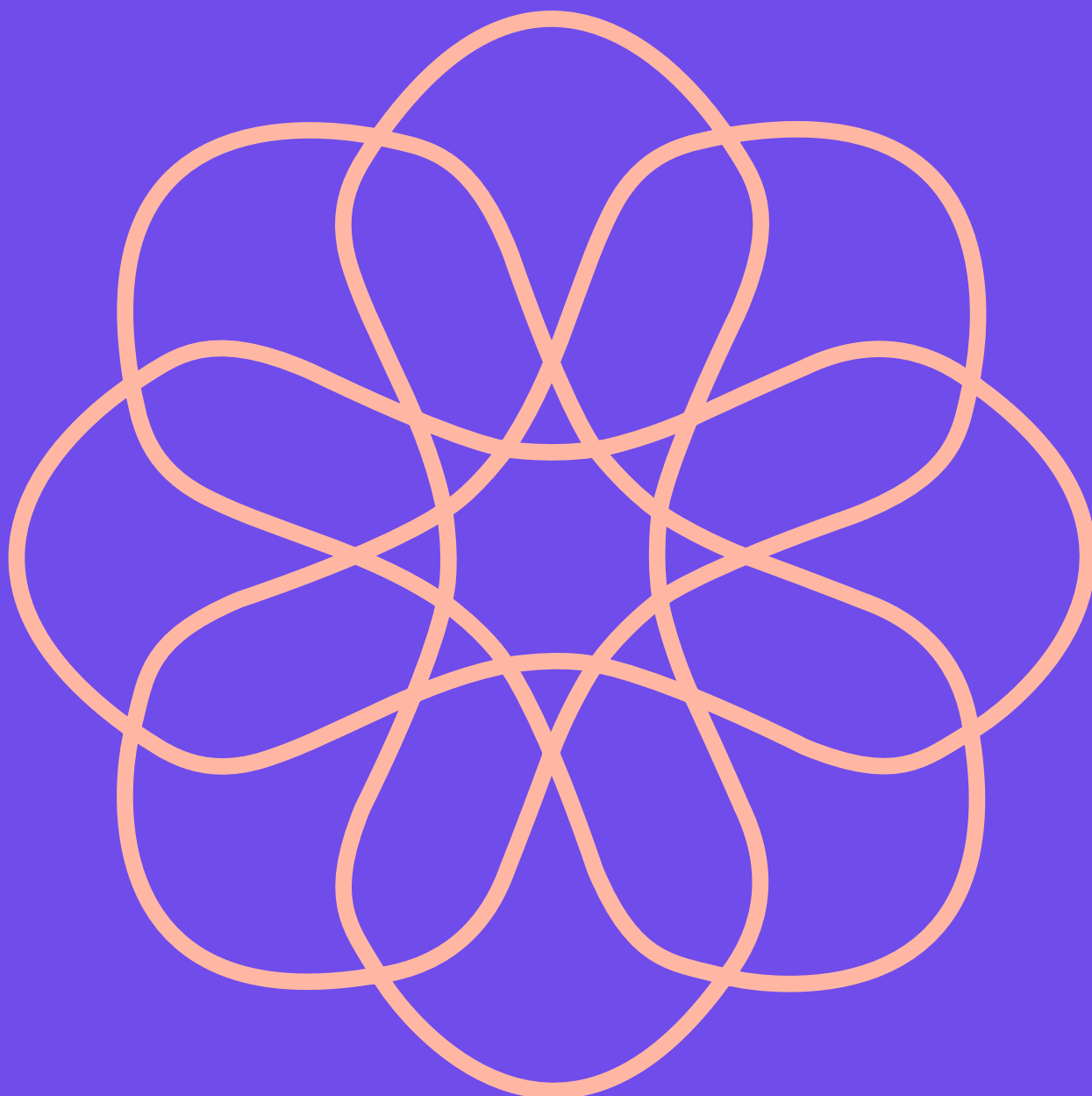




Hylleraas

Annual Report

2024



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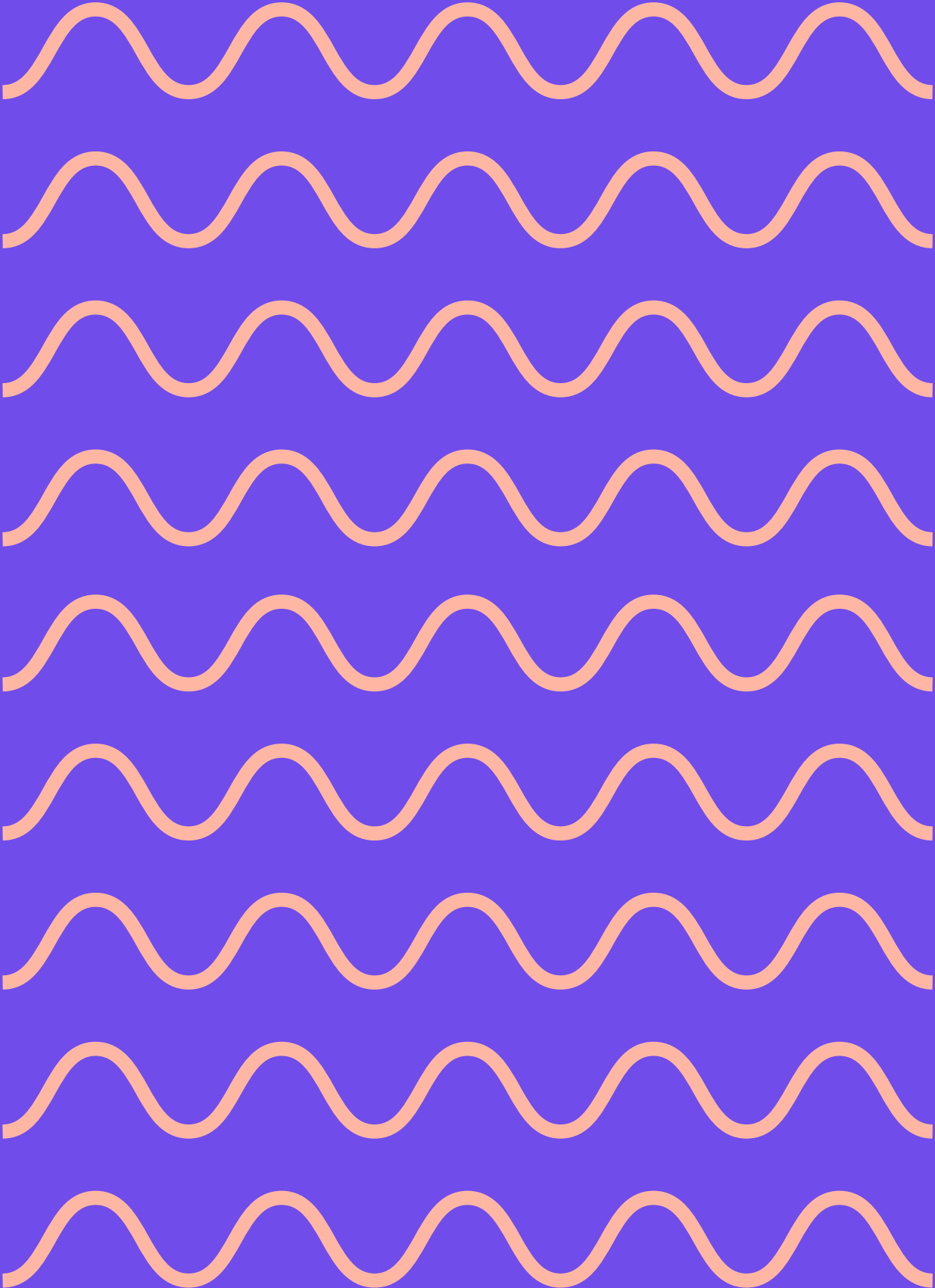


