussions with my office mate, PhD student Quentin Pitteloud, turned out to be very important for the devel-

opment of both my code and my skills, providing valuable comments and observations that made me discover so many more things than I could have done by myself.

How did you find Norway in general and Tromsø in particular?

I'm a big fan of mountains and stunning nature, so I've found myself very happy to be in this context. Norway is such a unique country, with an interesting culture and plenty of "unusual" activities for an Italian. I've always loved mountain sports and cold plunges. Thus, with Tromsø's weather and landscape, I was able to step up my game! Being there, and in the hope of staying, I quickly took up the challenge of learning the language, totally unaware of the "dialect situation", which slowed down my progress since they only taught Bokmål, whereas basically no-one is talking that up there. Fortunately, the effort was well worth it, as I got a PhD position in Tromsø the following autumn, thus continuing my journey in relativistic quantum chemistry, under Luca's supervision, as well as the one in the Norwegian language.



PhD candidate Jacopo Masotti from the Università degli Studi di Trieste *Photo: private.*

*Interview
with visiting researcher:*

Laura Sanchez Muñoz

Laura came for a 3-month PhD exchange at the Hylleraas Centre where she was learning about machine learning methods.

In particular, she received training on the implementation of graph neural networks to model excited-state processes in the photochemistry of lanthanide complexes. Laura is doing her PhD in the University of Barcelona, Spain, in the group of Jordi Cirera and Santiago Alvarez.

Why did you choose to visit the Hylleraas Centre and how did you learn about us?

I decided to visit the Hylleraas Centre because of its international reputation in theoretical and computational chemistry. During my PhD, I became increasingly interested in combining quantum chemistry methods with modern machine learning approaches. I learned about the Centre through scientific articles and conference presentations of Hylleraas principal investigators organized by the IQTC and RQTC, and it quickly became clear to me that it would be an ideal environment to broaden my expertise and collaborate with experts at the interface between chemistry and data science.

What was the impact of your research stay at the Hylleraas Centre on your scientific activities?

My stay at the Hylleraas Centre had a significant impact on both my PhD research and my scientific skills. I was able to deepen my understanding of graph neural networks and their application to the prediction of photochemical properties in lanthanide complexes. Working alongside Lucía Morán-González, Hannes Kneiding, and David Balcells allowed me to learn and incorporate new machine learning methodologies into my PhD project. The experience also helped me improve my coding skills, expand my academic network, and develop new collaborations for future projects.

What do you think about the social and scientific environment of the Hylleraas Centre? Were you able to participate in any activities?

I found the social and scientific environment at the Hylleraas Centre to be extremely welcoming and dynamic.

From the very beginning, I felt well integrated into the group. Scientifically, there was a strong culture of open discussion, collaboration, and exchange of ideas, which I really appreciated. I participated in group meetings, where I had the opportunity to present my work and get valuable feedback, and I also attended seminars from which I learned a lot about catalysis, MOFs, theoretical methods, and machine learning. In addition, I joined informal activities such as the seasonal parties and the “Waffles Day,” which helped me in meeting and connecting with other PhD students and researchers. This combination of high-level science and a friendly atmosphere made the experience quite enriching and a joyful chapter of my PhD.

How did you like Norway in general and Oslo in particular?

I enjoyed Norway very much, both culturally and in terms of lifestyle. Oslo is a beautiful and vibrant city, with a perfect balance between urban life and nature. I especially liked how easy it was to access parks, forests, and the fjord,



Laura with friends with the Oslo fjord on the background during the WATOC conference. Photo: Laura Sanchez Muñoz

which made my stay very pleasant and relaxing once outside of work. One of the things I enjoyed the most was being able to go hiking in the mountains and spend time in nature, which is something I truly value. Living in Oslo gave me the opportunity to experience a different culture and to enjoy a high quality of life during my research stay.

Can you mention a highlight of your stay?

A highlight of my stay was taking part in excursions with Lucía after long working days, which were a great way to relax and enjoy nature while sharing experiences outside the lab. In addition, having the opportunity to attend and experience the World Association of

Theoretical and Computational Chemists (WATOC) conference was particularly memorable. WATOC is one of the largest and most important international conferences in the field of computational chemistry and participating in it allowed me to broaden my scientific perspective, learn about cutting-edge research in this field, and connect with leading researchers in the community. These experiences, both social and scientific, made my stay at the Hylleraas Centre especially rewarding and memorable.

// Oslo offered a perfect balance of vibrant city life and easy access to nature, making my stay both enriching and deeply relaxing //

Incoming Visits

There were in total 12 visits and 10 unique visitors to the Hylleraas Centre in 2025.

Visitors to Oslo

Prof. Paul Walton	University of York, UK	30 Jan – 31 Jan
Prof. Ludwik Adamowicz	University of Arizona, USA	2 Feb – 31 Mar
MSc. Daniel Marke	Hannover Medical School, Germany	1 Apr – 30 Jun
MSc. Laura Sánchez	University of Barcelona, Spain	1 Apr – 30 Jun
Prof. Ludwik Adamowicz	University of Arizona, USA	8 May – 30 Jun
Dr. Jiali Liu	Evonik, Germany	14 Sep – 14 Dec
Prof. Angela K. Wilson	Michigan State University, USA	20 Sep – 24 Sep

Visitors to Tromsø

MSc Jan Beránek	University of Chemistry and	5 Jan – 6 Apr
MSc. Bryan Melo Flores	Slovak Academy of Sciences, Slovakia	25 Mar – 12 Apr
MSc. Tirthonkor Saikia	University of Helsinki, Finland	28 Apr – 11 May
Prof. Taye B. Demissie	University of Botswana, Botswana	8 Jun – 22 Jun
Prof. Angela K. Wilson	Michigan State University, USA	24 Sep – 26 Sep



Richard P. Feynman, Nobel Laureate 1965. In the early 1980s, Feynman proposed the idea of quantum computers, which may revolutionize computational chemistry. Photo credit: Harvey of Pasadena, courtesy AIP Emilio Segrè Visual Archives

“The physicist could never quite believe that the chemist knew what he was talking about when he described the arrangement of the atoms. For about twenty years it has been possible, in some cases, to look at such molecules [...] by a physical method, and it has been possible to locate every atom, not by looking at colors, but by measuring where they are. And lo and behold!, the chemists are almost always correct.”

Richard P. Feynman – on the concept of molecular structure, in *The Feynman Lectures on Physics* (1964)

EXTERNALLY FUNDED PROJECTS /

The financial support the Hylleraas Centre receives as a Centre of Excellence from the Research Council of Norway and from its host institutions constitutes a long-term secure funding allowing us to develop and pursue research projects that require a sustained effort over years. However, to reach the ambitious goals of the centre, additional funding is needed—to focus on particular research challenges and to pursue promising new research directions that may arise in the course of the work at the centre. In the following, we present the external research grant proposals that were approved for funding in 2025. Progress in these projects will in the future be reported as part of the activities of the research themes in the coming years.



Informal celebration of the QSTAR centre at the Department of Mathematics at UiO.

From left: Thordis Thorarinsdottir (Statistics, UiO), Joakim Bergli (Physics, UiO), Franz G. Fuchs (SINTEF), Nadia S. Larsen (Mathematics, UiO), Eric Bedos (Mathematics, UiO), Simen Kvaal (Hylleraas, UiO), Makoto Yamashita (Mathematics, UiO). Photo: Simen Kvaal.

QSTAR: Centre for Quantum Computing and Applications



RCN National Centre for Quantum
Technology Research
Simen Kvaal

At the end of 2025, four national centres for quantum technology were announced by the Research Council of Norway. Hylleraas PI Simen Kvaal was part of a consortium led by SINTEF researcher Franz G. Fuchs that submitted the proposal QSTAR: Centre for Quantum Computing and Applications. The centre comprises researchers from OsloMet, NTNU, Simula Research Laboratory, as well as international research partners QMATH in Copenhagen and Research Institutes of Sweden AB (RISE). Industry and government partners are also included, exemplified by IBM Norge, DNB Bank ASA, Kongsberg Discovery, and Norwegian National Security Authority (NSM). QSTAR will strengthen Norway's position in the field of quantum computing by

advancing fundamental research in key areas where the partners have distinctive expertise, namely fault tolerance, compilation, and quantum algorithms, while building a sustainable national academic community, fostering strong Nordic and European collaborations, and training the next generation of researchers and experts in quantum technology.

The centre is funded by RCN with 60 MNOK over 5 years and is scheduled to start on April 1, 2026. Hylleraas PI Simen Kvaal will work on quantum computing algorithms for quantum chemistry.



Project participants celebrating the election of the PERMEATE project as a UiO:Life Science Convergence Environment. From left: Ragnhild Elisabeth Heimtun Paulsen (Department of Pharmacy, UiO), Michele Cascella (Hylleraas PI, Department of Chemistry, UiO), Reidar Lund (Hylleraas affiliate, Department of Chemistry, UiO), Josefine Eilso Nielsen (Department of Pharmacy, UiO), Marit Inngjerdingen (Department of Pharmacology, UiO), and Ole Andreas Løchen Økstad (Department of Pharmacy, UiO). Photo: Reidar Lund.

PERMEATE: Peptides for Membrane Targeting and Synergistic Drug Delivery



UiO: Life Science Convergence Environment Reidar Lund and Michele Cascella

Hylleraas affiliate Prof. Reidar Lund at the Department of Chemistry, University of Oslo, leads the new UiO:Life Science Convergence Environment *PERMEATE: Peptides for Membrane Targeting and Synergistic Drug Delivery*, with Michele Cascella as one of the PIs. The project focuses on overcoming cell membrane barriers using peptides to facilitate the targeted delivery of therapeutic molecules, leveraging a multidisciplinary approach that combines expertise from computational sciences and chemistry to pharmacy and medicine.

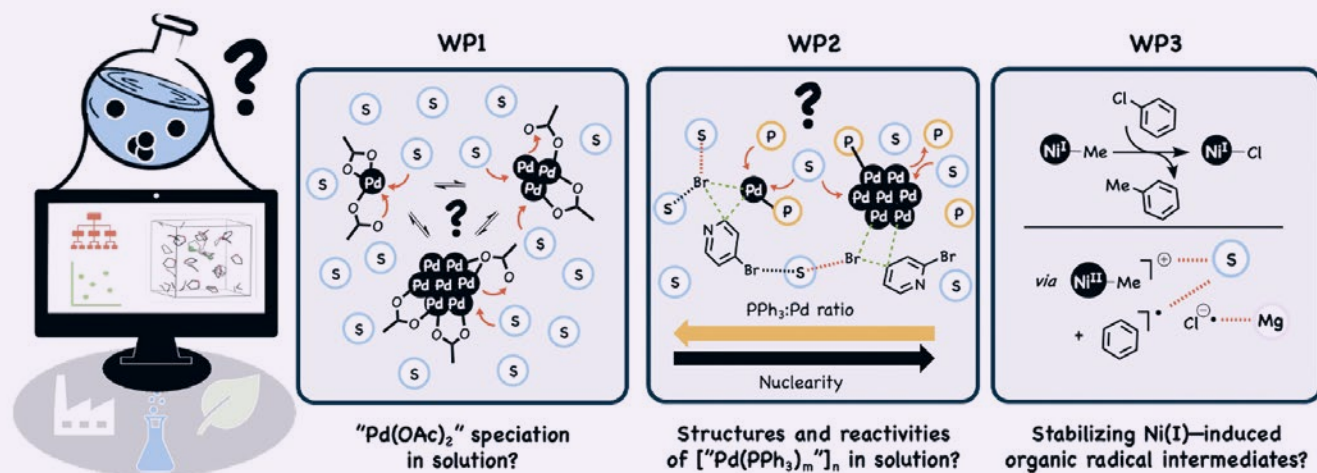
The primary objectives of the project are:

- Identify peptides to specifically target and permeate cell membranes of therapeutic relevance.
- Explore synergistic effects of peptides with small molecule therapeutics.
- Use peptides as a targeting molecule for drug delivery vehicles such as lipid nanoparticles (LNPs)

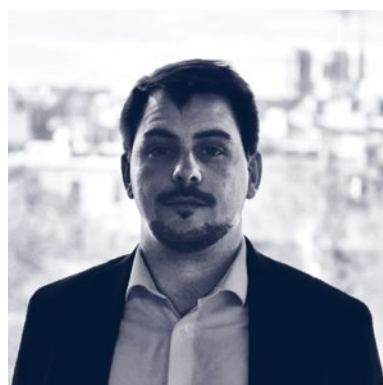
The secondary objectives are:

- Create experimental protocols for cancerous, healthy human and microbial model cell membranes.
- Establish predictive models for peptide-induced transport and cell membrane deformation.
- Create a training hub for young scientist to prosper in a multidisciplinary environment that connects experts ranging from theoretical modelling to biomedical applications.

PERMEATE has received sufficient resources, including three PhD students and a postdoc, to pursue the entire process; from understanding the underlying molecular interactions through simulations and structural studies, to relating these findings to cellular uptake. This knowledge will then be used to develop medical applications against bacterial infections and cancer.



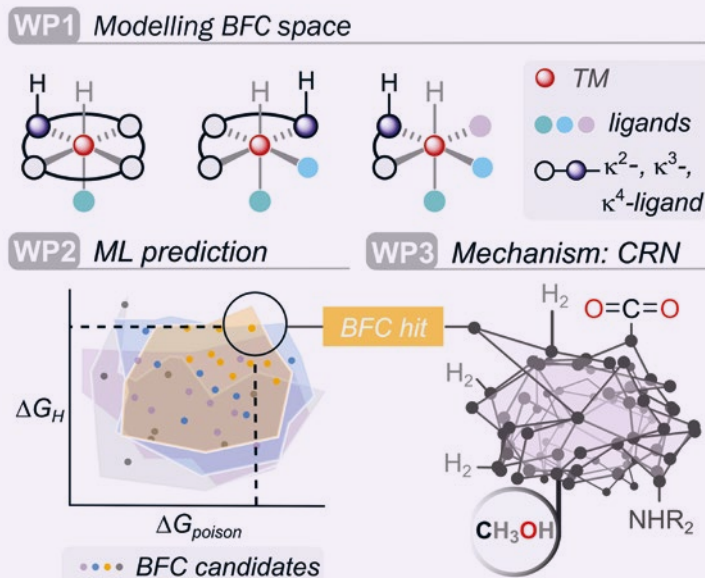
DEEP-CAT: Controlling the Structure of Transition-Metal Catalysts by Tuning their Chemical Environment



EU Marie Skłodowska-Curie Actions
Postdoctoral Fellowship
Jordan Rio

DEEP-CAT will investigate how cross-coupling reactions at palladium are influenced by thermodynamic conditions and solvent, as well as the local chemical environment. This will be done combining reliable quantum-mechanical approaches with novel machine-learning methods involving neural-network potentials.

Jordan will work at the Hylleraas Centre in Oslo under the supervision of Michele Cascella, David Balcells, and Ainara Nova, and in collaboration with Odile Eisenstein.



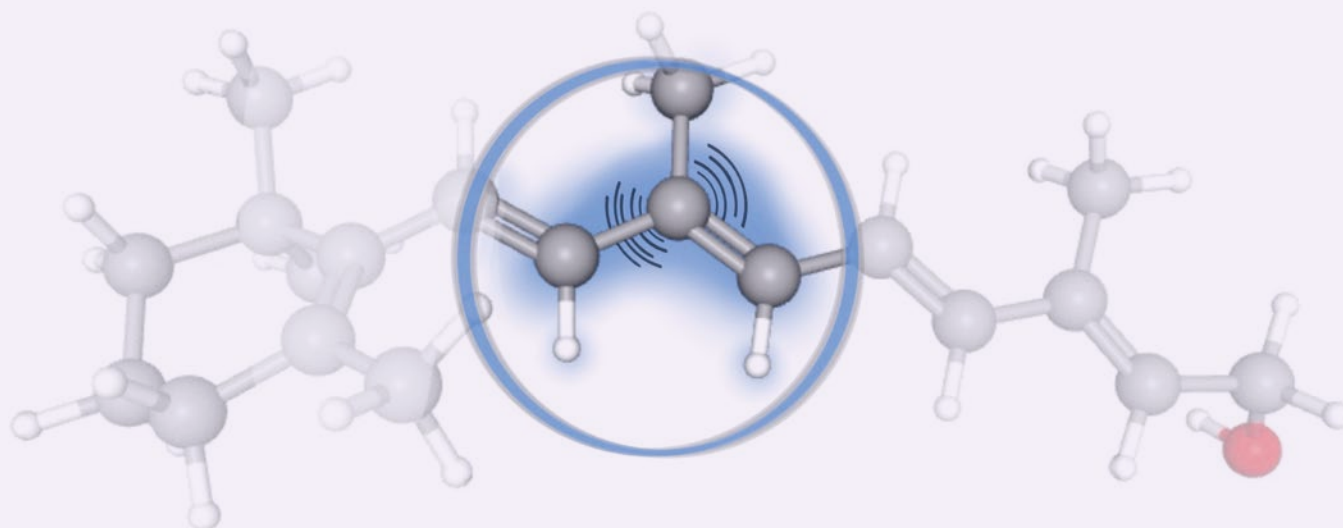
BIFUCCO₂: Machine Learning-Enhanced Design of Homogeneous Bifunctional Catalysts for CO₂ Hydrogenation



EU Marie Skłodowska-Curie Actions
Postdoctoral Fellowship
Lucía Morán González

BIFUCCO₂ aims to identify efficient catalysts for CO₂ hydrogenation reactions among a generated library of bifunctional molecular complexes by using data-driven strategies and quantum mechanics calculations. This project will also involve mechanistic studies through the automated generation of chemical reaction networks and microkinetic modelling.