UiT The Arctic
University of Norway



Norwegian
Centre of
Excellence

The Research Council of Norway



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 2024, 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.

mn.uio.no/hylleraas/ →



Contents

From the Directors	06	→
→	From the Board of Directors	08
From the Young Researchers	10	→
→	2024 in Brief	12
Research Highlights	22	→
→	Almlöf-Gropen Lecture Series	30
Meetings and events	36	→

Alumni Talks	48	Ph.D. Defences	52
→	Visits and Mobility	58	
Externally Funded Projects	68	→	
→	Research Theme Activity Reports	72	
Hylleraas Members	112	→	
→	Publications 2024	124	
Funding and Staff Report	130	→	

From the Directors

The year 2024 was the first full year of operation with the new leadership and research themes at the Hylleraas Centre. The centre maintained its high scientific productivity level from the year before and achieved its primary ten-year success criterion of scientific impact. With artificial intelligence and quantum technology high on the strategic and political agenda nationally and internationally, it is reassuring that our recent research puts us at the centre of these areas within chemistry and physics.

Measured in terms of peer-reviewed publications, members of the Hylleraas Centre maintained the high level of productivity from 2023, with 83 papers published in 2024. In line with the goals of the Hylleraas Centre, the 83 papers were published in scientific journals covering a broad range of disciplines, from mathematics and computer science to biochemistry and molecular biology, with most papers in physical chemistry and chemical physics. Shortly into our eighth year of operation, at the end of 2024, the Hylleraas Centre surpassed its primary success criterion of scientific impact as demonstrated by 500 publications in international journals with more than 6500 citations and an H-index of 40.

We are particularly pleased to observe that 11 young researchers, more than half of them PhD candidates, from the Hylleraas Centre gave 17 oral presentations at international meetings around the world, including in the UK and USA, in 2024. This is an indication that our focus on recruitment of international top talents is fruitful, and a strong in-

centive to continue the efforts to improve our career-development support for young researchers. An important step in this direction was taken in 2024 as we organized the third career-development workshop with participants from all University of Oslo-based Centres of Excellence. This workshop series has been an important arena for exchanging ideas and sharing experiences on career development, and we look forward to implementing new initiatives aimed at improving on-boarding procedures and the identification and documentation of transferrable skills. We are grateful to Olaug Kristine Bringager for leading the organizing committee through all three workshops in 2018, 2019, and 2024.

The Annual Hylleraas Meeting is important to the centre activities and to maintain the close ties between members working in Oslo and Tromsø. The 2024 edition of the meeting was held at Sanner Hotel in Hadeland north of Oslo and organized by Marinella de'Giovannetti and Oliver Macphail Bohle, the

Oslo representatives of the Young Researcher Parliament (YRP). Our sincere thanks go to them for ensuring the success of the Hadeland meeting.

Several other impactful events were organized by centre members in 2024:

- Hylleraas School (Inga Schmidtke, Tonje Reinholdt Haugen, Michal Repisky, David Balcells, Simen Reine)
- Hylleraas Hackathon (Magnus Ringholm)
- Session at the 18th International Congress on Catalysis (Ainara Nova)
- Young CAS Workshop: Can ice be described from first principles? (Sigbjørn Løland Bore)
- CECAM Workshop: Computational chemistry across scales and disciplines (Michele Cascella)
- DFT in chemistry – dispute at inception and rise to prominence (Trygve Helgaker)
- NordCO₂ symposium on sustainable chemistry (Ainara Nova)

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

During 2024, much effort has been invested in the organization of the 13th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC), which will take place in June 2025 in Oslo with an expected attendance of about 1000 scien-

«Shortly into our eighth year of operation, at the end of 2024, the Hylleraas Centre surpassed its primary success criterion of scientific impact»

tists from all parts of the world. Former director, professor emeritus Trygve Helgaker chairs the organization committee, and we would like to thank him for his tireless efforts in 2024.

With several RCN Fripro and other grants still running, relatively little new funding has been awarded to centre members in 2024. In spring 2024, however, the EU Horizon Europe MSCA Doctoral Network *Complex Lipid Membranes for Science and Technology (CLIMB)* was awarded to an international consortium with Hylleraas PI Michele Cascella and Hylleraas affiliate Reidar Lund as leaders of the network node in Oslo. We congratulate Michele and Reidar with this important achievement.

With the end of the Hylleraas Centre less than three years in the future and with the call for the next round of Norwegian Centres of Excellence expected in mid-2025, we are pleased to see the excellent quality and high impact of the research conducted at the centre. In particular, we are excited about the opportunities created by the new research themes installed in 2023 and the enthusiasm of our researchers, senior as well as young researchers, which place us in a strong position within the fields of quantum technology and artificial intelligence for chemistry.

Professor Nathalie Reuter, University of Bergen, stepped down as a member of the Hylleraas Board of Directors in

January 2024. We express our appreciation for her contributions to the Board and extend our sincere thanks, and we are pleased to welcome Prof. Ida-Marie Høyvik as new member of the board. Høyvik is a professor of theoretical chemistry at the Norwegian University of Science and Technology in Trondheim. Her experience will bring important insights to the Hylleraas Board in the second period of operation.

Our congratulations and best wishes are extended to the seven young centre members who defended their PhD theses in 2024: Mahika Luthra, Ryan Scott Wilkins, Magnar Bjørgve, Lin Xue, Hannes Kneiding, Sahil Gahlawat, and Marinella de'Giovannetti.

Throughout 2024, Communication Adviser Cathrine Strøm worked hard on revising our communication procedures, leading to more frequent updating of the news section of the Hylleraas

web pages. We are grateful to Cathrine for her efforts.

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

Finally, we would like to thank all members and affiliates of the Hylleraas Centre for their excellent work in 2024, as detailed in this report.



Prof. Thomas Bondo Pedersen
Director



Prof. Luca Frediani
Deputy Director

From the Board of Directors

The Hylleraas Centre is now well within the second period, which started last year. A focus area in 2024 has been the consolidation of the strategy for the rest of the Centre lifespan, with special attention to a possible future application for another Centre of Excellence (SFF).

A recurring theme throughout the year has been the strategy towards another application for a third Centre of Excellence (SFF) which will follow CTCC (2007-2017) and Hylleraas (2017-2027).

The board is pleased to note that the reorganization of the centre's Research Themes and leadership in mid-2023 has been successful, with high productivity in terms of scientific publications and dissemination at international meetings. In particular, the board is happy to see that the Hylleraas Centre is a leading research environment within artificial intelligence (AI) for chemistry and computational tools for quantum-technology (QT) developments. Both AI and QT are research areas with great national and international strategic importance, and the board encourages the Hylleraas Centre to pursue research in these directions and to seek new collaborations with top-tier research groups in Norway and abroad.

The board also applauds the centre's efforts towards increased visibility, including increased participation of junior as well as senior members at interna-

tional scientific events and participation in outreach activities directed towards student recruitment. Importantly, the board strongly supports the establishment of a new communication system in 2024. This ensures continuous news updates at the Hylleraas website, showcasing the centre activities to the public as well as to the scientific community.

The Hylleraas Centre has managed throughout the years to attract additional external funding, especially from calls within the FRIPRO program at the Research Council of Norway and other funding agencies aimed at excellent science, including the European Research Council. In 2024, a Marie Skłodowska Curie Actions Doctoral Network was awarded to a consortium that includes Hylleraas PI Michele Cascella and Hylleraas affiliate Reidar Lund at the University of Oslo. We congratulate them with the new grant. Most PIs at the centre currently have one or more active projects, limiting the possibility to apply for more funding. The board supports several initiatives that are planned for 2025, including new FRIPRO proposals and AI, QT, and SFF centre proposals.

«The board is happy to see that the Hylleraas Centre is a leading research environment within artificial intelligence for chemistry and computational tools for quantum-technology developments»

In the past few years, the board has been concerned with making sure the Hylleraas Centre would be able to reach its full potential. An important action in this respect has been the establishment of RTo – Hylleraas Software Platform to exploit synergies between the research themes internally and to facilitate external collaborations. We are pleased to see that this activity is now well supported across the centre, in Oslo and in Tromsø.

An issue in the past few years has been the sufficient availability of computing resources, upon which the research at

the Hylleraas Centre is critically dependent. The board is pleased to see that both UiO and UiT have provided a lifeline to the Centre though additional resources for computing, smoothening the transition to the user contribution system without jeopardizing the centre's research output and quality.

Prof. Natalie Reuter, who has given her invaluable contribution to the board from the beginning of the Hylleraas Centre in 2017, decided to step out at the beginning of 2024. We thank Prof. Reuter for her very active engagement

in the work of the board. The board has been very pleased to welcome Prof. Ida-Marie Høyvik from the Norwegian University of Science and Technology in Trondheim as a new member. We are certain that she will contribute significantly to the board discussions in the final period of the Hylleraas Centre.

We conclude by expressing our thanks to the leadership of the Hylleraas Centre for their work and wish the centre a successful continuation in 2025, a defining year with several new proposals.



Unni Olsbye (chair)
Professor
Dept. Chemistry
UiO



Ida-Marie Høyvik
Professor
Dept. Chemistry
NTNU



Atle Jensen
Professor
Dept. Mathematics
UiO



John Sigurd Mjøs
Professor
Dept. Chemistry
UiT



Aslak Tveito
Professor
Simula Research
Laboratory

From the Young Researchers

The Young Researchers Parliament (YRP) aims to ensure a favorable working environment for early career researchers at the Hylleraas Centre. The YRP is composed of Postdocs, PhD candidates, Master students, and visiting students at the centre. Four representatives, two from Oslo and two from Tromsø, are elected to be the voice of the young researchers in the management team at the Hylleraas Centre. Their role is to serve as a communication bridge between young researchers and the management team, facilitating the exchange of concerns, ideas, and management discussions. Additionally, the YRP organizes the Hylleraas Annual Meeting.

This year's annual meeting was held at Sanner Hotel in Hadeland over three days and was organised by the YRP representatives of the Oslo node. This is one of the two annual events between members in Oslo and Tromsø. The young researchers had informed the YRP representatives that they were interested in learning more about grant proposal writing, which served as a central theme for this year's annual meeting, since most of the young researchers are early-career academics.

The YRP representatives invited two external speakers: Asbjørg Dyveke Johnsen (Research advisor at UiO), who gave a talk on the practical aspects of grant proposal writing, and Per Magnus Kommandantvold (Special Adviser, RCN), who provided an overview of the ERC, MSCA and FRIPRO calls. We also had Simen Kvaal deliver a highly relevant talk on the responsible use of generative AI in research. Michele Cascella presented a talk on the philosophical problem of knowledge, which resulted in some very interesting questions and discussions afterward.