Lucía will work at the Hylleraas Centre in Oslo under the supervision of Ainara Nova, and David Balcells.



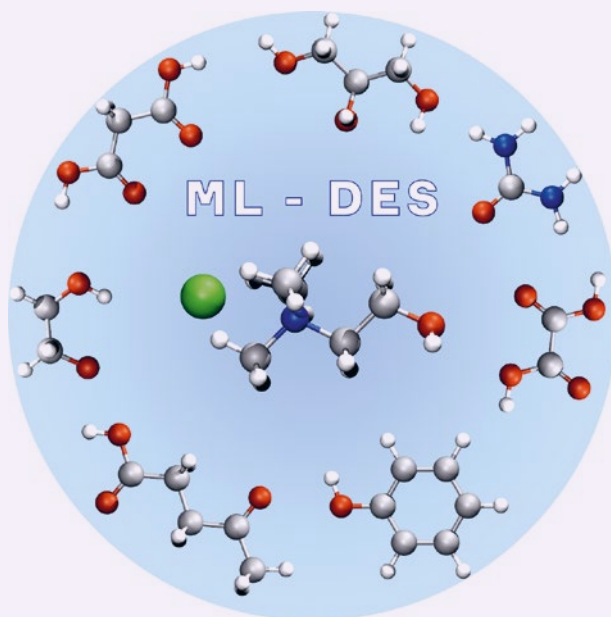
HOOD: High-order geometric derivatives with multilevel coupled cluster theory



HOOD seeks to develop methodology for the efficient calculation of geometric derivatives of molecular properties at the coupled-cluster level, involving the multilevel coupled-cluster functionality of the eT program and the symbolic functionality framework of SymResponse.

Josefine will work at the Hylleraas Centre in Tromsø under the supervision of Magnus Ringholm.

EU Marie Skłodowska-Curie Actions
Postdoctoral Fellowship
Josefine Hvarregaard Andersen



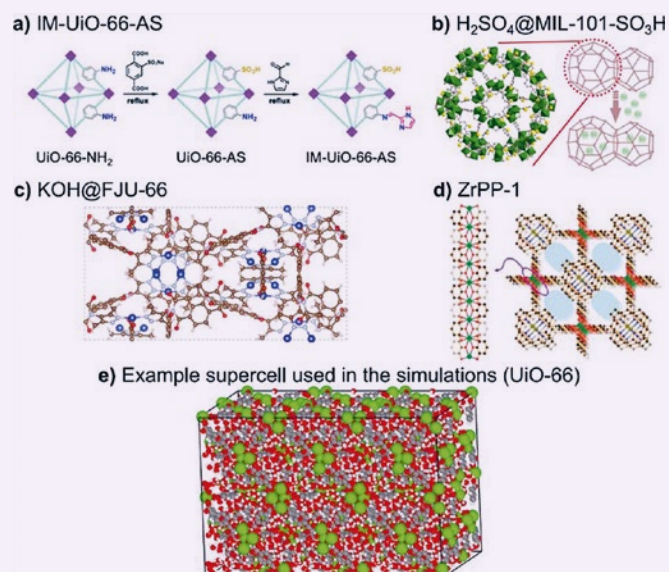
ML-DES: Developing Efficient Machine Learned Potentials for Deep Eutectic Solvents



EuroHPC Joint Undertaking
Regular Access
Marco Bortoli

The project ML-DES aims to develop a fast and accurate interatomic potential to simulate an ensemble of deep eutectic solvents (DESs) composed of choline chloride and a variety of H-bond donor molecules using a machine learning (ML) approach. Thanks to this potential, exploration of the structure and properties of different DESs will improve the range of application of these non-toxic and environmentally friendly solvents that are a promising substitute to more traditional volatile organic compounds.

The funding provides a total of 260000 GPU hours to be used on the supercomputer LUMI and involves Marco Bortoli as PI with the collaboration of Hylleraas alumnus Sondre Eliasson, Hylleraas PhD student Manuela Leal Nader, and MSCA postdoc Jordan Rio.



Ionic conductivity in metal-organic frameworks from first principles



EuroHPC Joint Undertaking
Regular Access
Henrique Musseli Cezar

The project aims to understand how to make metal-organic frameworks (MOFs) better conductors for protons and hydroxide ions. To achieve this, machine learning interatomic potentials will be developed from first-principles calculations to describe various MOFs and their interaction with water. These potentials will then be used to simulate ion conductivity in both pristine and defective systems. The results are expected to provide clear guidelines for improving conductivity in MOFs.

Working with Sigbjørn Løland Bore, Henrique will utilize the LUMI supercomputer. The project was granted a total of 7.9 million CPU hours and 408,756 GPU hours



The MRChem group at the Hylleraas Annual Meeting in September 2025. Photo: Marco Bortoli.

Parallelization of the MRChem code: Development Phase

EuroHPC Joint Undertaking
Development Access
Luca Frediani

Quantum chemistry is a very useful and routinely applied tool in chemical research, providing insight by modelling geometries, reaction mechanisms, molecular properties and more. Our software, MRChem, is a quantum chemistry code based on Multiwavelets which stands out by being capable of performing DFT calculations at very high precision due to the use of an adaptive grid and precise error control for each operation. With the advent of artificial intelligence and machine learning, it is of paramount importance to be able to provide such methods with precise and reliable reference data for training and validation.

From December 2025 until June 2026, Luca and the MRChem group will use the granted 200,000 CPU hours on the MareNostrum5 cluster to fine tune the development of the parallelization strategy of the MRChem software to adapt it to the EuroHPC machines.

RESEARCH THEME ACTIVITY REPORTS /

At the Hylleraas Centre, we develop and apply computational methods to understand, interpret, and predict new chemistry, physics, and biology of molecules in complex and extreme environments.

99 RT1: MOLECULAR QUANTUM
MECHANICS / **107** RT2/6:
MULTISCALE MODELLING AND
COMPLEXITY / **113** RT3/4:
MATTER-FIELD INTERACTIONS /
118 RT5: CHEMICAL
TRANSFORMATIONS / **123** RT7:
MACHINE LEARNING AND
MATHEMATICAL METHODS /
129 RT0: HYLLERAAS SOFTWARE
PLATFORM

Our work is organized into six research themes (RTs):

- RT1: Molecular Quantum Mechanics
- RT2/6: Multiscale Modelling and Complexity
- RT3/4: Matter-Field Interactions
- RT5: Chemical Transformations
- RT7: Machine Learning and Mathematical Methods
- RT0: Hylleraas Software Platform

Each RT has its own deliverables, directed towards the common goal of the centre: develop an integrated approach to the investigation of complex molecular systems in electromagnetic fields and in extreme environments, including:

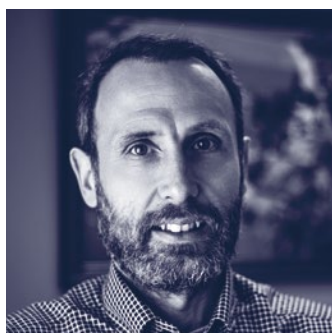
- accurate and efficient modelling of complex systems in space and time
- understanding matter–field interactions and extreme environments

We aim to treat systems containing from a few to thousands and even millions of atoms, to unravel their response to short laser pulses and strong fields, and to explore processes extending from attoseconds to microseconds.

In the following, the 2025 activity report is provided for each of the RTs.

RT1: Molecular Quantum Mechanics

Molecular quantum mechanics is the application of the laws of quantum mechanics to study chemical systems. While this is commonly interpreted as electronic structure and dynamics within the Born–Oppenheimer approximation, research in RT1 is based on the wider definition where both electronic and nuclear degrees of freedom are treated quantum mechanically, either with or without the Born–Oppenheimer approximation. The central motivation is to develop accurate computational tools to understand, interpret, and predict molecular properties and reactivity, including laser-induced processes down to the attosecond time scale.



Principal investigators:
Thomas Bondo Pedersen and
Luca Fredian

Laser-induced molecular quantum dynamics

A major goal of RT1 is to enable fully quantum-mechanical simulations of laser-induced dynamics without assuming the Born–Oppenheimer approximation at any stage. In effect, this means that the electrons and atomic nuclei are treated on the same footing without localizing the latter at fixed spatial positions at any stage. To this end, we are working on two different approaches. One is based on real-space grids with emphasis on pseudo-spectral methods. While highly accurate, such grid-based methods suffer from enormous computer memory requirements. As an alternative, unconventional but highly promising approach, we also develop methods based on one- and many-body Gaussian wave packets. The propagation of these is, however, extremely numerically challenging within the framework of the time-dependent variational principle. To overcome this challenge,

we collaborate closely with RT7 on Rothe propagation, which turns the wave-function propagation into an optimization problem at each time step, thus enabling error control relative to a chosen reference propagation. For more details on the developments of Rothe propagation, we refer to the RT7 activity report.

One of the key questions addressed in 2025 is whether the Gaussian wave packets can correctly capture ionization and dissociation dynamics induced by strong laser fields. Following up on previous work done in collaboration with Dr. Aleksander P. Wozniak from University of Warsaw and Prof. Ludwik Adamowicz from University of Arizona, we published a paper on Rothe propagation of Gaussian wave packets for 2D models of an electron in a Coulomb-like potential and a heavy particle moving in the Morse potential [1].



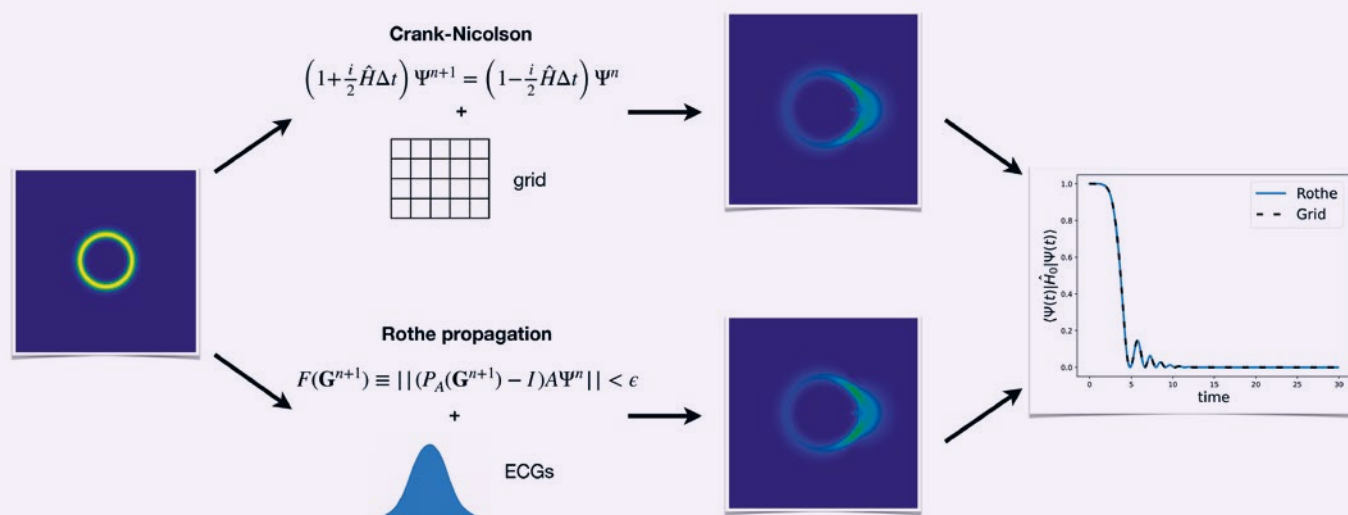


Figure 1: Laser-induced quantum-mechanical motion in a Morse potential, comparing highly accurate grid-based results with those obtained by Rothe propagation of Gaussian wave packets. The two approaches yield virtually identical results. The curve on the right shows that the final state is completely orthogonal to the ground state (shown to the left), demonstrating the enormous adaptability of the Gaussian wave packets in the Rothe propagation scheme. Reproduced from ref. [1] under CC-BY 4.0 license.

Figure 1 illustrates the differences between conventional propagation, here with the Crank-Nicolson scheme, and the stepwise optimization of Rothe propagation for the Morse model. Starting from the same initial state, the ground state, the time evolution is virtually identical with both schemes after application of a very strong electric-field impulse. For the Coulomb-like model, Figure 2 similarly documents that Rothe propagation of Gaussians yields accurate results if the optimization problem at each time step is sufficiently tightly converged. Importantly, only a few dozen Gaussians are required to reproduce unbound (ionization) electron dynamics with high angular-momentum quantum numbers.

Correlated electron dynamics

Laser-driven electron dynamics remains an important goal of RT1, and we have in 2025 continued our long-standing efforts on developing the coupled-cluster methods for this purpose. Together with Prof. T. Daniel Crawford and doctoral student Zhe Wang at Virginia Tech, we have presented the first implementation of the time-dependent coupled-cluster singles and doubles with approximate triples (CC3) model [2] using fixed, atom-centered (conventional) Gaussian basis functions. The mathematical foundation underpinning this work was also developed in 2025, as described in the activity report of RT7. In the future, the ambition is to expand the formulation to Gaussian

wave packets such that continuum-continuum interactions can be described with unprecedented accuracy, including processes such as non-sequential double ionization and relaxation processes such as Auger decay.

In ref. [2], we study linear absorption spectra and frequency-dependent polarizabilities and hyperpolarizabilities and show that simulations may be considerably accelerated using graphical processing units (GPUs). A particularly important finding of this work is that single-precision arithmetic may be applied without significant loss of accuracy (Figure 3), at least for the types of weak-field processes studied in ref. [2].

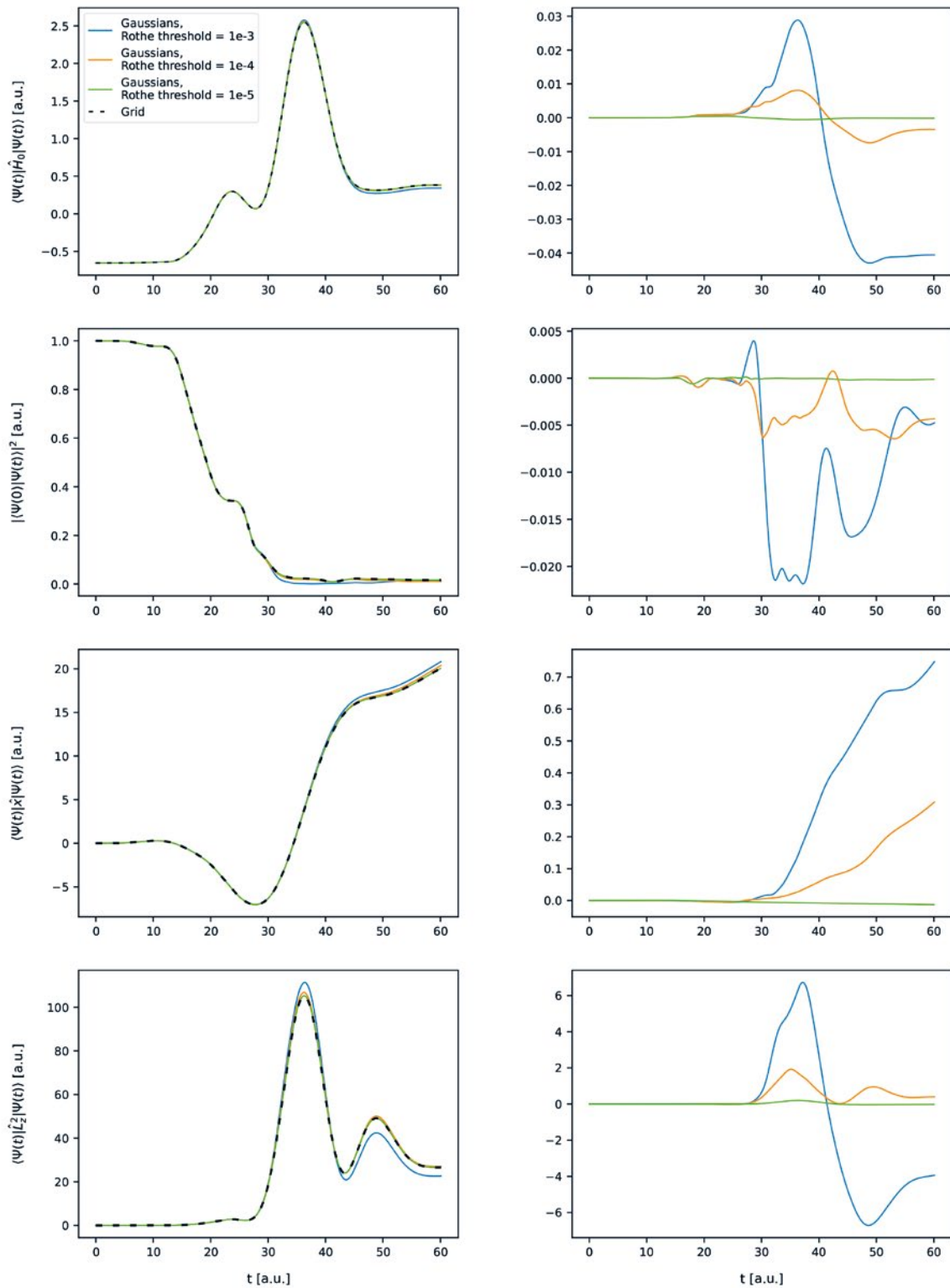


Figure 2: Laser-induced quantum-mechanical motion in a Coulomb-like potential, comparing highly accurate grid-based results with those obtained by Rothe propagation of Gaussian wave packets. The left column shows (from top to bottom) the time evolution of the energy, the ground-state survival probability, the position, and the angular momentum. The right column shows the errors relative to the grid-based reference simulation for different Rothe optimization tolerances. Note that the scale on the y-axis of the right-column plots is two orders of magnitude below that of the left-column plots. Reproduced from ref. [1] under CC-BY 4.0 license.