Our last talk was given by Trygve Helgaker, who gave a concise account of his career as a theoretical chemist, providing valuable advice and tips for the young researchers in the audience. The last item on the program was the 5-minute presentations, where the PhD and master's students gave everyone a short update on their projects.

The YRP visitor programme offers valuable opportunities for young researchers to expand their academic perspectives. By welcoming distinguished professors and researchers from other institutions, the programme acts as a crucial platform for collaborative discussions, organising seminars, and promoting knowledge-sharing initiatives at the Centre. On behalf of the YRP, UiO representatives invited Prof. Stefan Grimme for a virtual visit to the Hylleraas Centre in Oslo on the 8th of March. During his visit, he gave a seminar to the entire Centre on his new low-cost electronic structure methods for large systems. In addition to the seminar, he had individual meetings

«By welcoming distinguished professors and researchers from other institutions, the YRP visitor programme acts as a crucial platform for collaborative discussions, organising seminars, and promoting knowledge-sharing initiatives at the centre»

with members of the Hylleraas Centre, including PhD students.

A subset of the YRP visitor programme is the alumni talks, which allows the YRP to invite former members of the Hylleraas Centre to come and give a seminar. This year, the YRP representatives of the Oslo node invited Dr. Hima Bindu Kolli to share her experiences and transition from academia to industry, as well as discuss her current research.

At each node of the Hylleraas centre, there are two elected YRP representatives. In Tromsø, Tonje Reinholdt Haug-

en stepped down in March and, in Oslo, Marinella de'Giovanetti stepped down in September. Both spent approximately two years as YRP representatives. The young researchers elected Helena Hradiská (Tromsø) and Manuela Leal Nader (Oslo) as the new representatives. We, on behalf of everyone at the Hylleraas Centre, would like to thank Tonje Reinholdt Haugen and Marinella de'Giovanetti for their hard work and contributions to the YRP and the whole Hylleraas Centre.

Elected YRP representatives 2024:



Oliver Macphail Bohle



Manuela Leal Nader

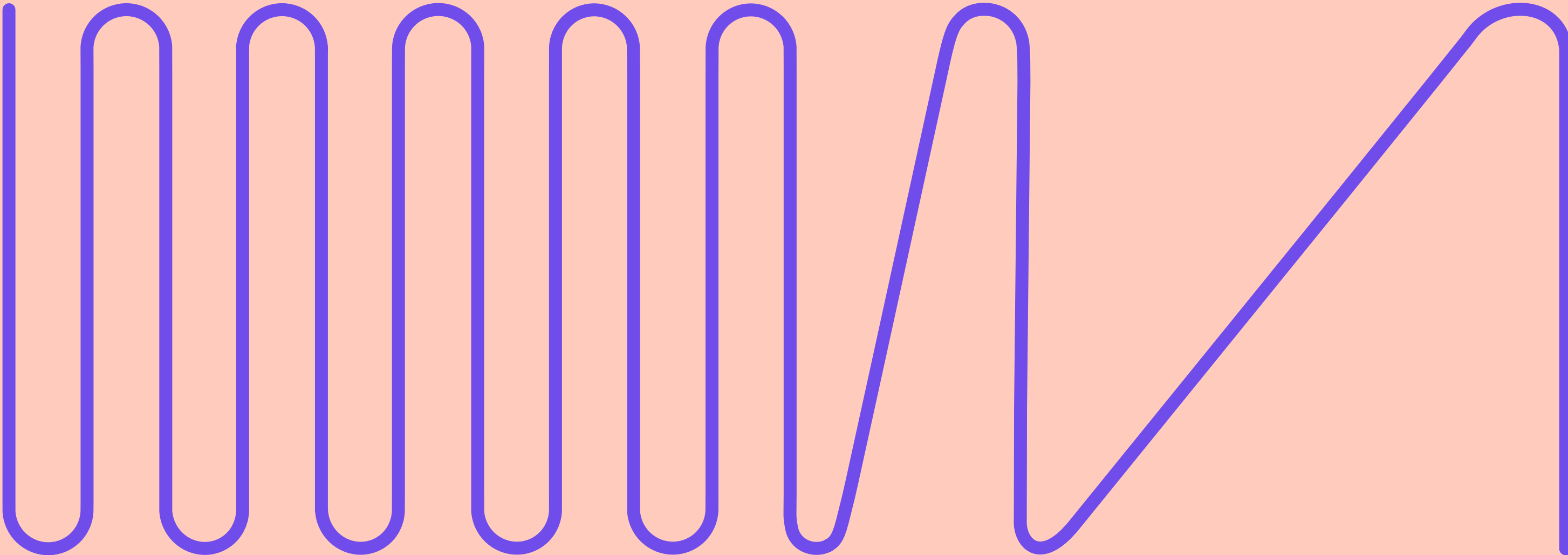


Quentin Pitteloud



Helena Hradiská

2024 in brief



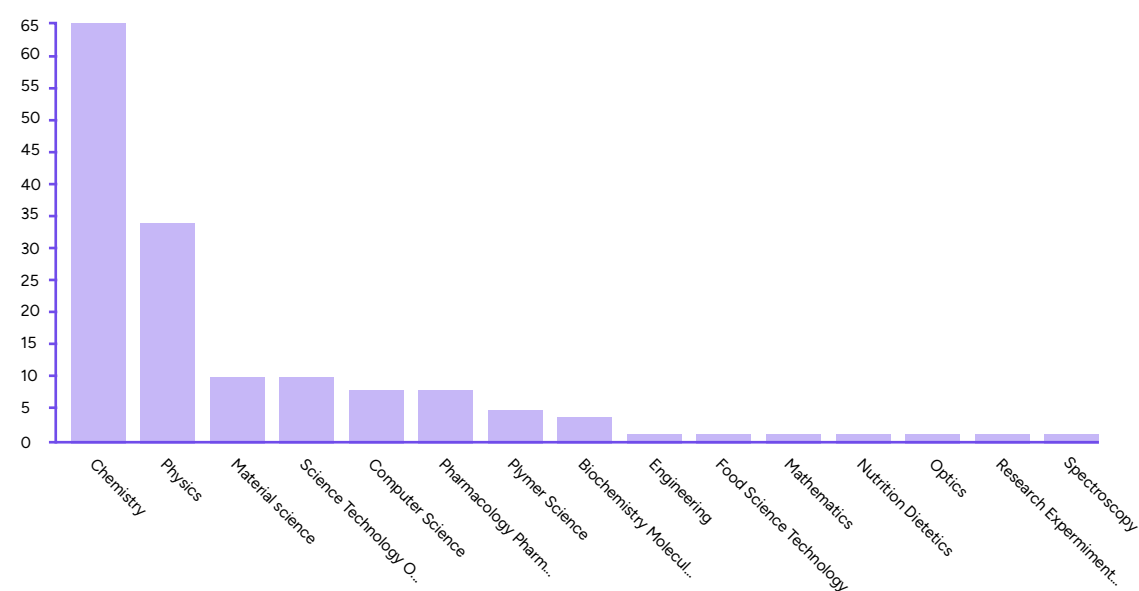


Figure 1: Categorization of the Hylleraas publications in 2024 into Research Areas.
Illustration generated by Clarivate Web of Science.

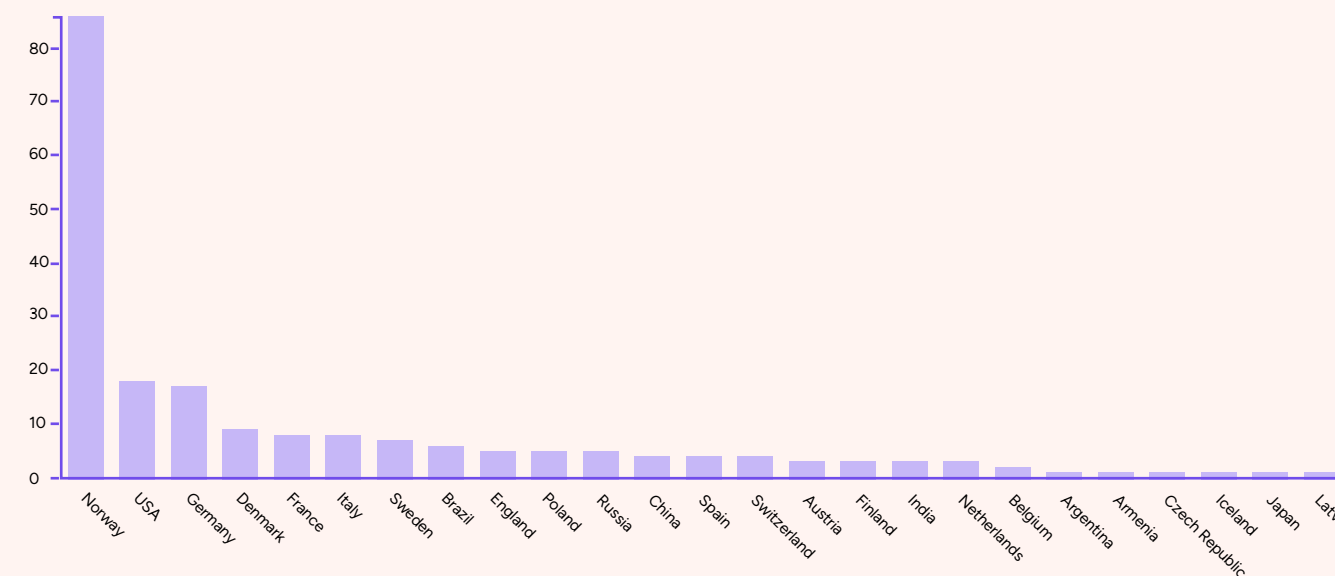


Figure 2: International collaboration is crucial to the Hylleraas Centre, here illustrated by the country of affiliation of our co-authors in 2024. Figure generated by Clarivate Web of Science.

Publications

Members of the Hylleraas Centre produced 83 scientific articles in 2024, bringing our total scientific production to 489 publications. Roughly 10% of these – 10 in 2024, 46 in total – were published in journals with an impact factor greater than ten. Specifically, in 2024, we published two articles in the Journal of the American Chemical Society, two in ACS Catalysis, two in Nature Communications, one in Angewandte Chemie, one in Small Science, one in Science Advances, and one in Nature Computational Science. At the end of 2024, the articles

published by the Hylleraas Centre since its opening in 2017 had been cited about 6500 times (excluding self-citations), with an H index of 40.

International collaborations are very important to the Hylleraas Centre. Since 2017, we have published papers in collaboration with authors from 49 countries across all continents. The historically most frequent countries are USA (104 papers), Germany (86), France (54), England (52), and Denmark (43). In 2024, we published papers on a wide range of Research Areas with collaborators from 30 countries, see Figs. 1 and 2.

About one half of these articles are devoted to theoretical and methodological developments, the other half being computational studies, often carried out in collaboration with experimentalists. Roughly 17% of our papers in 2024 were on quantum dynamics or machine learning methods with applications to molecular systems. These methodologies are key to the development of quantum technologies and chemical artificial intelligence, subjects of great national and international interest.

Meetings and conferences

Several meetings were organized by Hylleraas members in 2024. The *Hylleraas Hackathon* was held at Skibotn near Tromsø on April 22–26, organized by Magnus Ringholm, with about 30 participants. The *Annual Hylleraas Meeting* took place at Sanner Hotell near Gran on August 19–21 and was organized by YRP representatives Marinella de'Giovannetti and Oliver Macphail Bohle (Figure 3), with 51 participants. As always, the meeting offered opportunities for both scientific discussions (Figure 4) and social activities (Figures 5 and 6).

At the 18th International Congress of Catalysis, a major event with more than 2000 participants, Ainara Nova co-organized a symposium on *Computational Approaches at the Atomic Scale of Catalysis – Unifying Concepts to Tackle Dynamics in Computational Catalysis* on July 17 in Lyon, France. Shortly after the summer break, on August 26–30, Sigbjørn Løland Bore organized the YoungCAS workshop *Can Ice be Described from First Principles?* at the Hylleraas premises in Oslo.