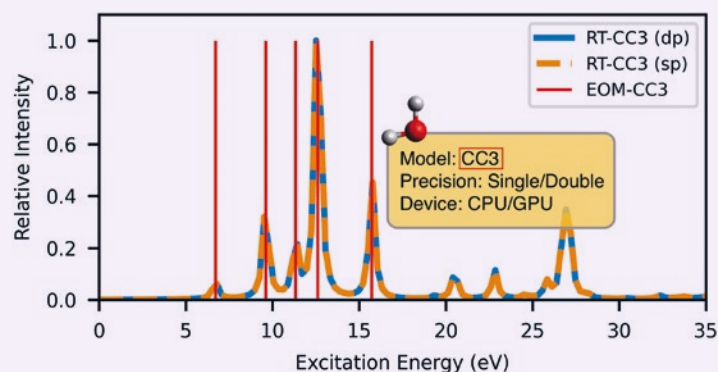


Figure 3: Linear absorption spectrum computed from CC3 simulations and compared with conventional equation-of-motion CC3 excitation energies (vertical red lines). Importantly, single-precision arithmetic can be used to accelerate simulations with negligible loss of numerical accuracy relative to double-precision arithmetic, thus enabling efficient use of GPUs. Reproduced from ref. [2] under CC-BY 4.0 license.

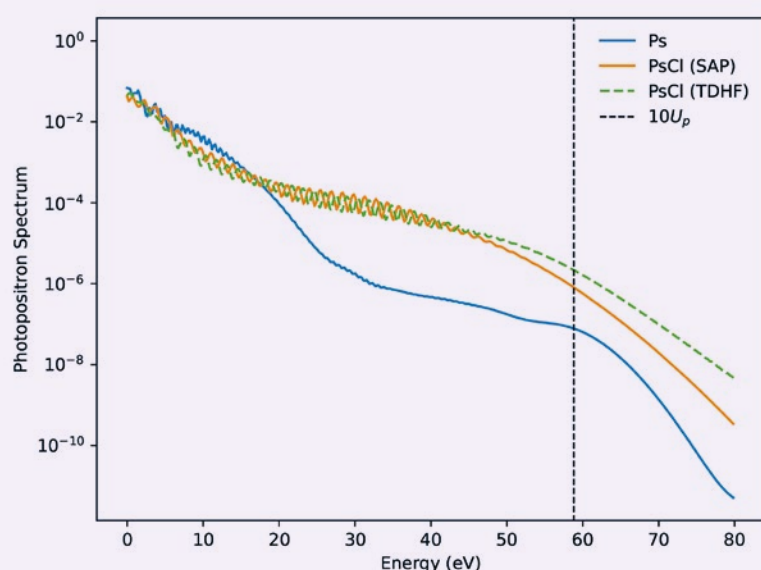


Figure 4: Photopositron spectra of Ps and PsCl, the latter obtained from TDHF and SAP simulations (the Ps simulation is numerically exact). The driving laser field is a four-cycle pulse with 800 nm carrier wavelength and a peak intensity of 1014 W/cm². The dashed vertical line indicates an estimate of the maximum achievable energy of the positron (U_p is the ponderomotive energy) obtained from the so-called “Simple Man’s model.” Figure by Einar Aurbakken.

Ultrafast dynamics of positronic matter

Positronium (Ps) is the hydrogen-like “atom” formed by an electron and its antiparticle, the positron. When the electron and positron collide, the pair is annihilated producing gamma radiation. The positron annihilation is the fundamental process exploited in positron emission tomography (PET) and its recent extension, positron imaging (PI). Relatively little is known about the short-lived states of a positron bound to an atom or molecule, however, despite the great interest in them for improved medical diagnostics. A key quantity, the positron binding energy, has proven

challenging to compute theoretically and, moreover, has only been experimentally measured for a limited number of molecules.

Noting that the lifetime of such systems typically is on the order of tens of nanoseconds, we have in 2025 completed a study of laser-induced dynamics in PsCl aimed at predicting ultrafast spectroscopic signals from this system and thus to aid future direct observations of it [3]. This is a collaboration with Dr. Antoine Camper from the Department of Physics at UiO. Camper is also affiliated with the antimatter project, AEGLS, at CERN where experi-

ments of the type proposed by us may soon become possible.

In this study, we have used the time-dependent Hartree-Fock (TDHF) model with a pseudo-spectral representation of the electronic and positronic orbitals. While correlation (electron-electron and electron-positron) effects are neglected in this approach, the simulations are converged with respect to radial grids and angular expansions. Since an experimental sample will contain Ps in significantly higher concentration than the target system PsCl, we searched for spectroscopic signals of the latter that are well separated from those of Ps.

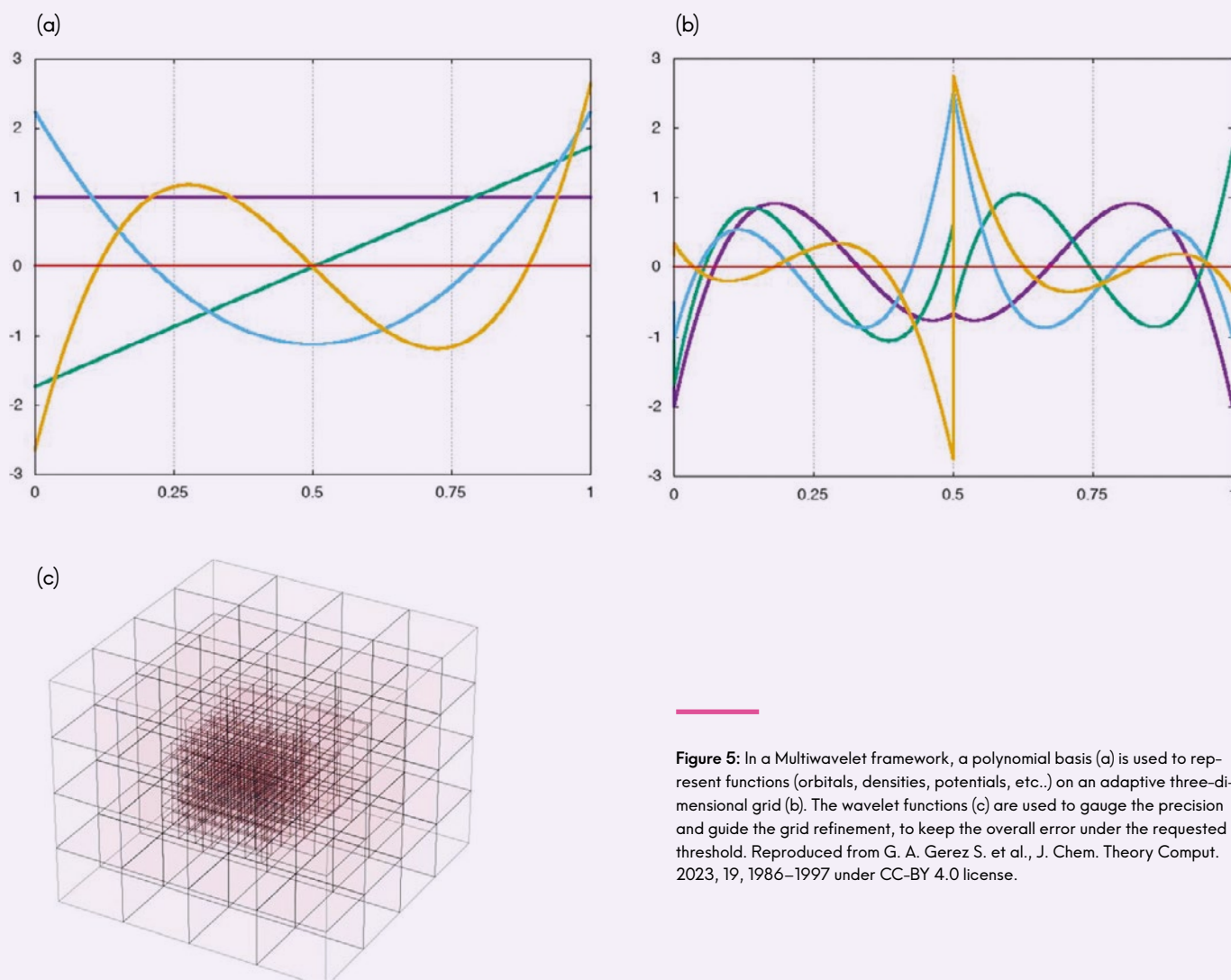


Figure 5: In a Multiwavelet framework, a polynomial basis (a) is used to represent functions (orbitals, densities, potentials, etc..) on an adaptive three-dimensional grid (b). The wavelet functions (c) are used to gauge the precision and guide the grid refinement, to keep the overall error under the requested threshold. Reproduced from G. A. Gerez S. et al., *J. Chem. Theory Comput.* 2023, 19, 1986–1997 under CC-BY 4.0 license.

Figure 4 shows the TDHF predictions for strong-field photopositron spectra of Ps and PsCl along with the prediction from a “single-active positron” (SAP) model for PsCl where the electron density is fixed at its ground-state value and only the positronic orbital is propagated. Evidently, the TDHF model predicts that peaks between roughly 20 to 45 eV should indicate the presence of PsCl in the sample. Including correlation in the treatment—a project we are about to initiate—will obviously change the PsCl peak positions but will not fundamentally alter the prediction.

Multiwavelets

Multiwavelets (MWs, Figure 5) provide a systematically improvable real-space representation with simultaneous localization in real and Fourier space, enabling adaptive grids and compressed high-precision representations of orbitals and electron densities. Building on this foundation, the Tromsø node expanded the methodological and application scope of MW-based quantum chemistry in the MRChem software package during 2025, spanning correlation methods, robust force calculations, time-dependent operators, and core-level spectroscopy.

The group was strengthened by several new members in 2025: Researcher Inga Lena Schmidtke (PhD, UiO, Oslo 2025), Postdoc Marcus Takvam Lexander (PhD, NTNU, Trondheim 2025), Researcher Tarek Scheele (PhD, University of Bremen 2025), two new PhD students Niklas Göllmann (MSc, University of Münster, 2025) and Jacopo Masotti (MSc, University of Trieste, 2025), and finally Researcher Valentyn Abramov (MSc, PSTU, Mariupol 2022).

Several exciting new activities have been initiated in 2025. Although they have not led to publications yet, they will lay the foundation for several results in

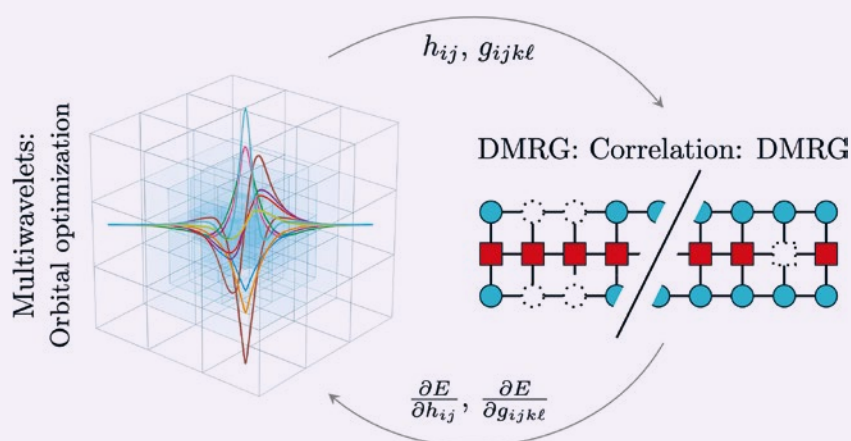


Figure 6: The Combined DMRG-MW procedure. Orbitals are optimized with multiwavelets in the complete basis, whereas configuration coefficients are obtained via DMRG. 1- and 2-electron integrals are passed from the MW solver to the DMRG solver, while 1- and 2-reduced density matrices are fed back to the MW optimizer. Reproduced from ref. [4] under Creative Commons license.

the coming years. Ylva Os has been working on the implementation of LibXC in MRChem to expand the available exchange–correlation functionals. LibXC is the de-facto standard library for approximate density-functionals both in quantum chemistry and in materials science and is regularly updated with new functionals. This will therefore be a welcomed and long-awaited feature for MRChem, allowing us to provide additional benchmarks to the community.

Tarek Scheele and Bin Gao are implementing explicit magnetic fields: the use of Multiwavelets is here especially interesting to investigate possible limitations of Atomic Orbital bases when strong external magnetic fields are introduced.

Peter Wind has done extensive development of mrcpp to support multicomponent functions and native complex-valued functions which will enable

several developments such as magnetic-fields, time evolution, and relativistic methods.

Quentin Pitteloud has worked on Clifford-algebra formulations of 2- and 4-component relativistic methods, to obtain a formulation which could consistently take advantage of the Kramers Time Reversal Symmetry for many-electron systems (beyond the trivial two-electron case).

Niklas Göllmann who started his PhD project last year on large and condensed-phase systems, has started the implementation of subsystem DFT methods with MWs, an expertise he has acquired during his master in Münster. As a connected preliminary study, he has implemented a simple population analysis tool for dimers (tested now on water and benzene dimers) which can give interesting insight in electron distribution among two monomers, free from any AO basis misinterpretations.

Jacopo Masotti who started his PhD project last year on the implementation of relativistic methods, has been working on 4-component relativistic methods in MRChem. In particular, he has been working on the reformulation of 4c methods in terms of the squared Dirac operator.

Inga Schmidtke has started using MRChem to obtain benchmarks for energy, gradients and geometry optimizations, taking advantage of our recently published work on gradients.

Evgueni Dinvar has worked on direct optimization methods on Grassman manifolds. The flexibility of MW methods allows one to explore optimization methods in ways that are not amenable to AO treatments and that could potentially make optimization in electronic structure both more efficient and more robust, especially for correlated wave functions and excited states.

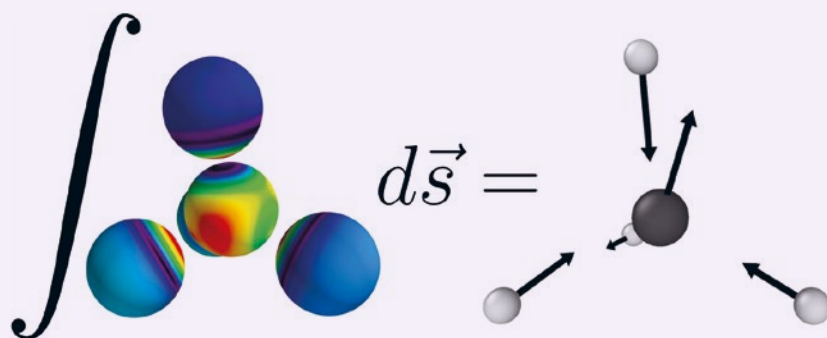


Figure 7: Forces acting upon a given nucleus in the MW framework are calculated as surface integrals over a spherical domain around the selected nucleus. This mitigates numerical issues making the calculation more precise. Reproduced from ref. [5] under CC-BY 4.0 license.

We have finalized several publications which consolidated our development of MRChem to reach the goal of a widely used and feature complete code. We made progress along several method-development directions, ranging from the introduction of correlation, the computation of robust nuclear gradients, to time propagation, core-ionization energetics, and algorithmic advances for multiconfigurational optimization with a Newton-type algorithm.

In ref. [4] (Figure 6) we combined a MW representation for orbitals with a DMRG approach to strong-correlation solver. DMRG calculations can be carried out with a comparatively small basis yet keeping the full flexibility of the MW orbital optimizer in the complete basis set. Basis-set incompleteness issues are absent, and convergence to the correct solution is achieved with an active DMRG space of small size.

Precise nuclear gradients are a known numerical stress test for MW methods because they probe quantities extremely sensitive to local errors. Reference [5] provides a reformulation that improves robustness (especially at “moderate” precision settings), making geometry optimization and related property calculations more practical in routine applications (Figure 7).

Core-ionization energies demand extremely good description of the core orbitals, which are generally less well described by AO bases, with the assumption that the chemically relevant orbitals are the valence ones. This assumption is missing for core properties, and the benefit of an adaptive MW basis becomes apparent. To overcome the collapse of the core-ionized state (either towards a valence ionization or due to delocalization of the hole) we coupled our MW method with the Maximum Overlap Method (MOM) which effectively constrains the hole to

stay localized at the correct nucleus. As shown in ref. [6], this enables stable and physically meaningful core-ionized solutions (Figure 8).