On October 1–3, Michele Cascella co-organized the CECAM Workshop on Computational Chemistry Across Scales

and Disciplines to honor the scientific contributions of Prof. Ursula Röthlisberger from the Swiss Federal Technology Institute of Lausanne (EPFL), Switzerland. The workshop was held at CECAM headquarters at EPFL with 55 participants (Figure 7). In addition to being the former supervisor of Michele, Prof. Röthlisberger was a member of the Scientific Advisory Committee of the Hylleraas Centre from 2017 to 2023. On November 7–8, Trygve Helgaker co-organized the seminar *DFT in Chemistry – Dispute at Inception and Rise to Prominence* at the Royal Swedish Academy of Sciences in Stockholm, Sweden. Delivered by



Fig. 3. YRP representatives Oliver Macphail Bohle and Marinella de'Giovannetti organized the Hylleraas Annual Meeting in 2024. Photo: Cathrine Strøm. Fig. 4. Rasmus Vikhamar-Sandberg (left) and Evgueni Dinvyay discussing science at the Annual Meeting in 2024. Photo: Cathrine Strøm. Fig. 5. Hylleraas members preparing for a hike during free time at the Hylleraas Annual Meeting 2024. Photo: Cathrine Strøm. Fig. 6. Conversations during a coffee break at the Hylleraas Annual Meeting at Sanner Hotel, Gran, in 2024. From left: Manuela Leal Nader, Henrique Musseli Cezar, Michele Cascella, Jan Ingar Johnsen, and Rasmus Vikhamar-Sandberg. Photo: Cathrine Strøm. Fig. 7. Participants at the CECAM Workshop co-organized by Michele Cascella in honor of Prof. Ursula Röthlisberger. Photo: CECAM. Fig. 8. Illustration from the presentation of Trygve Helgaker at the Royal Swedish Academy of Sciences on Nov. 9, 2024. Screenshot from the recording posted at the YouTube channel of the Royal Swedish Academy of Sciences.

leading scientists from around the world, the presentations can be watched at the YouTube channel of the Royal Swedish Academy of Sciences (Figure 8). At the end of 2024, on December 13, Ainar Nova organized the *NordCO₂ Workshop on Sustainable Chemistry* at the University of Oslo, marking the end of the Nordic Consortium for CO₂ Conversion, a Nordic research network led by Nova and funded by Nordforsk since 2017.

In connection with the disputation of Mahika Luthra, Ainar Nova and David Balcells organized a *Symposium in Com-*

putational Catalysis on January 25 in Oslo, featuring the opponents Prof. Feliu Maseras, Institute of Chemical Research of Catalonia, Spain, and Assistant Professor Maren Podewitz, Technical University of Vienna, Austria. On February 12, the *Workshop on Chemical Bonding and Materials of the Future* was organized in Tromsø, with Dr. Cina Foroutan-Nejad from the Institute of Organic Chemistry of the Polish Academy of Sciences as the main speaker.

Professor Fernanda Duarte from University of Oxford, UK, delivered the 2024

Almlöf–Gropen Lecture, *Exploring chemical reactivity in the age of automation and machine learning*, on September 17 in Oslo and September 19 in Tromsø. At both events, the Almlöf–Gropen Young Speakers were Tonje Reinholdt Haugen from Tromsø and Marinella de'Giovannetti from Oslo. The title of Tonje's lecture was *Investigating cyclic peptides interactions with lipid bilayers using computational methods* while that of Marinella's lecture was *Grignard meets machine learning: cracking Grignard chemistry with neural network potentials*.



Fig. 9. Ainar Nova during the roundtable on career pathways for young researchers in Nanchang, China. Photo: The China Association for International Exchange of Personnel. Fig. 10. Telluride, Colorado, at 2600 m altitude in the Rocky Mountains, viewed from the gondola connection to Mountain Village. Photo: Thomas Bondo Pedersen. Fig. 11. Michele Cascella presenting at the Chemistry@Sete meeting, celebrating the 75th birthday of Odile Eisenstein. Photo: Marco Bortoli. Fig. 12. Poster-prize winner Inga Schmidtke (left) with Odile Eisenstein (centre) and Marinella de'Giovannetti (right). Photo: private.

Dissemination

The members of the Hylleraas Centre gave a total of 77 oral presentations in 2024. Of these, 18 presentations were given by young members and 10 by senior members and visitors as Friday seminars at the centre. The remaining 49 presentations were given by Hylleraas members at international meetings and conferences.

Ainar Nova gave a keynote lecture at the 2nd *International Sustainable Development and Innovation Forum* in Nanchang City, Jiangxi Province, China, and participated in a roundtable on career path-

ways for junior researchers (Figure 9). David Balcells gave an invited talk on generative artificial intelligence for transition-metal complexes at the *Gordon Research Conference on Computational Chemistry* in Portland, USA. Almost at the same time, Thomas Bondo Pedersen gave an invited talk on electron dynamics driven by strong laser fields at the *Telluride Science and Innovation Center workshop on New Developments in Coupled-Cluster Theory* in Telluride, Colorado, USA (Figure 10). Michele Cascella gave an overview of the Grignard reaction from a multiscale perspective at the Chemistry@Sete conference organized

on the occasion of the 75th birthday of Hylleraas affiliate professor Odile Eisenstein (Figure 11).

A total of 28 Friday seminars were given at the Hylleraas Centre in 2024, of which seven were given by guests to the centre. One of these was given by the YRP-invited speaker, Prof. Stefan Grimme from the University of Bonn, Germany, on March 8. Unfortunately, Prof. Grimme was unable to travel to Oslo and his lecture, *New 'Low-Cost' Electronic Structure Methods for Large Systems*, was delivered digitally, on Zoom.



Fig. 13. Erik Tellgren (left) supervising Piotr Dawid Ul, a talented student from Ullern senior high school, at the Hylleraas Centre in Oslo. Photo: Cathrine Strøm.

«During the autumn semester Piotr Dawid Ul, a talented student at Ullern high school, visited the Hylleraas Centre in Oslo to do a research project under the supervision of Erik Tellgren (Figure 13). Piotr used quantum-chemical calculations using our in-house software London to explore chemical bonding in mixed helium and hydrogen clusters subject to strong magnetic fields».

At the 45th International Conference on Coordination Chemistry held at Fort Collins, Colorado, USA, PhD student Inga Schmidtke (Figure 12) won a prize for her poster *Computational insights into ethylene hydrogenation via Rh(III)dimers*.

Following the signing of the collaboration agreement on quantum technology between the Faculty of Mathematics and Natural Sciences at the University of Oslo and the Niels Bohr Institute at the University of Copenhagen, Denmark, on May 14 in Oslo, the first scientific meeting between the two parties was organized in Copenhagen on October 30. At this meeting, Thomas Bondo Pedersen represented the Hylleraas Centre and presented its research lines with direct relevance for the second quantum revolution.

Outreach

The Hylleraas Centre was visited by *Talentsenteret i realfag* (part of Oslo Vitensenter at the Norwegian Museum of Science and Technology) on January 17, 2024. The visiting students carried out exercises related to quantum chemistry, attended talks by Trygve Helgaker, Hanan Gharayba, and Erik Tellgren, and visited the mass spectrometry laboratory with Mauritz Ryding.

On February 27, the Swedish government-owned multinational power company Vattenfall published the article *Five better things to do with carbon dioxide* on its website. This article is an interview with Ainara Nova who describes how the research carried out in the NordCO₂ consortium under her leadership can be used to produce valuable

materials such as methanol, polymers and plastics, synthetic fuels, carbonate minerals, and even food from CO₂.

In 2024, the French newspaper *Le Monde* published a series of six articles on “scientific cold cases.” On July 15, as the first of the six cold cases, *Le Monde* published the article *La réaction de Grignard, à l'origine des parfums, démasquée par les Arsène Lupin de la chimie* (The Grignard reaction, the origin of perfumes, unmasked by the Arsène Lupins of chemistry). The ingress of the *Le Monde* article states, in English translation: “For over a century, the Grignard reaction has enchanted industry, fascinated researchers, and traumatized students. In 1912, the Nobel jury awarded this recipe for manufacturing complex alcohols, which are the source of perfumes, fertilizers, and medicines. How-

ever, its mechanism had never been elucidated. Until an astonishing duo of chemists tackled the mystery.” The “astonishing duo of chemists” denotes Michele Cascella and Odile Eisenstein, and the article highlights the computational detective work done under their leadership at the Hylleraas Centre over the past five to six years on the Grignard reaction.

During the autumn semester Piotr Dawid Ul, a talented student at Ullern high school, visited the Hylleraas Centre in Oslo to do a research project under the supervision of Erik Tellgren (Figure 13). Piotr used quantum-chemical calculations using our in-house software London to explore chemical bonding in mixed helium and hydrogen clusters subject to strong magnetic fields. He found that exotic chemical bonds are

possible and shared his findings in the form of a 9-page written report.

Faglig-pedagogisk dag is an annual event at the University of Oslo aimed at high school teachers. On October 31, 2024, Thomas Bondo Pedersen presented the research themes of the Hylleraas Centre for about 40 chemistry teachers – twice the attendance compared with 2023 – from high schools in and around Oslo.

With artificial intelligence on everyone’s lips in 2024, Simen Kvaal published the article *KI er bullshit!* (AI is bullshit!) in *Khrono*, the Norwegian news outlet for academia, on December 5. Simen argues that one should always think of the output of large language models as “bullshit,” meaning that one must assume that the output from, e.g., ChatGPT is incorrect or not true.

Training and career support

Seven members of the Hylleraas Centre – four in Oslo, three in Tromsø; five male, two female – defended their PhD thesis in 2024: Mahika Luthra (UiO), Ryan Scott Wilkins (UiT), Magnar Bjørgve (UiT), Lin Xue (UiO), Hannes Kneiding (UiO), Sahil Gahlawat (UiT), and Marinella de’Giovannetti (UiO). At the end of the year, a total of 30 PhD candidates had completed their degrees at the Hylleraas Centre.

The 2024 edition of the *Hylleraas School* was organized by a committee composed of Inga Schmidtke, Tonje Reinholdt Haugen, Michal Repisky, David Balcells, and Simen Reine, and held at Hadeland north of Oslo on January 9-12 with 57 participants. The scientific theme of the 2024 edition of the Hylleraas School was spectroscopy and optical properties and



Fig. 14. Thomas Bondo Pedersen opening the KUPP3 career development workshop at the Norwegian Academy of Science and Letters in Oslo on October 29. Photo: Frithjof Bringager.



Fig. 15. Kenneth Ruud was elected member of the International Academy of Quantum Molecular Science in 2024.

featured a guest lecture on experimental attosecond spectroscopy by Antoine Camper from the High Energy Physics group at the University of Oslo.

Following the highly influential career-development workshops organized in 2018 and 2019, Trygve Helgaker, Olaug Kristine Bringager, and Thomas Bondo Pedersen organized the third workshop, KUPP3, on October 29 at the Norwegian Academy of Science and Letters in Oslo with assistance from Prof. Ragnhild Eskeland from CanCell, Prof. Ragnhild Brøvig from RITMO, and Senior Adviser Else Marie Lingaas from the Research and Innovation Administration at the University of Oslo. The KUPP3 workshop was attended by all Centres of Excellence at the University of Oslo and focused on sharing of experiences and on outgoing support for young researchers, including identification and documentation of transferable skills (Figure 14).

Young Researcher Parliament

The Young Researcher Parliament (YRP) invited Prof. Stefan Grimme from the Mulliken Center for Theoretical Chemistry at the University of Bonn, Germany, to deliver a guest lecture at one of the regular Hylleraas Friday seminars on March 8. The YRP also organized an

alumni talk featuring Dr. Hima Bindu Kolli, Rutherford Appleton Laboratory, UK. A second alumni talk was organized in November but had to be cancelled in the last minute.

The Hylleraas Annual Meeting in August 2024 was organized by the YRP representatives Marinella de'Giovannetti and Oliver Macphail Bohle at Sanner Hotel in Gran.

In 2024, Helena Hradiská succeeded Tonje Reinholdt Haugen as YRP representative in Tromsø, while Manuela Leal Nader succeeded Marinella de'Giovannetti in Oslo. Hradiská and Nader join Quentin Pitteloud and Oliver Macphail Bohle as YRP representatives.

Visitors

In 2023, a total of 24 researchers visited the Hylleraas Centre, with 19 in Oslo and 6 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

With several senior members running RCN Fripro grants already, the Hylleraas Centre attracted relatively little new funding following the record years 2020 and 2021.