Reference [7] shows that it is possible to perform stable and efficient Newton-type optimizations for multiconfiguration self-consistent-field problems when the orbital representation is obtained using MWs. The restricted two-electron setting provides a test environment for diagnosing convergence behavior and algorithmic stability, with a view toward generalization.

Describing electron dynamics using MWs is the subject of refs. [8] and [9]. Reference [8] constructs a multiresolution approximation of the free-particle propagator by representing the associated semigroup directly in a multiwavelet basis. The technical bottleneck is that the representation involves integrals of highly oscillatory

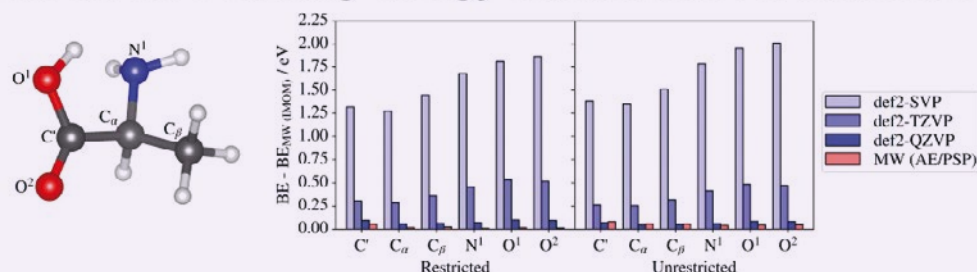
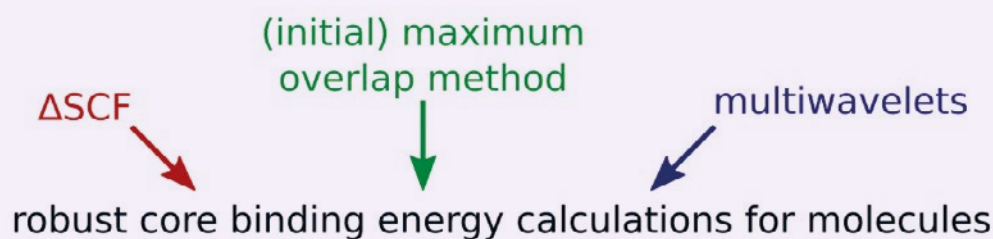


Figure 8: The combination of the Maximum Overlap Method and a MW approach allows to compute precise core-ionization energies in all-electron framework without risking delocalization or collapse of the core-ionized state. Reproduced from ref. [6] under CC-BY 4.0 license.

functions, which are difficult to discretize reliably with earlier approaches. The paper's key methodological contribution is an efficient contour-deformation discretization, establishing a robust operator representation usable as a building block in time-dependent MW algorithms.

Reference [9] delivers the algorithmic integration pathway for the time-dependent Schrödinger equation in the multiresolution framework. It combines symplectic splitting (separating kinetic and potential contributions) with the multiwavelet semigroup representation of the free-particle operator and uses contour deformation to obtain an effective discretization. The implementation is validated through numerical simulations and precision benchmarks, documenting the step from a well-defined representation to a usable propagation tool.

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RT2/6: Multiscale Modelling and Complexity

To study large-scale responses to local perturbations, we develop methods, software, and virtual-reality tools bridging electronic structure, condensed matter, and the mesoscale. We apply these methods to bio-soft matter and address mechanisms associated with health threats like bacterial drug resistance.



Principal investigators:
Michele Cascella and
Bjørn Olav Brandsdal

In 2025, we continued with the development of multi-scale models toward computational strategies incorporating physics-based approaches with data-driven protocols and successfully applied them to systems of chemical and biochemical interest. We have advanced the use of empirical valence bond (EVB) and molecular dynamics (MD) simulations to understand and predict the temperature dependence of enzymatic reaction rates. A central theme has been to connect microscopic free-energy landscapes and protein dynamics to macroscopic observables such as activation parameters and temperature optima, with particular emphasis on cold adaptation and rational enzyme design. These projects share interests and objectives with RT5, RT7, and RT0.

Machine learning for multiscale modelling: Neural network interaction potentials.

Machine learning interatomic potentials (MLIPs) are increasingly becoming the

go-to method for simulating the time evolution of chemical systems in first-principles investigations. These potentials predict the atomic forces needed for dynamic propagation in milliseconds, bypassing the need to numerically solve complex electronic structure problems. This capability enables the study of large systems over extended timescales, such as microseconds, for supercooled water [11].

Developing MLPs presents challenges, especially concerning reliability, with primary issues being simulation crashes and inaccurate thermodynamics. In 2025, significant effort was put into establishing robust workflows for active learning of MLPs and simulations. This included developing a software tool called HyAL. HyAL automates the creation of MLPs by automating tasks such as sampling new training set geometries, training models, and performing high-throughput electronic structure calculations. Its modular

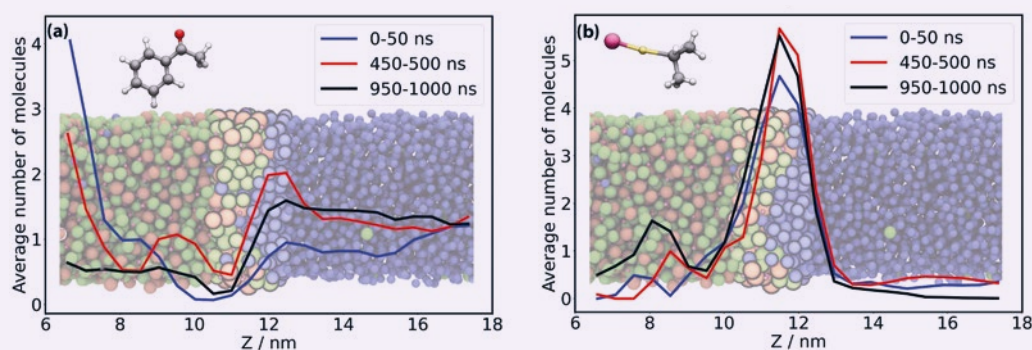


Figure 1: Localization acetophenone (panel a) and Grignard reagent (panel b) in a binary solution composed of non-miscible DES/THF liquids, monitored molecular dynamics simulations. The molecular components of DES are depicted as green/orange spheres; THF molecules are depicted as ice-blue spheres. Reproduced from ref. [4] under CC BY 4.0 license.

design enables seamless integration of new software as it emerges. This resulted in a new publication [12].

In 2026, the focus will shift from pure development to the application of hyal. Specifically, we aim to publish two application papers examining ice friction and water in metal-organic frameworks (MOFs). These efforts align with H₂O-MOF NFR, EuroHPC, and YoungCAS projects under Bore.

Multi-scale modelling of Grignard reactions in Deep Eutectic Solvents.

In the past years, research at the Hylleraas Centre dissected the molecular details of the Grignard reaction, revealing how the process of carbon-carbon bond formation follows a manifold of possible mechanisms, determined by the multiple reacting chemical species present in solution [1]. Incoming MSCA postdoc Jordan Rio, at the time PhD student in the group of

Prof. Marie-Eve Perrin (Université de Lyon) visiting the Hylleraas centre, extended the study to the characterization of the Schlenk species of organozinc [2].

Due to their high reactivity, main-group organometallic reagents like organolithium and organomagnesium must be kept inert in atmosphere at low temperature, and strictly accept dissolution in weakly-dielectric, aprotic solvents like ether. It had been very surprising when work carried in the group of Prof. Eva Hevia (University of Bern, Switzerland) showed that, by dissolving the substrate in deep eutectic solvents (DES), these processes can be carried out on the benchtop, in air at room temperature [3]. Deep eutectic solvents are composed of substances that are individually solid, but, if mixed in proper stoichiometric ratios, melt forming a glassy liquid. Surprisingly, the organometallic reagent, added to the DES from an organic solution in drops while rapidly

stirring, works in these conditions and gives better yields than in the standard setup. The use of DES as the main solvent would reduce the amounts of expensive, environmentally unfriendly organic solvents. Thus, this setup seems to offer multiple advantages, both for chemical efficiency, and for reduced environmental impact. In fact, how mixing DES with ether favours the Grignard reaction defies chemical intuition; moreover, its effectiveness is strongly dependent on the nature of the substrate, and of the organic residue. Like for the prototypic Grignard reaction, also in this case molecular simulations were crucial to determine of the molecular intricacies behind this setup. Specifically, MSCA postdoc Marco Bortoli investigated acetophenone and *i*-PrMgCl in a (1:2) choline chloride:glycerol (ChCl:Gly) DES solution using classical molecular dynamics simulations. Computer models revealed how the Grignard compound rapidly migrates toward the liquid/liquid

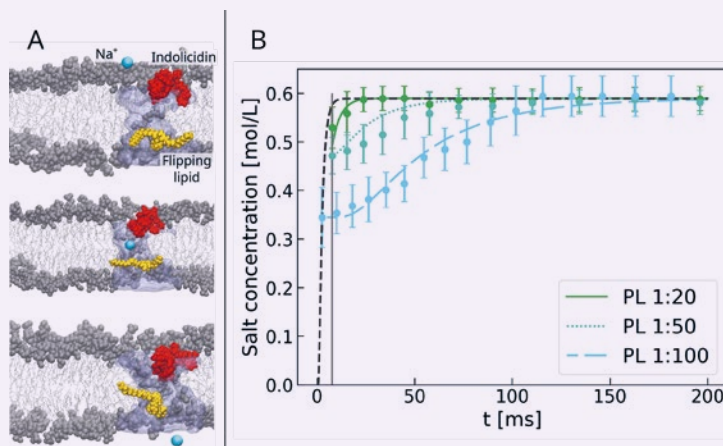


Figure 2: Transient pore formation and ionic equilibration model. (Left): MD reveal that ions permeate through a lipid bilayer, when a transient water pore associated with lipid flipping (yellow) induced by AMP (red) is formed. (Right) diffusion model (straight lines) with a statistical presence of 0.8, 0.1, and 0.05 pores per vesicle quantitatively explain the experimental ion discharge into the core of the nucleosome in the presence of peptide:lipid ratios equal to 1:20, 1:50, and 1:100. Figure from ref. [8] under CC BY 4.0 license.

interface (Figure 1). At the same time, acetophenone is surface-active in DES. The surface-enriched concentration of the substrate thus facilitates the reaction before the protic solvent can degrade the Grignard reagent. Computational data were supported by a several experimental data, which included liquid diffraction, neutron reflectometry, NMR, and interfacial tension measurements, performed in partners labs in Sweden, Switzerland, and the UK [4]. Having understood the origin of improved reactivity observed in mixed ether/DES, currently, multi-scale models employing QM/MM molecular dynamics are being performed at the Hylleraas Centre, to further explain the origin of selectivity in this process.

This project has been supervised by profs. Michele Cascella and Odile Eisenstein. Together with researcher Sigbjørn L. Bore, in 2025 they wrote a perspective article dedicated to the ability of molecular simulations, also

empowered by machine learning, to characterise main group chemistry in the years to come [5]. This work is in collaboration with RT5.

A new paradigm in the mechanism of activity of antimicrobial peptides.

Antimicrobial peptides (AMPs) are part of the innate immune system across all living organisms, including humans. Although AMPs are highly diverse and vary in composition, size, and charge density, they all display high potency and broad-scope antibacterial activity. Importantly, bacterial cells are less susceptible to develop resistance against AMPs than against conventional antibiotic drugs. In fact, AMPs have retained their efficacy despite a long evolutionary coexistence with bacteria.

In fact, the primary mode-of-action of AMPs is through a physical and nonspecific perturbation of the bacterial membranes, while conventional

antibiotics target metabolic pathways or specific bacterial enzymes that more prone to react to evolutionary pressure. However, this mechanism is also the main reason for very high AMP cytotoxicity and weak specificity. Understanding the mechanisms by which AMPs recognise, bind, and perturb cellular membranes is key to the rational development of bacteria-specific peptide sequences that could be used in alternative with conventional antibiotics. In the past, scientists have been proposing a mechanism of action involving the folding and self-assembling of AMPs in the core of the membrane, to form structured pores that would significantly increase the permeability of the membrane, destroying the homeostasis of the cell. In fact, so far, structural studies have not been able to clearly identify the presence of such self-assembled structures. On the contrary, there has been accumulation of indirect data that have challenged the necessity of the formation of,

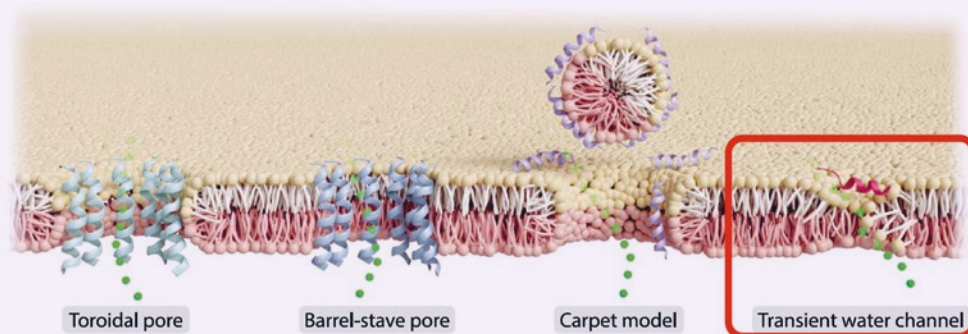


Figure 3: Different model mechanisms of action for AMPs in the literature. The red box highlights the transient water channel model proposed by Koynarev et al. [8]. Figure from ref. [9] under CC-BY-NC-ND 4.0 license.

well-folded, self-assembled units composed of a minimal critical number of AMP.

In the past years, Hylleraas affiliate Prof. Reidar Lund employed combinations of advanced small-angle X-ray and neutron scattering techniques to characterise lipid dynamics in model liposomes exposed to antimicrobial peptides [6]. His studies pointed at a direct action of AMPs associated with increased lipid mobility within and across liposomes already at AMPs concentrations too low to be compatible with any self-assembling. Moreover, SAXS data revealed that AMPs resided peripherally to the membrane and did not have strong tendency to incorporate transversally across the lipid leaflets. Past molecular dynamics simulation studies by former PhD student Manuel Carrer and researcher Henrique M. Cezar, supervised by Cascella and Prof. Il Thereza Soares characterized the molecular details of AMP-induced lipid

flipping across the bilayers [7]. That study identified that lipid flipping is induced by individual, peripherally bound AMPs, and that such events are accompanied by the formation of transient water channels. Intrigued by this finding, PhD student Vladimir Koynarev used time resolved X-ray scattering to further explore the dynamics of liposomes under osmotic shocks. He found that while, as expected, osmotic gradients produce the collapse of the liposomes, in the presence of AMPs, the structure of the liposomes remain intact. Time-resolved X-ray scattering also provided, for the first time, a measure of the kinetics of ion penetration inside the liposomes. Interestingly, he could demonstrate that equilibration of the osmotic pressure occurs in a timescale of the millisecond, varying with the concentration of the peptides.

PhD student Manuela Nader re-analysed MD data by Carrer et al [7],

identifying the spontaneous diffusion of sodium and chloride ions through the transient water channel produced by AMP-induced lipid flipping. Those data were used to determine the diffusion coefficient of the ions through the membrane, which was then employed in a Fickian diffusion model. Fitting to the experimental data, we determined that the statistical presence of a minimal fraction of water channels is sufficient to explain quantitatively the ion diffusion observed in the experiment (Figure 2). Our diffusion model validates once more a mechanism that sees AMPs induce the formation of transient water channels; on the contrary, ion diffusion through structured pores would be too fast to be compatible with the experimental kinetic data.

The work by Koynarev, Nader and others [8] has been recently reviewed in a commentary appeared in the Proceedings of the National Academy of Sciences of the USA [9], where it has

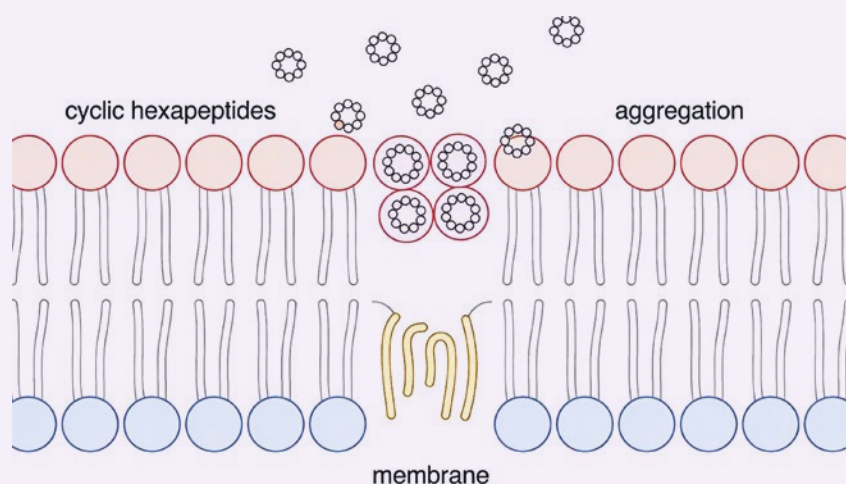


Figure 4: Peptide aggregation drives membrane disruption. Illustration: Tonje Reinholdt Haugen.

been presented as a new paradigm for the mechanism of AMPs, on par with the others historically established in the literature (Figure 3).

EVB simulations of enzyme temperature dependence

We have further developed and applied our EVB/MD workflow for computing temperature-dependent activation free energies and extracting activation enthalpies and entropies from Arrhenius-type analyses of simulated reaction free energies. This approach has been used to quantify how changes in active-site preorganization, protein flexibility and solvation contribute to the balance between enthalpic and entropic effects along the reaction coordinate.

A major focus has been cold-adapted versus mesophilic enzymes, where we use EVB simulations at multiple temperatures to probe how psychrophilic catalysts achieve high turnover at low

temperature while often sacrificing thermal stability. Building on earlier work on computational design of cold-adapted enzymes, we are exploring design principles that decouple catalytic efficiency from thermal robustness, aiming at enzymes with tailored temperature profiles for biotechnological applications (see also Research Highlight in the present report).

Chorismate mutase has served as a benchmark system for validating our protocol for accurate computation of thermodynamic activation parameters from EVB simulations and for dissecting the relative roles of enthalpy and entropy in catalysis [14]. In parallel, we have continued with EVB/MD studies of the glycosidase Mall and of proline racemase, extending the methodology to mechanistically distinct enzyme classes and to reactions where temperature effects on both catalysis and conformational equilibria are expected

to be pronounced. Of particular interests, is the observed non-linear Arrhenius behaviour of Mall, which apparently seems to be caused by key substrate-enzyme interactions disappearing at elevated temperatures.

Antimicrobial peptides and membrane simulations

In addition to enzyme catalysis, we have an ongoing activity on atomistic and coarse-grained MD simulations of antimicrobial peptides interacting with realistic membrane models. This work is motivated by the urgent need for new antibacterial strategies that bypass classical small-molecule resistance mechanisms and exploit membrane disruption as an alternative mode of action. In particular, we are studying cyclic hexapeptides designed as minimalist, drug-like antimicrobial scaffolds, which allow systematic variation of sequence and physico-chemical properties within a compact architecture.

// This work provides molecular-level design-rules that can guide the development of next-generation antibiotics //

The simulations probe peptide binding, insertion, and aggregation at lipid bilayer surfaces, followed by possible transitions to transmembrane states and pore-like defects. We find that peptide aggregation at the membrane interface is a key driver of membrane perturbation and correlates strongly with experimentally observed antimicrobial activity (Figure 4), suggesting that the ability to form higher-order assemblies is at least as important as single-molecule binding affinity [15]. By linking sequence, aggregation propensity and membrane response, this work provides molecular-level design rules that can guide the development of next-generation cyclic peptide antibiotics with improved potency and selectivity.

Other published works

In 2025, studies on chromatin [10] and self-assembly of non-conventional surfactants [11] appeared in the literature. These works were presented in past annual reports, thus they are not discussed here in detail.

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RT3/4: Matter-Field Interactions

The goal of RT3/4 is to develop high-accuracy quantum dynamics methods to simulate ultrafast laser-driven processes in molecules and periodic magnetic systems, and theory and methods for strong-field chemistry and simulations of spectra from magnetic white dwarf stars.



Principal investigators:
Michal Repisky and
Erik Tellgren

Relativistic Methods and Phenomena

In 2025, Torsha Moitra, Lukas Konecny, Marius Kadek, and Michal Repisky, in collaboration with Ofer Neufeld (Technion) and Angel Rubio (MPI Hamburg), demonstrated a new route to ultrafast electronic chirality in molecules [1]. The team showed that a single monochromatic circularly polarized laser pulse can induce long-lived chiral electronic currents in an oriented achiral molecule, without any nuclear motion (Figure 1). Using real-time TDDFT simulations, they linked these currents to induced magnetic dipole moments, directly accessible via attosecond time-resolved electronic circular dichroism (TR-ECD). The resulting electronic wavepacket oscillates rapidly in handedness at harmonics of the driving laser frequency, with chiral currents persisting after the pulse. This work establishes a molecular-current analogue of high harmonic generation and enables attosecond control of

transient chirality, with potential impact on spintronics, ultrafast magnetism, and reaction dynamics.

In 2025, Lukas Konecny, in collaboration with the group of Angel Rubio (MPI Hamburg), published a landmark study in Physical Review X documenting the development and implementation of four-component relativistic quantum electrodynamical density functional theory (QEDFT). This work represents an important step toward accurately describing how molecules interact with quantized light fields, such as those found in optical cavities [2]. Building on this foundation, the study demonstrated that QEDFT can describe molecular spectra under strong light-matter coupling, including systems where relativistic effects are essential. To make such simulations feasible for large and complex systems, an efficient exact two-component (X2C) QEDFT approach was introduced shortly thereafter [3], achieving high accuracy at significantly

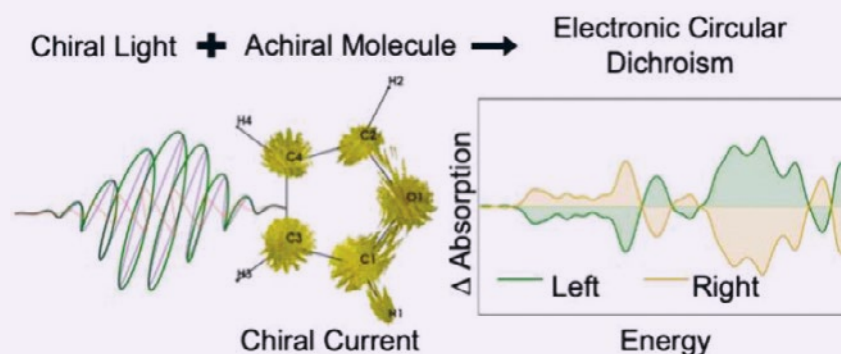


Figure 1: A single circularly polarized laser pulse can induce long-lived chiral electronic structure in an achiral molecule. Reproduced from ref. [1] under CC-BY 4.0 license.

reduced computational cost. Together, these advances enable simulations that were previously out of reach, such as two-dimensional spectroscopies and collective light–matter interactions in extended molecular systems. Applications to molecules in optical cavities revealed the formation of polaritonic states and showed that collective coupling can locally modify chemical bonding, highlighting the potential of relativistic QEDFT for cavity chemistry and polaritonic materials (Figure 2).

In 2025, a new publication showcased recent developments in the ReSpect program, an open-access DFT software platform designed to model spectroscopic processes while treating relativistic effects in a fully variational manner [4]. Recent works have focused on making these simulations faster and more practical, without sacrificing accuracy. At the theoretical level, the developments centered on exact two-component (X2C) model Hamiltoni-

ans, which provide an efficient yet highly accurate way to capture relativistic effects while keeping calculations manageable. These advances enable the study of complex, time-dependent phenomena—such as laser-driven dynamics and cavity QEDFT—that were previously computationally demanding. By combining advanced capabilities with open access, ReSpect continues to support researchers across a wide range of disciplines, helping to broaden the use of relativistic approaches and enabling new discoveries in fields where these effects are essential.

Advances in Response Theory

In 2025, Magnus Ringholm, in collaboration with Patrick Norman (KTH Stockholm), introduced a new theoretical framework for describing response properties of non-stationary electronic states within a self-consistent field approach [5]. The work extends conventional response theory by incorporating relaxation effects directly

into the Liouville equation of motion. The proposed density-based formulation builds on concepts familiar from established wavefunction-based response theories, while offering a more general and flexible perspective applicable to approximate electronic states. The study clarifies how traditional wavefunction-based approaches relate to this broader framework and highlights situations where the new formulation provides clear advantages. At the same time, key challenges and current limitations are identified, helping to define priorities for future methodological development. Together, these advances lay the groundwork for response theories capable of addressing a wider range of time-dependent and non-equilibrium electronic phenomena.

In 2025, Bin Gao and Magnus Ringholm developed and published SymResponse, a unified and extensible framework designed to simplify and

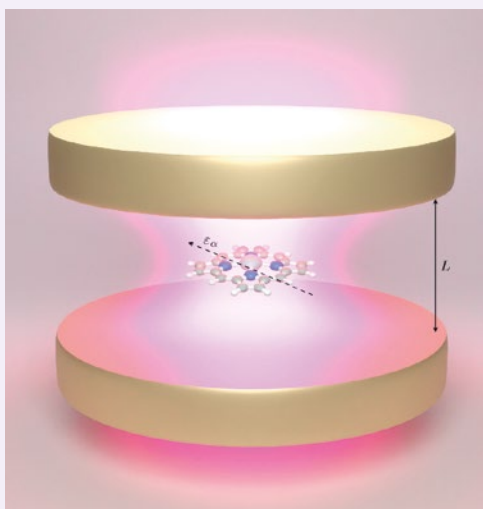


Figure 2: Schematic representation of a Fabry-Pérot cavity with a Hg-porphyrin complex embedded between the cavity mirrors. The relativistic QEDFT framework enabling first-principles simulations of this system was developed by Lukas Konecny and collaborators, as discussed in Ref. [2]. Reproduced from ref. [2] under CC-BY 4.0 license.

accelerate the implementation of response theory across a wide range of electronic-structure methods [6]. The framework provides a flexible foundation for formulating and evaluating response functions in a consistent and transparent manner. SymResponse operates at a symbolic level, allowing response functions to be represented as symbolic expressions that can later be evaluated numerically using user-defined routines. By building on established symbolic libraries, the framework separates formal theory development from numerical implementation, significantly lowering the barrier to extending response theory to new models. As a proof of concept, SymResponse has been applied to response theory at the Hartree-Fock, density functional theory, and coupled-cluster levels. The framework also supports the use of established elimination strategies to reduce computational cost. Overall, SymResponse provides a versatile and scalable platform for developing,

testing, and extending response-theoretical methods.

In 2025, Magnus Ringholm and Kenneth Ruud, in collaboration with Jógvan Magnus Haugaard Olsen and colleagues at the Technical University of Denmark, presented a comprehensive workflow for simulating harmonic IR and Raman spectra of molecules in solution using a polarizable-embedding quantum-mechanics (PE-QM) approach [7]. The proposed multiscale strategy partitions the system into a quantum-mechanical core region and a surrounding environment described by a fragment-based polarizable embedding model. The workflow provides practical guidance covering structure generation, property calculations, and postprocessing, offering a clear roadmap for reliable simulations of solute-solvent systems. Benchmark studies assessed the accuracy of key approximations, clarifying both the strengths and limitations of the approach. Applications

to acetone in three different solvents, with direct comparison to experimental IR and Raman spectra, demonstrate the reliability of the PE-QM workflow for modeling solute-solvent systems (Figure 3).

Strong magnetic fields and magnetic properties

Hylleraas affiliate Stella Stopkowicz with co-workers have reported three studies related to strong magnetic fields. In the first study, the effect of basis set errors in strong magnetic field calculations was investigated [8]. Specifically, they considered molecular orbitals expanded in finitely many Gaussian-type orbitals with London gauge factors. They used the London program package and CFour program package to get such finite-basis set results at the Hartree-Fock level of theory. As case studies, they considered various electronic states of the helium atom and the helium dimer as well as the methyldine radical (CH) and

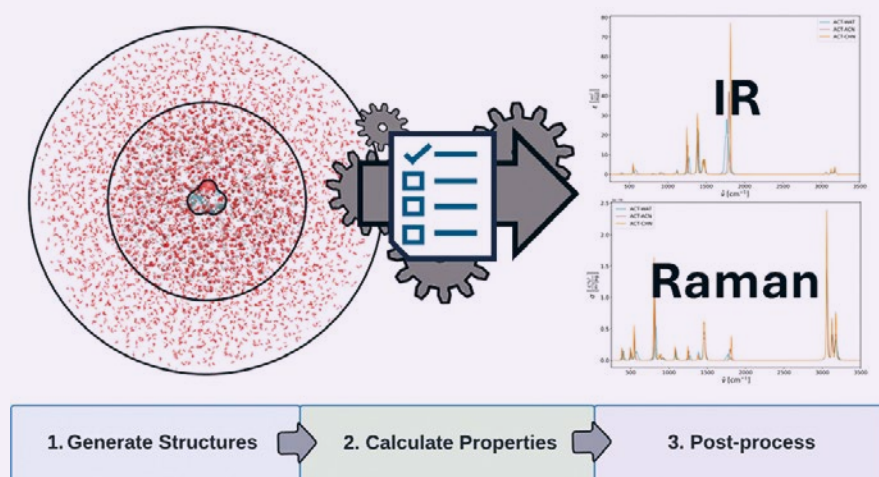


Figure 3: Outline of the PE-QM workflow for modeling solute-solvent systems and simulating their IR and Raman spectra. Reproduced from ref. [7] under CC-BY 4.0 license.

the water molecule. They then compared these finite-basis results to reference results obtained using multiresolution approaches, implemented in the ZNEMO and MADNESS program packages. This comparison showed that basis set errors increase rapidly with magnetic field strength in the range 0.5 to 1.0 atomic units (or about 120 to 235 kT). Beyond 1 atomic unit, the authors do not recommend standard basis sets.

In the second study, the implementation of a high-quality method for excited states of molecules in strong magnetic fields was reported [9]. The equation-of-motion coupled-cluster formalism was adapted at the EOM-CCSD(T) level to requirements of strong magnetic fields and calculations of spin-flip, ionization, and electron-affinity energies. The authors then used their computer code implementation to study atoms and molecules of interest in astrophysics and the spectra of magnetic

white dwarf stars. Moreover, the application to the CH radical indicated that the spin-flip, ionization, and electron affinity adaptations of the EOM-CC method can provide more physical approximate results, less influenced by spurious symmetry breaking.

The third study considered the unitary coupled cluster method for molecules in strong magnetic fields [10]. The motivation is that standard coupled cluster theory may result in approximate energies that are complex numbers, even though the correct energy is a manifestly real valued. In the absence of a magnetic field, this difficulty can often be circumvented by forcing all intermediate quantities to real values. However, in the presence of a magnetic field, a complex valued wave function is necessary for even qualitatively correct results. Unitary coupled cluster theory (UCC) does not suffer from this difficulty. Stopkowicz and co-workers compared

two versions, UCC2 and UCC3, to standard coupled cluster calculations. For the water molecule and boric acid $B(OH)_3$, the standard calculations gave imaginary parts of the energy on the order of 10 microhartree and 500 microhartree, respectively. By contrast, the UCC methods provide energies without the unphysical imaginary part.

At the Oslo node, Jha and Tellgren have started a research project aimed at unifying a popular practical density functional approach (meta-GGA functionals) with the proper theoretical setting for calculations of magnetic properties. Meta-GGA functionals utilize the kinetic energy density in approximate models. An important intermediate quantity in such models has also found use in a widespread chemical visualization tool in the form of the Electron Localization Function. For accurate magnetic properties, density functional approaches should include a dependence on the paramagnetic current

// Extreme magnetic environments demand new theoretical tools. Our work bridges fundamental method development with applications ranging from molecular spectroscopy to magnetic stars //

density, though models and software implementations that take this into account are not yet available. However, a framework for unifying the two approaches was established in previous work at the Hylleraas center—the key ingredient turns out to be a generalization of the kinetic energy density that enters in meta-GGA functionals to a kinetic energy tensor. Within this framework, Jha and Tellgren have as a first step started developing generalizations of the Electron Localization Function, with the longer-term goal to make improved exchange functionals.

Personnel and Funding

Research in RT3/4 in 2025 has been supported by the RCN (FRIPRO) project *EPR and paramagnetic NMR of solids from relativistic two- and four-component density-functional theory* led by Kenneth Ruud and Michal Repisky.

In the Oslo node, currently E. Tellgren (researcher) is primarily active in RT3/4 and to support the work, Gautam Jha was hired for a two-year position starting in August 2025. Hylleraas members Pedersen (professor) and Laestadius (Prof. II adjunct; assoc. prof. at OsloMet) contribute partially to RT3/4.

Tromsø RT3/4 research team in 2025 consists of Kenneth Ruud (professor), Michal Repisky (researcher), Magnus Ringholm (researcher), Lukas Konecny (postdoc), Marc Joosten (PhD), Vanda

Le (PhD), and Rasmus Vikhamar-Sandberg (PhD). From October, Josefine Hvarregaard Andersen joined the Hylleraas Centre (UiT node) as an MSCA postdoctoral fellow, supervised by Magnus Ringholm. In the project HOOD – Higher-Order Geometric Derivatives, she will develop new methods for simulating advanced vibrational spectroscopies within multi-level coupled-cluster theory.

In addition, Hylleraas adjunct Assoc. Prof. Stella Stopkowicz, Saarland University, have contributed to research in RT3/4.

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RT5: Chemical Transformations

In RT5, we use computational methods to elucidate reaction mechanisms and to design more sustainable processes in close collaboration with experimental groups. Our approach integrates computation-guided identification and characterization of reaction intermediates with comprehensive reactivity studies, including microkinetic modeling for highly complex reaction networks.



Principal investigators:
Ainara Nova and
Abril Castro

Reactivity with bi-functional catalysts

Organometallic complexes combining an acid site, usually a transition metal, with a basic site on a ligand, and reacting by metal-ligand cooperative mechanisms are called bi-functional catalysts (Figure 1). One of the most popular bi-functional catalysts for CO₂ hydrogenation to methanol is the Ru-MACHO. This reaction requires an amine as a co-catalyst, enabling CO₂ conversion at low concentrations. The understanding of this reaction and the design of more sustainable catalysts for it are the main focus of Mohamed Eid Safy's PhD thesis, under the supervision of Nova. In his first work, he combined conformational sampling (CREST/GFN2-xTB) with DFT methods to explore the main reaction pathways for CO₂ hydrogenation to formic acid and for formamide hydrogenation to formaldehyde, which is then hydrogenated to yield methanol.[1] The mechanisms with the lowest DFT energies were refined

with DLPNO-CCSD(T) to construct a microkinetic model, which yielded a methanol turnover number (TON = 4.4) very close to the experimental value (3.3) under representative conditions. The experimental work was performed in LIKAT, Rostock (Germany), by PD Raquel Jimenez-Rama in collaboration with Prof. Matthias Beller. In addition, a sensitivity analysis of the MKM model was used to determine the transition state and catalyst resting state having the strongest influence on the methanol TONs, which were the DMF hydrogenation TS and the Ru-formate complex, respectively. This information is highly relevant to the following catalyst design work.

Ru-MACHO also catalyses the methanol-to-syngas reaction. Since Ru-CO species were detected during the CO₂ hydrogenation to methanol, Dr. Jiali Liu from Evonik, who visited Nova's group in 2024 and 2025, studied this reaction to determine the mechanism for the CO

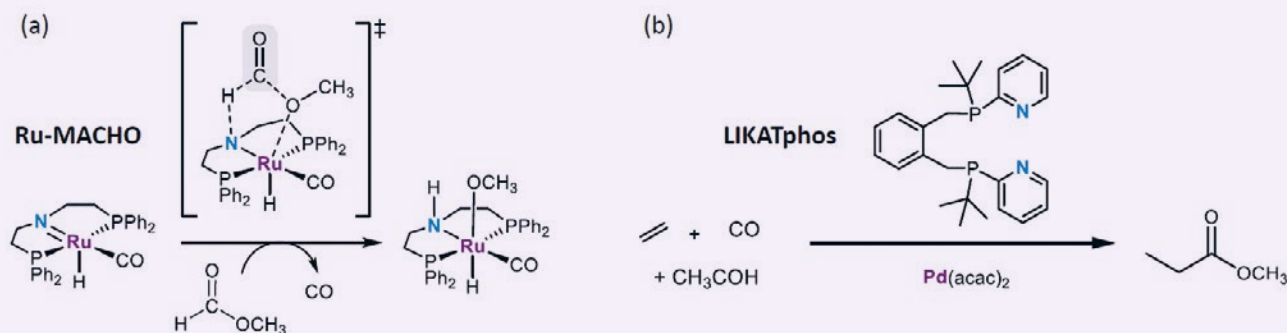


Figure 1: Two reactions involving bifunctional catalysts with the acid and basic sites in purple and blue, respectively: a) the decarbonylation of methylformate and b) the methoxycarbonylation of ethylene. Illustration: Ainara Nova.

formation.[2] In this study, multiple plausible pathways were computed in both methanol and toluene using DFT methods and the SMD solvation model. The complete catalytic cycles indicate that CO formation proceeds primarily via methyl formate, generated from formaldehyde and methanol. CO release occurs through an outer-sphere mechanism, in which CO is directly liberated from the methyl formate intermediate to form a Ru-OCH₃ species (Figure 1a). To connect theory to experiment, a microkinetic model coupled to a batch autoclave liquid-vapour description was used. The microkinetic model successfully reproduced the experimentally observed temporal evolution of CO and H₂ turnover numbers. Its analysis suggests that the reaction is limited by Ru-CO formation and by reaction thermodynamics.

DFT calculations of thermodynamic parameters, such as hydricity, and spectroscopic properties of manganese

complexes similar to Ru-MACHO were the focus of Øystein Senstad Alve's master's thesis. Senstad passed his examination in June 2025, supervised by Castro and co-supervised by Nova.

Other bifunctional catalysts studied by Liu, in collaboration with Nova, Safy, and Jimenez-Rama, are the Pd complexes formed by combining the racemic, meso, and epimerized LIKATphos ligand with a Pd salt (Figure 1b).[3] These systems catalyse the methoxycarbonylation of ethylene, with activity varying with the ligand stereochemistry. The function of the pyridine group is to facilitate methanol deprotonation during the addition of the methoxide group to the acyl substituent. Experimentally, the racemic LIKATphos exhibited the highest catalytic activity, the meso form the lowest, and the epimerized ligand an intermediate performance. The computational study of the reaction mechanisms using DFT methods showed a correlation between

catalyst activity and the energy difference between the Pd-CO and Pd-hydride intermediates, which was used to rationalise the experimental results.

There is an interest in transferring the activity of bi-functional catalysts to single-atom heterogeneous systems. The feasibility of this idea using N-doped graphene has been explored by Aurore E. F. Denjean, who defended her PhD in September 2025. Her thesis, entitled "Structure, Reactivity, and Dynamics of Transition Metals for Catalysis Applications: A Computational Journey from Molecular to Single-Atom Systems", was supervised by Balcells and co-supervised by Nova.

C-H activation reactions

The selective oxidation of C-H bonds by bio-inspired copper (Cu) complexes incorporated into metal-organic frameworks (MOFs) is the primary objective of the CUBE project, in which

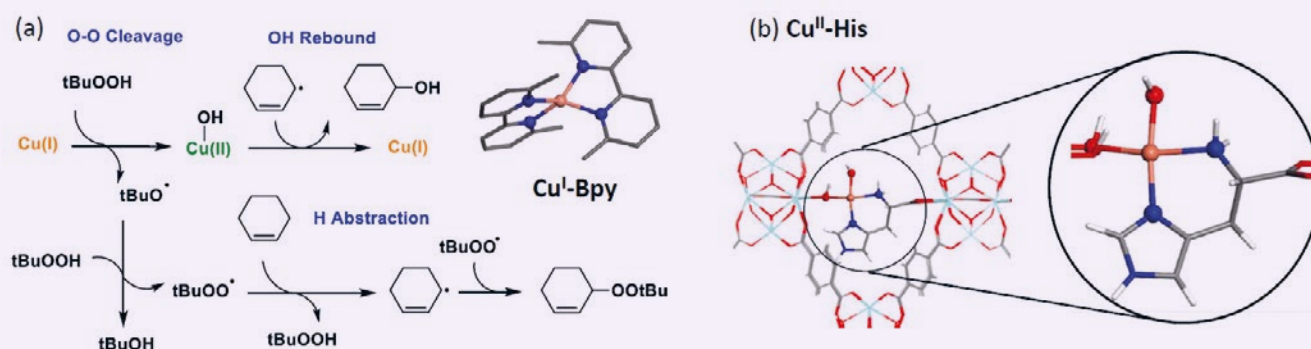


Figure 2: a) Reaction mechanism for the C-H oxidation of cyclohexene by Cu^I-Bpy. b) Structure for the Cu^{II}-His site found in the Cu-UiO-66 MOF. Illustration: Ning Cao and Ainara Nova.

the PhD student Ning Cao and the PDs Lucía Morán-González and Nishamol Kuriakose contributed in 2025. Their work involved applying computational methods to elucidate reaction mechanisms, support the experimental characterisation of Cu-sites into MOFs, and inform the design of more active and selective systems. Some of the work reported in 2025 includes the mechanistic study of the oxidation of cyclohexene with tert-butyl hydroperoxide (tBuOOH) catalyzed by **Cu^I-Bpy** (Figure 2a).^[4] By using DFT methods, Cao found that the tBuOO[•] radical serves as the primary active species for the C-H activation reaction. Furthermore, steric hindrance from the Cu ligands causes the tBuO[•] radical to diffuse rather than undergo hydrogen atom abstraction to form a Cu(II)-O[•] species, explaining the observed products. This information provides critical insights into ligand-driven selectivity important in catalyst design. Ongoing efforts by Cao and Morán-González are rationalizing the

formation of products over time in the presence and absence of O₂, using microkinetic modelling.

In addition to studying reactivity using molecular systems, Cao has used periodic models to assist in the characterization and reactivity of Cu sites in a histidine-modified Cu-UiO-66 MOF.^[5] Experimentally, this system was characterised by in situ X-ray Absorption Spectroscopy (XAS) under redox conditions, using H₂ as the reducing agent and O₂ as the oxidising agent at 150°C. Using MCR-ALS, a method for decomposing spectra from mixtures into those for pure species, four distinct Cu species were observed in the MOF during the employed redox protocol. With the help of DFT optimized structures, XAS simulations successfully reproduced the experimental spectra, revealing variations in Cu coordination environments involving penta- and tetra-coordination species. Additionally, the geometry optimization and energy

calculations for reaction intermediates during the redox process provided insight into reactivity, such as the lack of reaction observed on the Cu sites anchored to the histidine ligand (**Cu^{II}-His**, Figure 2b), in contrast to those on the Zr nodes.

An alternative strategy to mimic enzymes in Cu(I) MOFs is to incorporate guest molecules to modulate the active Cu microenvironment without complex organic synthesis. This strategy has been used by the catalysis group using phenol and propionamide as guest molecules.^[6] Cao's contribution to this work was to determine the preferred coordination mode of propionamide to Cu by evaluating different structures and reaction thermodynamics using periodic models with DFT methods. Our calculations together with spectroscopic characterization using XAS showed that propionamide coordinates to the cuprous center as an N-coordinated iminol, one of the tautomers of

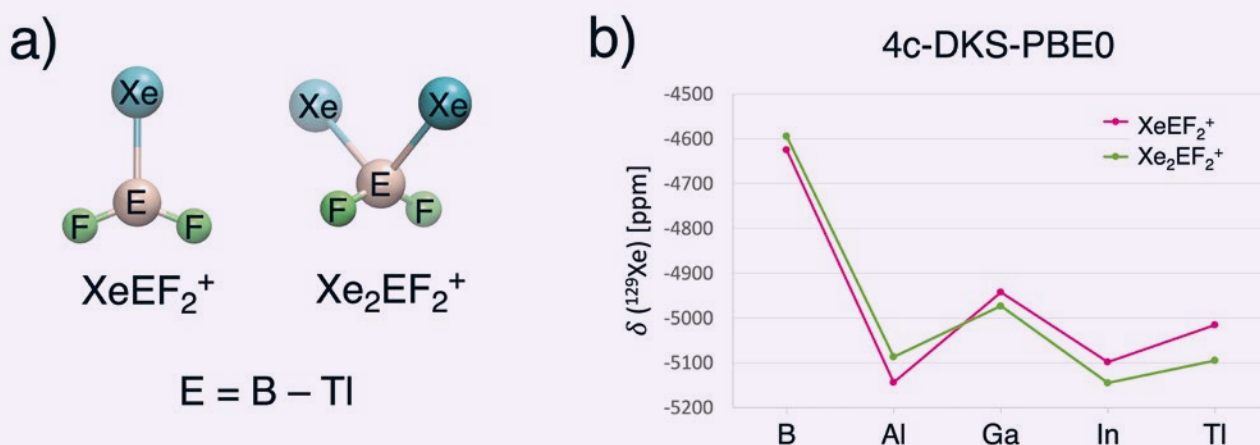


Figure 3: a) Minimum-energy structures of the XeEF_2^+ and Xe_2EF_2^+ species ($\text{E} = \text{B-Tl}$), and b) Predicted ^{129}Xe NMR chemical shifts using the 4c-DKS-PBE0 method. Illustration: Abril Castro.

propionamide, while phenol remains unabsorbed. Although propionamide successfully modulated the center initially, its impact on long-term performance was limited as the molecule was displaced under reaction conditions.

Cao defended his thesis entitled “Computational Studies of Biomimetic Cu Metal Organic Systems” in May, 2025. The same month, Inga Lena Schmidtke, also defended her PhD thesis, entitled “Investigations into transition metal complex reactivity – A computational perspective on C-H and C=C bond activation reactions” supervised by Nova. One of the manuscripts included in her thesis, involving the C-H bond activation and coupling of methane and toluene, was submitted for publication in 2025.

Covalent bonding and extreme shielding in xenon-icosagen fluoride cations

Under the supervision of Castro and in

collaboration with distinguished universities in Mexico, our group explored the chemistry of noble-gas compounds by predicting stable xenon compounds that form covalent bonds with a range of icosagens.

The computational protocol used a genetic algorithm to explore the potential-energy surfaces of the XeEF_2^+ and Xe_2EF_2^+ ($\text{E} = \text{B-Tl}$) cations, resulting in global-minimum structures featuring Xe-E bonds (Figure 3a). High-level ab initio calculations indicated that these species are thermodynamically viable at room and higher temperatures, with all considered dissociation pathways being endergonic. Detailed bonding analyses reveal strong covalent Xe-icosagen interactions for B, Al, and Ga, while In and Tl form weaker bonding character that suggests more ionic-like interactions.

PhD candidate Alberto Guerrero calculated the ^{129}Xe NMR chemical

shifts in both XeEF_2^+ and Xe_2EF_2^+ species to provide an additional probe for the Xe-icosagen interactions. Employing state-of-the-art relativistic methods, the predicted spectra show extreme shielding of the Xe nucleus, consistent with the strong electron-withdrawing character of the EF_2^+ fragments (Figure 3b).

Published in *PCCP* journal, this study expands the known chemistry of Xe-icosagen compounds beyond the previously reported XeBF_2^+ , identifying XeAlF_2^+ and XeGaF_2^+ as promising targets for experimental synthesis and characterization.[7]

Personnel and Funding

In 2025, Drs. Lucía Morán-González, Nishamol Kuriakose and Mauricio Portioli Franco joined RT5. Morán-González started as a researcher in the CUBE project and continued as MSCA Postdoctoral fellow, after her project, BIFUCCO2, was funded by the EU.

// Guerrero's poster "Analyzing the electronic structure of Pt(II) complexes via ^{195}Pt NMR" was awarded a Best Poster prize at WATOC 2025 //

Nishamol Kuriakose started as a researcher in the CUBE project in September, and Mauricio Portioli started with a postdoctoral position funded by the MSCA EU Co-fund DStrain project.

Dr. Inga Lena Schmidtke left RT5 after finalizing her PhD to join RT1 as a researcher in Tromsø working with Frediani, while Dr. Ning Cao continued in RT5 as a researcher in CUBE. Dr. Aurore Denjean finalised in RT5 after she defended her PhD. Mohamed Eid Safy moved from a MSCA COMPSCI PhD student to a researcher contract, thanks to a UiO: energy seed funding grant to initiate a collaboration with Assoc. Prof. Martin Nielsen, from the Technical University of Denmark.

RT5 received three visitors in 2025: Dr. Jiali Liu from Evonik (Germany) for a three-month visit, Dr. Mauricio Portioli Franco from the University of Campinas (Brazil) for an 8 month-visit, and MSc student Eri Karoline from the University of Tromsø for a one-week visit.

Most of our MSc and PhD students, and PDs presented posters at the WATOC 2025 conference, where Guerrero's poster entitled "Analyzing the electronic structure of Pt(II) complexes via ^{195}Pt NMR" was awarded a prize sponsored by the Journal of Computational Chemistry. His poster stood out from more than 800 posters presented, highlighting the high quality and visibility

of RT5 work in computational spectroscopy and transition-metal chemistry. In addition, Ning Cao gave an oral presentation at the EuropaCat conference in Trondheim, and Mohamed E.A. Safy was invited to present his work at a HySchool Webinar and contributed with an oral presentation at the NKS Quantum/Computational Chemistry Annual Meeting in Tromsø.

Lucía Morán-González participated as a teacher in two workshops: the Summer School in Machine Learning and Artificial Intelligence in Synthetic Chemistry at the University of Helsinki (Finland); and the Cheminformatics, Automation and Machine Learning in Chemistry (CAMLC25): from fundamental concepts to emerging techniques, in Zaragoza (Spain).

Nova was invited to five conferences and workshops: the conference "Catalytic Conversations: Integrating Theory and Experiments in Homogeneous Catalysis" that took place in Barcelona (Spain) to celebrate the 70th anniversary of Prof. Agustí Lledós; the XXVI European Conference on Organometallic Chemistry (EuCOMC 2025) in Bern (Switzerland), the workshop "Boosting Computational Catalysis with Machine Learning: Current Challenges, Limitations, and Opportunities, in Zurich (Switzerland), the 7th Quantum (Bio-) Inorganic Chemistry Conference (QBIC VII), in Berlin (Germany) and the "2a Reunió de Química Teòrica i Computac-

ional" organized by the Catalan Chemical Society in Barcelona (Spain). In addition, she participated in two outreach activities organised by the Department of Chemistry at the University of Oslo: "Live after studies" and a student gathering on Artificial Intelligence (AI).

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RT7: Machine Learning and Mathematical Methods

RT7 focuses on the development of machine learning (ML) and mathematical methods (MM) and their application to a broad range of problems in chemistry, physics, biology, and computer science. Regarding ML, the main activities include the computation of large datasets, the development of novel graph representations, generative methods, active learning approaches, and machine learned interatomic potentials. Regarding MM, the main activities include analysis of electronic-structure methods and development of novel time-integration schemes. A long-term goal is to integrate the ML and MM lines of research, focusing on topics like the development of unconventional ML methodologies for chemistry.



Principal investigators:
David Balcells and
Simen Kvaal

Datasets

In 2025, we extended the tmQM dataset series by adding tmQMg* to it. tmQMg* provides electron excitation data (wavelengths, intensities, and solvatochromism) at the TD-DFT wB97xd def2SVP level of theory for 74k metal complexes [1] extracted from the Cambridge Structural Database (CSD). This work was part of the NFR CatLE-GOS FRIPRO project led by David Balcells, which finished this year, and it was done in collaboration with Hannes Kneiding, who contributed with the computation and curation of the data, now already available on the Internet with open access. Besides the article published in the ACS JCIM journal, Hannes presented the work in a poster at the WATOC 2025 conference in Oslo.

Other incipient work on metal complex datasets for machine learning that started in 2025 under the supervision of David Balcells includes: 1) the bimetallic frustrated Lewis pairs dataset designed

by Miguel Ángel Gaona Fernández (postdoc in the DSTrain COFUND project), 2) the tmQM-RDF knowledge graph dataset developed by Luca Cibinel (PhD student in collaboration with the INTEGRATE Centre of Excellence at the UiO Department of Mathematics), and 3) the kinetics, X-Ray, and high throughput experimental data collected by PhD students Michael Augello, Flavie Le Rai, and Lucas Bitencourt Theodoroviez (EU DN DEMO project, in collaboration with partner institutions in Slovenia, Italy, and France).

ML representations for MOFs

Continuing the work done in 2024 in autocorrelation functions for graph-to-vector (g2vec) transformations, this year we extended the in-house atom-atom bond-bond bond-atom (AABBA) representation [2] to metal organic frameworks (MOFs) [3]. In contrast with other g2vec approaches for machine learning, AABBA encodes both atomic

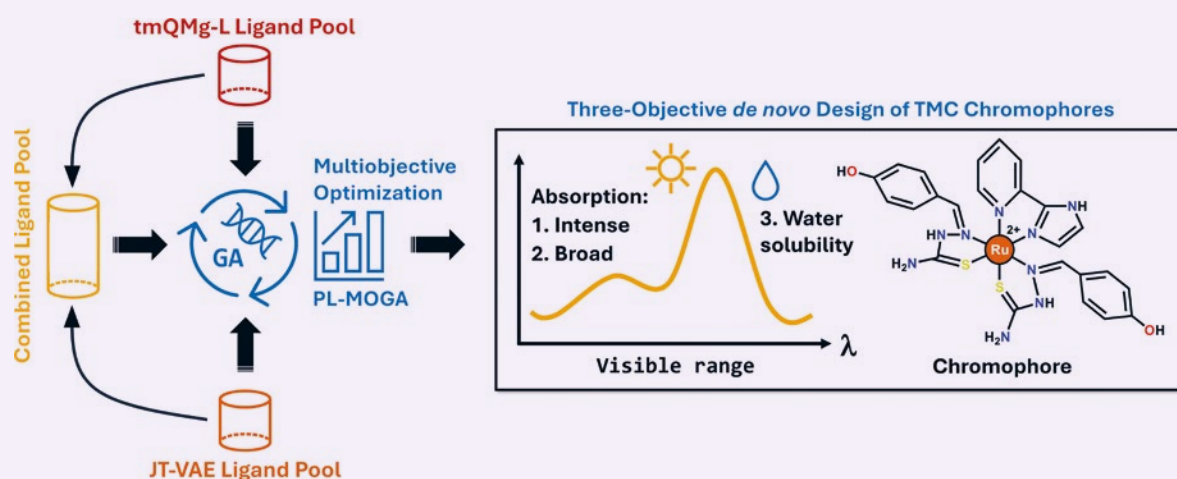


Figure 1: Evolution of ruthenium chromophores with known and AI-made ligands. Illustration: David Balcells.

and bond information from the nodes and edges that form molecular graphs. In the extended version of the code, the algorithm now supports the modular nature of MOFs, which is based on combinations of metal oxides with organic linkers. The work was done by Nishamol Kuriakose (postdoc in the EU HYSTRAM project), in collaboration with Lucía Morán-González (MSCA postdoc), Jørn Erik Betten (former MSc student, now PhD candidate at SIMULA), and Hannes Kneiding, under the supervision of David Balcells. Besides the preprint published in *ChemRxiv*, the work is currently under review, and it was presented in a talk by Nishamol at the ACS 2025 Spring Meeting in San Diego, USA.

Inverse design of metal complexes

After exploring high throughput virtual screening approaches to palladium-catalyzed cross-coupling reactions with DFT [4], we turned our attention to generative AI with deep learning

methods. In particular, we continued the work started in 2024 on the junction tree variational autoencoder (JT-VAE) for metal complexes, which was peer-reviewed and published in *JACS Au* this year [5], where it was highlighted among the most-read articles of the journal. For this model, we developed a string encoding of different metal-ligand bond types, including denticity and hapticity through metallacycle fragments. The work was started by Magnus Strandgaard (2024 visitor from Jensen's group in Copenhagen) and continued in collaboration with Hylleraas members Trond Linjordet and Arron Burnage (both postdocs in the NFR CatLEGOS FRIPRO project), together with Hannes Kneiding, who also explored its use with SMILES representations supporting metal complexes [6]. Future work on generative AI shall focus on diffusion models, in collaboration with Trond Linjordet (currently in a postdoctoral position with Ruben Staub at ICRD in Hokkaido University, Japan), and catalysis, for

which we recently wrote and published a perspective [7], together with Ainara Nova, PI in RT5.

Evolutionary deep learning

Following a perspective published in 2024 [8], we have been exploring the potential synergies between evolutionary and deep learning methods. In particular, we have extended the work initiated by Alejandra Pita-Milleiro (visitor from IIQ Sevilla, Spain) on chromophores with potential use in photovoltaic technologies. The central concept of this project is to use the PL-MOGA genetic algorithm developed by Hannes [9] for the three-objective optimization of ruthenium chromophores that maximize 1) light absorption intensity in the visible, 2) light absorption broadness in the visible, and 3) solubility in water. In this framework, PL-MOGA uses a pool of genes originating from either the CSD or the JT-VAE model, the latter thus being "AI-made" (Figure 1). This year we published a preprint with



Figure 2: David Balcells participating in scientific discussions in the CECAM “ML Advances for Molecular and Materials Property Prediction” workshop in the University of Notre Dame (South Bend, USA). Photo: Yamil Colon.

the computational results [10], while starting a collaboration with the experimental group of Alejandra to attempt the synthesis and characterization of the chromophores evolved. This work was presented in several invited talks in international conferences (Figure 2), including a Telluride Science Center Workshop (USA), and the CECAM Workshops held in the Max Planck Institute for the Physics of Complex Systems (Dresden, Germany) and the University of Notre Dame (South Bend, USA), and also in invited lectures in research institutions abroad, including the University of Barcelona (Spain) and the City University of Hong Kong (China).

Coupled-cluster theory

The QOMBINE project is an RCN Fellesløft IV large-scale interdisciplinary researcher project funded jointly by RCN and the Faculty of Mathematics and Natural Sciences. The project consortium comprises physicists, chemists, and mathematicians, is led by

Prof. Nadia S. Larsen (Department of Mathematics), and has a total budget of 25 MNOK, with project time frame 2022—2027. QOMBINE is interdisciplinary and seeks to develop new mathematical methods for central problems of quantum technology. Among the topics to be developed is a new mathematical foundation for coupled-cluster theory, the most popular quantum-chemical computational method besides DFT. Simen Kvaal, Sergiy Neshveyev (Mathematics), and Nadia S. Larsen, together with PhD students Håkon R. Fredheim (Hylleraas) and Snorre Bergan (department of Mathematics), use operator algebra theory and differential geometric notions to unify theory for electrons, protons, and other elementary particles, possibly also more exotic particle-like phenomena such as anyons and Majorana fermions. The latter are important building blocks in the development of putative topological quantum computers. On the other hand, a version

of coupled-cluster theory called unitary coupled-cluster theory is classically intractable, but very fast on a quantum computer. Thus, the chemistry arm of QOMBINE aims not only at a better understanding of coupled-cluster calculations to be run on quantum computers, but also better understanding of how to build future quantum technologies. The QOMBINE project introduced a new, exciting research direction and interdisciplinary collaboration for the Hylleraas centre, involving several departments, including the industry sector. As of December 2025, the group is nearing the completion of a major mathematical study of error estimation in coupled-cluster theory, and Håkon R. Fredheim has submitted his PhD thesis, to be defended in January 2026.

Density-functional theory

A central research topic at the Hylleraas Centre is the mathematical development of density-functional

Rothe's Method: Adaptive Gaussian Optimization for Time-Dependent Orbitals

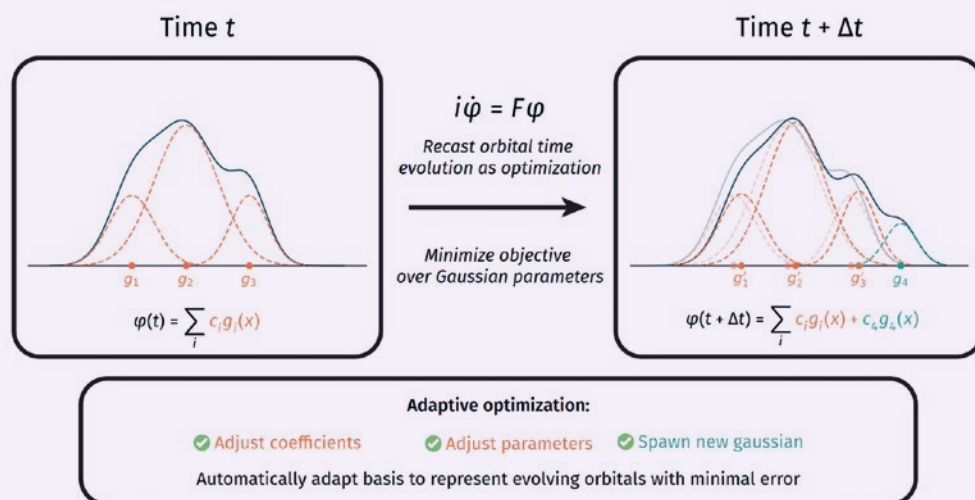


Figure 3: Illustration of Rothe's method applied to time-dependent Hartree–Fock and Kohn–Sham theory. Reproduced from ref. [18] under CC-BY 4.0 license.

theory, in its various forms. Hylleraas members have pioneered the Moreau–Yosida regularization technique in formal DFT (MY-DFT), and this continues to be a fruitful research topic. In particular, the ERC Starting Grant project *REGAL* of Prof. Il Andre Laestadius (Associate Professor at OsloMet, 20 % at Hylleraas) aims to make MY-DFT a practical tool.

The Dicke model is a model for the archetypal collective matter–light interaction, describing a large number of identical spins interacting with a single photon mode. Vebjørn H. Bakkestuen *et al.* [11] studied a DFT formulation of this model. This establishes a firm theoretical foundation for developing practical approximation methods to predict properties of systems where light and matter couple strongly.

A special case of the Dicke model is the quantum Rabi model, with a single spin.

Systems where light and matter couple strongly are increasingly important, e.g., polaritonic chemistry of molecules in cavities with radiation. In a study in *J. Phys. Chem. A* [12], Vebjørn H. Bakkestuen and coworkers use the Rabi model to demonstrate how quantum–electrodynamical DFT (QEDFT) can reduce a coupled light–matter problem to a description in terms of a few key variables. A central result is that QEDFT's central ingredients can be worked out essentially explicitly, providing a transparent, mathematically sound reference that helps validate QEDFT concepts and functional development.

An important problem in DFT is the inversion of the Kohn–Sham mapping: Find the exchange–correlation potential that reproduces a given ground-state density. In a study, Michael F. Herbst, Vebjørn H. Bakkestuen and Andre Laestadius address this issue for periodic solids [13]. Reliable inversion,

which is numerically hard, is a key tool for benchmarking DFT and for learning why approximate functionals succeed or fail. The authors produce an inversion algorithm grounded in a Moreau–Yosida regularized DFT.

In a related study, Oliver M. Bohle, M. Lotfigolian, Andre Laestadius, and Erik I. Tellgren develop a Moreau–Yosida regularized density-to-potential inversion method for periodic systems, e.g., crystals, focusing on Hartree–Fock exchange [14]. The method is demonstrated in a one-dimensional periodic setting, showing that one can feasibly recover a local potential that reproduces the effect of exact exchange.

A generalization of DFT that allows for nonlocal single-particle potentials is reduced density matrix functional theory (RDMFT). While the mathematical foundation of ordinary DFT has been known for a long time, a similar foundation for RDMFT has been lacking. In a

// A deeper understanding of quantum systems requires both rigorous theory and practical algorithms. Our research advances both, laying foundations for the next generation of quantum chemistry and materials science //

study submitted to Archives of Rational Mechanics and Analysis [15], Håkon R. Fredheim and Simen Kvaal address this challenge, and in the process obtain a refined and simpler analysis of traditional DFT.

Time evolution

At the Hylleraas centre, RT1 and RT7 both have strong activities regarding developing propagation algorithms for molecular systems. In particular, time-dependent coupled-cluster (TDCC) methods have been studied and employed over several years. In a study in *J. Phys. Chem. A* [16], Simen Kvaal, Håkon R. Fredheim, Mads G. Højlund, and Thomas B. Pedersen analyzed the abstract time-dependent bivariational principle, which is little-studied, yet forms the foundation for TDCC methods. In this article, they obtained several key results, including the identification of two mutually complementary bivariational principles. The theory was applied to the formulation of many of the common

TDCC formulations in the literature.

The Rothe method (Figure 3) is an unconventional wavefunction propagation technique pioneered by the Hylleraas group. The method is based on discarding traditional ODE integration techniques for wavefunction parameters in favor of time stepping formulated as an optimization problem. Two studies have been published in 2025:

Simon E. Schrader, Thomas B. Pedersen, and Simen Kvaal published a study of Rothe's Method for multidimensional wavepacket propagation applied to the Henon–Heiles model in two to four dimensions [17]. Explicitly correlated gaussians numbering only a few dozen were sufficient to capture essentially exact dynamical spectra for this model, even in four spatial dimensions.

Simon E. Schrader, Håkon E. Kristiansen, Thomas B. Pedersen, and Simen Kvaal

conducted a second study [18], where Rothe's method was applied to propagating time-dependent Hartree–Fock and Kohn–Sham theory, demonstrating that linear combinations of 30–100 gaussians can be time stepped successfully, reproducing high-quality grid calculations also in this case.

Oberwolfach workshop “Mathematical Methods in Quantum Chemistry”

On 10–14 March 2025, Simen Kvaal and Thomas B. Pedersen attended the Mathematisches Forschungsinstitut Oberwolfach (MFO) workshop “Mathematical Methods in Quantum Chemistry”. On Thursday 13 March, Kvaal gave a presentation “A mathematical approach to coupled-cluster theory”, outlining the findings of the QOMBINE projects efforts.

Visitors and personnel

PhD student Laura Sánchez came from the group of Prof. Jordi Cirera (IQTC,

University of Barcelona, Spain) for a 3-month exchange under the supervision of Lucía Morán-González and David Balcells. Laura worked on the development of graph neural networks to model excited-state processes in the photochemistry of lanthanide phosphors. The research stay of Laura was fully funded by the Spanish Ministry of Research.

External funding

DEMO Doctoral Network, EU, 2023–2027, 0.5 MEUR share (3.5 MEUR total).

DSTrain COFUND, EU, 2023–2027, 0.5 MEUR share (4.5 MEUR total).

QOMBINE, RCN Large Interdisciplinary Researcher Project, 2022–2027, ~ 4 MNOK share (25 MNOK total)

QSTAR, RCN National Center for Quantum Technology awarded 2025 (2026–2030), ~5 MNOK share (60 MNOK total)

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RT0: Hylleraas Software Platform

Throughout 2025, the Hylleraas Software Platform was further developed and advanced to support research activities both within the Centre and beyond.



Principal investigators:
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In 2025, the Hylleraas Software Platform (HSP, Figure 1) continued its development as a central research infrastructure for the Centre, building on the progress reported in previous years and with particular emphasis on consolidation, robustness, and integration across scientific applications and computing environments. The year was characterized by maturation of core functionality and optimization of the platform for reliable large-scale and production-level calculations. Additional targeted adaptations to new high-performance computing (HPC) architectures were implemented, including the transition to two-factor-authenticated login on the national supercomputing clusters. In parallel, key components for visualization of electronic densities and molecular orbitals were consolidated and brought to maturity. These are now being used by researchers in RT1 and RT3/4, for visualization of both grid-based and Gaussian basis-based orbitals. A substantial effort was also

devoted to workflow automation, documentation, and user support. Together, these activities further strengthened HSP as a common platform for method development, high-performance computing, and data-driven workflows, and supported its sustained use across research themes and external collaborations.

Throughout the year, the HSP team maintained and expanded both internal and external collaborations through continued development and application of the platform. An important technical milestone was the completion of hyflow, a workflow engine developed as an integral part of HSP for the construction and execution of complex computational workflows. Hyflow provides six basic building blocks—-independent processes, dependent processes, conditional branching, fan-out, fan-in, and loops (including self-loops)—which can be combined to represent a wide range of automated and adaptive scientific

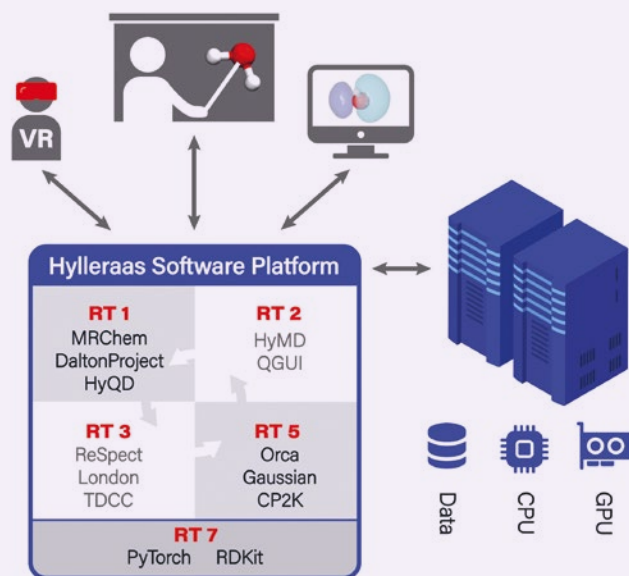


Figure 1: Illustration the Hylleraas Software Platform. Illustration by Morten Ledum.

workflows. Each step of such workflows is automatically inserted into an integrated database associated with the platform.

These workflow capabilities provide a key enabling abstraction for the active learning project in collaboration with Sigbjørn Løland Bore, which aims at the development of machine-learning interatomic potentials through iterative active learning cycles. The project addresses complex phenomena such as ion transfer processes, phase transitions, and chemical reactions. Its first results were published in *npj Computational Materials* [1] this year. The computational demands of this work (Figure 2), particularly the need for large-scale, automated, and reliable generation of training data and model validation, have driven further optimization and hardening of the platform, contributing significantly to its robustness, workflow automation, and readiness for sustained production use on HPC resources.

The collaboration with the Institut Laue–Langevin (ILL) in Grenoble, initiated in earlier years, was further consolidated in 2025 through close technical interaction and joint development. Morten Ledum and Simen Reine visited ILL in early 2025, where HSP was deployed and tested on ILL’s internal computing infrastructure, demonstrating seamless execution of electronic-structure software (including VASP) through the platform. This work helped clarify how HSP can serve as an integrating layer between experimental workflows and advanced simulations, and supported ILL’s decision to allocate additional resources to a deeper and more systematic integration of the platform into their computational environment. As part of this continued collaboration, a return visit to Oslo is planned for February 2026 to initiate implementation of more complex, production-level workflows and to prepare for broader adoption by the users of ILL. By using HSP, non-experts running experiments

with the ILL neutron beams will be able to easily run simulations in conjunction with their experimental investigations.

The Tromsø-based team collaborated closely with RT3 and RT4 and further developed a flexible framework within HSP for studies of molecular properties at different theoretical levels. This work resulted in a publication on unified molecular response functions [2]. The collaboration will continue in 2026 with a focus on simulations based on coupled-cluster and multiconfigurational self-consistent-field response theory.

HSP also played an important role in the Centre’s educational activities in 2025, notably at the Hylleraas School held at Hotel Hadeland, Gran (7–10 January 2025), where the platform was used for hands-on training in efficient use of electronic-structure codes, high-performance computing, and automated workflows. A major effort during the year was devoted to improving the

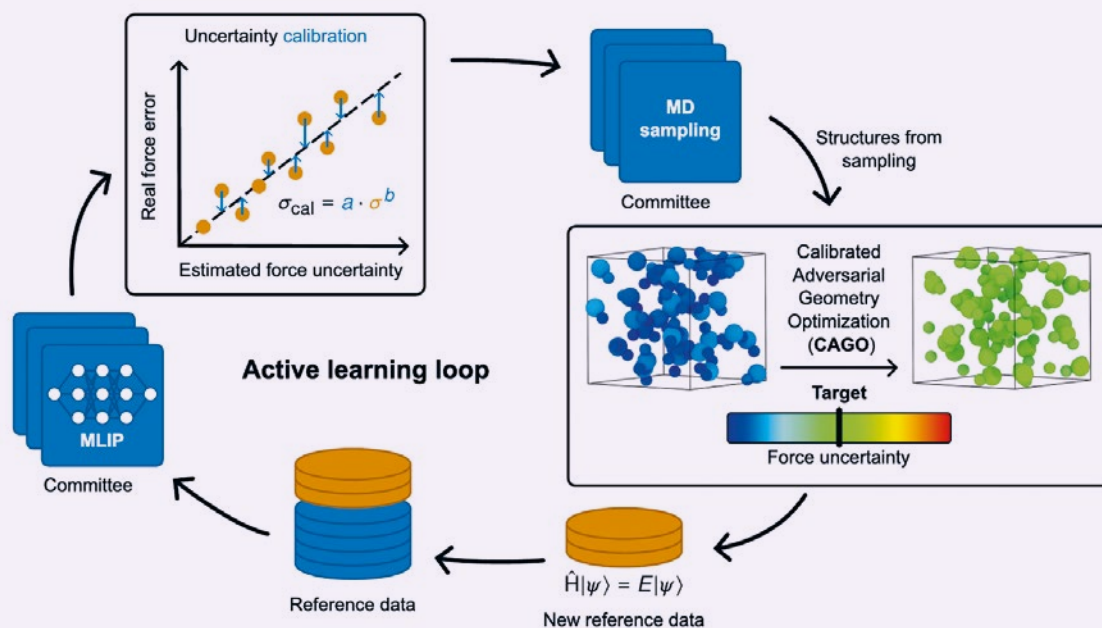


Figure 2: The HSP was essential for implementing an automated workflow to obtain machine-learned interatomic potentials. Reproduced from ref. [1] under CC-BY 4.0 license.

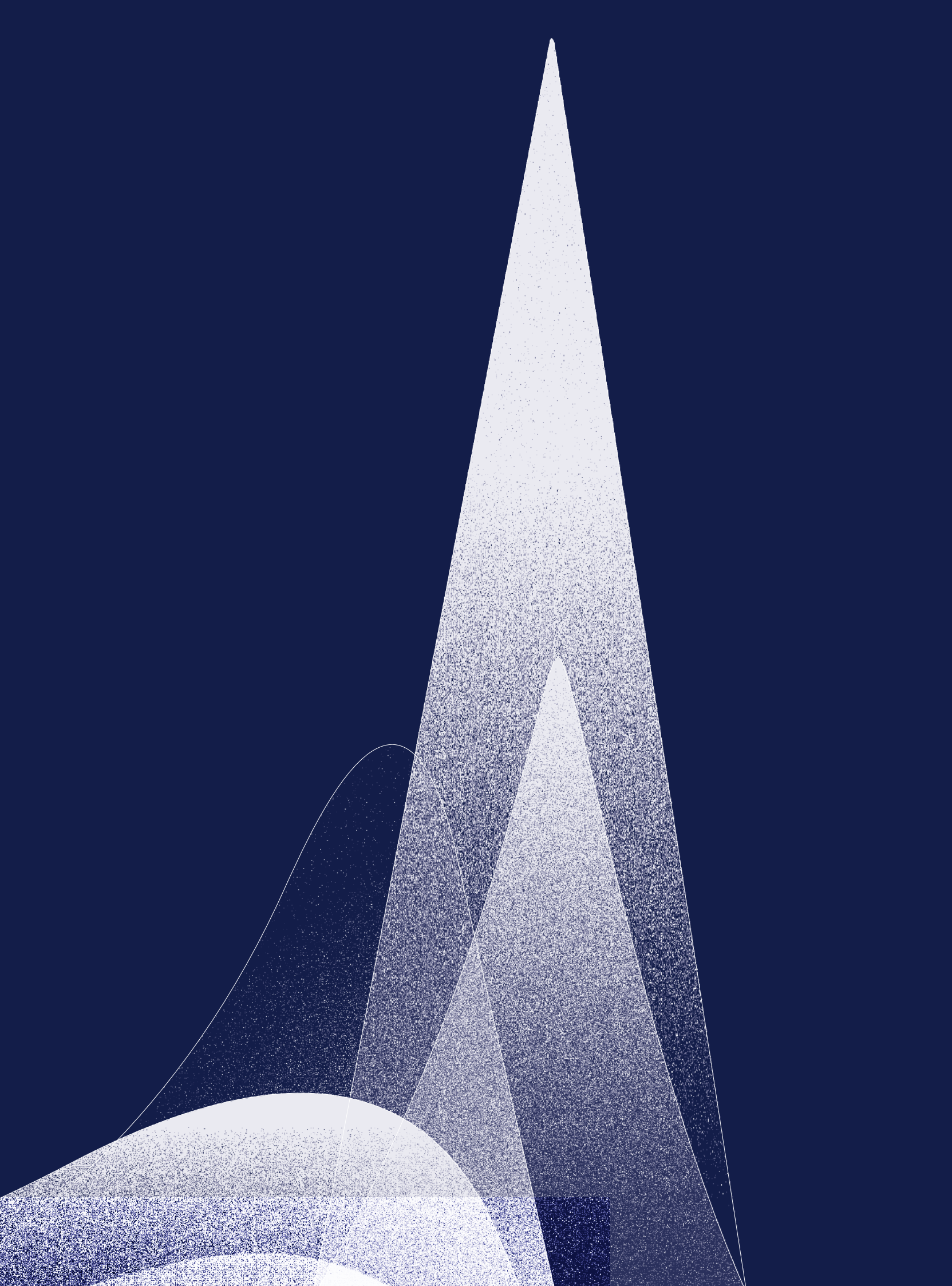
usability and transparency of the platform through technical optimizations and a thorough revision and expansion of the online documentation, including user guides, developer guides, and application programming interface references [3].

In summary, 2025 represented a year of consolidation and maturation for HSP. The platform's role as a shared research infrastructure within the Centre was further strengthened, its workflow and automation capabilities were significantly expanded, and key external collaborations—most notably with ILL—were advanced toward deeper and more strategic integration. The year also marked the first full year of contribution from Gabriel Gerez to the development of the platform.

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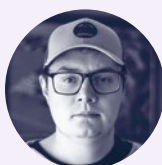
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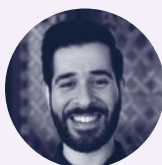
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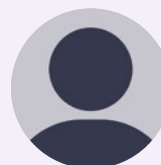
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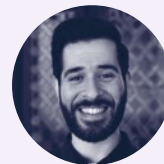
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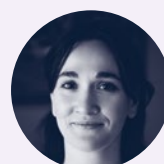
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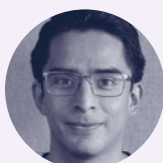
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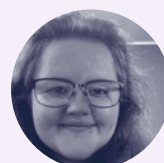
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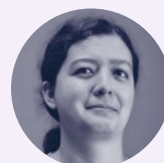
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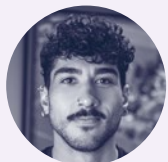
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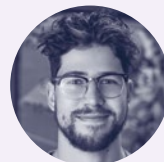
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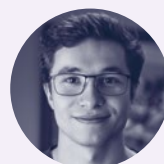
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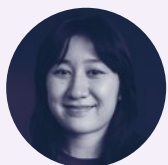
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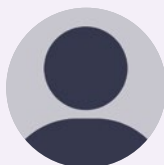
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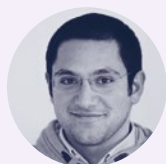


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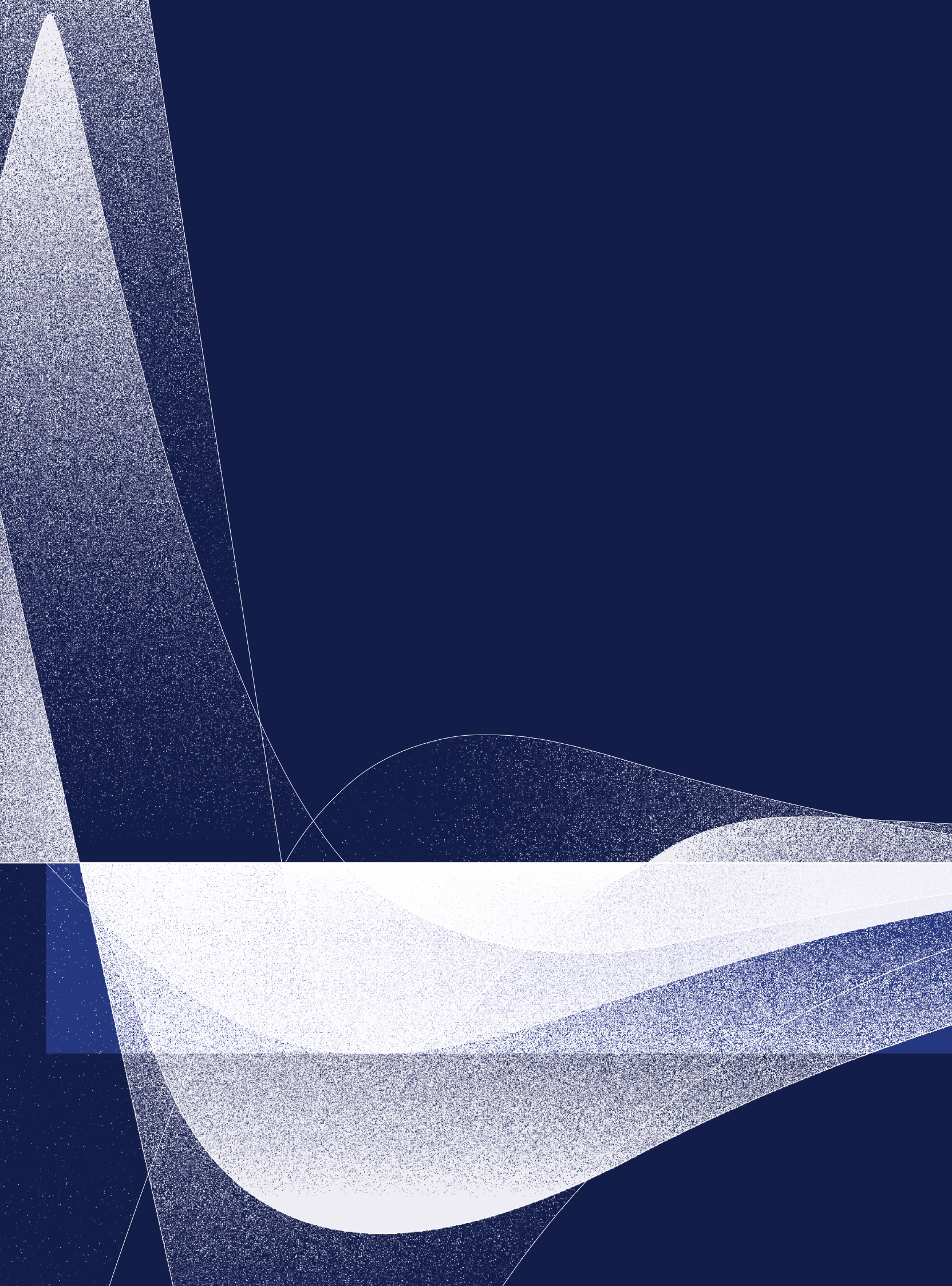
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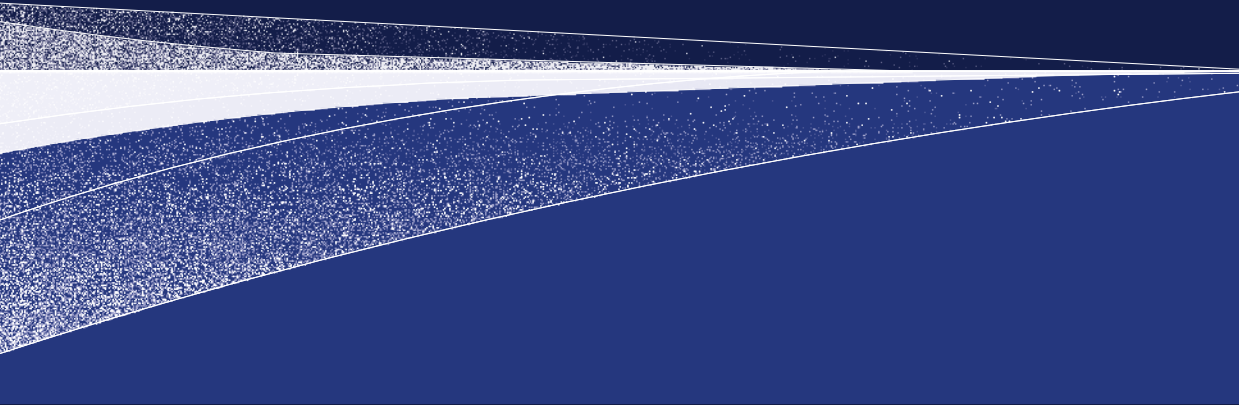
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FUNDING AND STAFF REPORT /

Funding (in NOK 1000)	2025
Basic funding as agreed in the Centre contract	
Funding from Research Council (CoE grant)	16 038
Funding from home institutions	19 252
Total basic funding	35 291
Additional funding from external projects	
Research Council funding	9 421
International funding	4 107
Public funding	0
Private funding	0
Total additional funding	13 582
Total funding	48 873

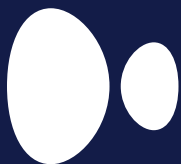
Staff Report (in man-years)	2025
Professors and researchers	23.9
PhD Candidates	13.9
Postdoctoral Fellows	5.7
Visiting Researchers	1.5
Administrative and technical staff	3.5
All staff	48.9

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