However, the Hylleraas Centre became part of a new Marie Skłodowska Curie Action (MSCA) Doctoral Network through the participation of Michele Cascella and Reidar Lund. The project, CLIMB (Complex Lipid Membranes for science and technology), will involve leading European lipid-research laboratories with strong complementarity in expertise and training capabilities. It will focus on the exploration of structural properties and of membrane-driven interactions that are key to the development of complex lipid-based nanostructures, mimicking the cellular environment and function as high-performance sustainable materials. One PhD student will be funded in Oslo, which will also serve as the host institution for several secondments.

Personnel

Kenneth Ruud (Figure 15) was elected member of the International Academy of Quantum Molecular Science.

Management

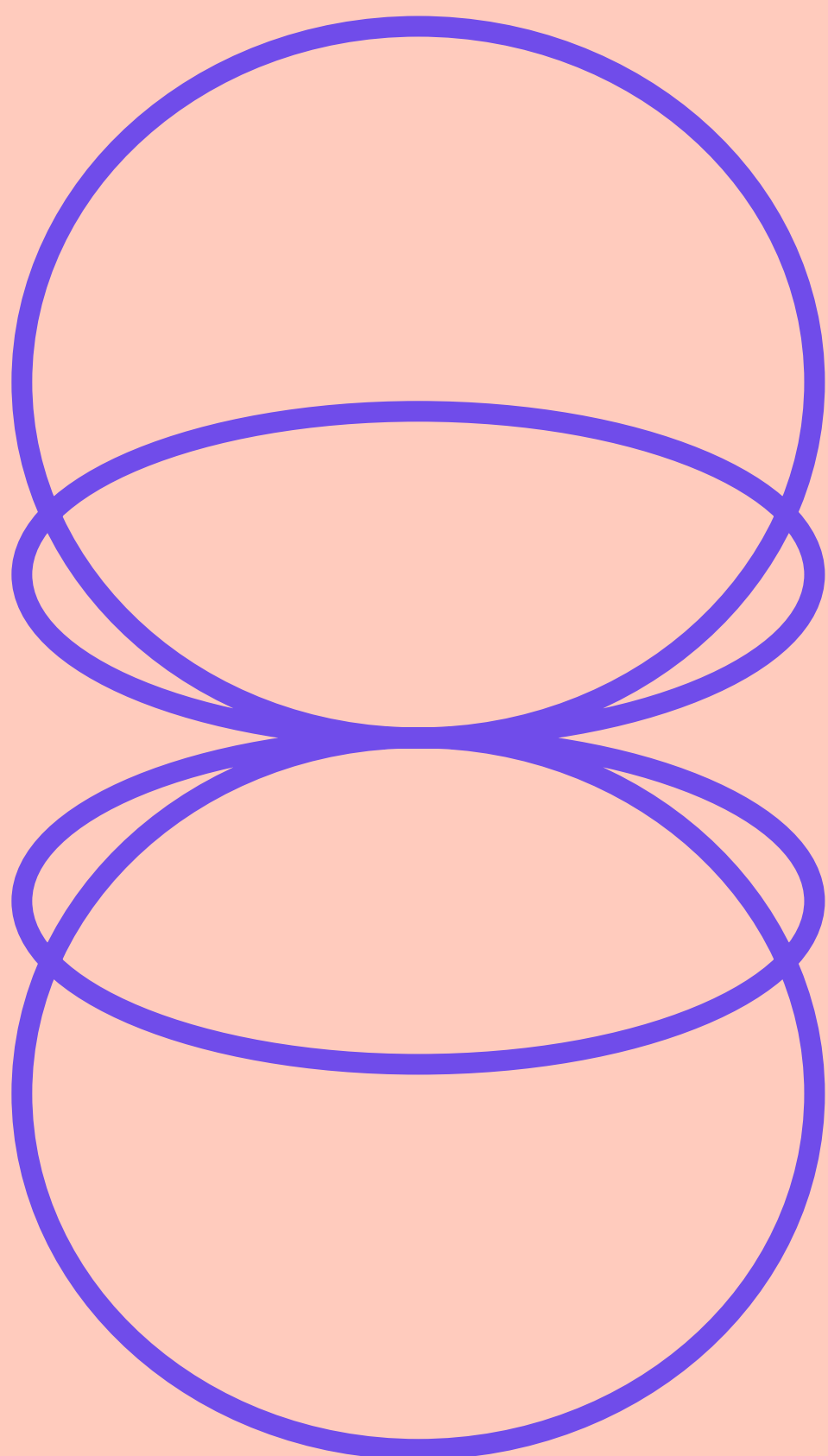
The Management Team met 11 times in 2023 (all months except July), while the Board of Directors met twice (March 20, November 6).



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)



Research Highlights

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.

Simen Kvaal

Computing dynamics of quantum systems using Rothe's method

The accurate simulation of the dynamics of quantum systems poses a monumental challenge. The complexity arises from the exponential growth in computational effort with the number of particles. Traditional methods employ large grids, and here we present our recent advances using a grid-free approach: Rothe's method and explicitly correlated gaussians. Our research shows that this is a promising approach to high-dimensional problems with many particles.

The law governing the time evolution of quantum systems is the *time-dependent Schrödinger equation*. This is a partial differential equation of immense complexity, the main complicating factor being that the effort required to simulate a collection of particles, e.g., electrons in an atom or molecule, grows *exponentially* with the number of particles. It is a major challenge to produce simulation techniques that both are affordable enough to be carried out on physical systems of interest and at the same time being accurate enough to produce predictions verifiable by experiment. The high demand for accuracy in chemistry makes this a daunting task, indeed. The demand for performing such simulations is growing, due to the progress in experimental techniques that operate on the attosecond scale.

Indeed, the 2023 Nobel prize in Physics was awarded to Pierre Agostini, Ferenc Krausz and Anne L'Huillier for "experimental methods that generate attosecond pulses of light for the study of electron dynamics in matter" [1].

The mathematical description of a quantum system's state is a *wavefunction* Ψ , a complex-valued function of time and space, yielding *all* the physical properties of the system [2]. Thus, the first major obstacle is to find a compact representation of this wavefunction. This is in general hard, since when a molecule is subject to strong perturbations such as external laser fields, the wavefunction becomes very complicated, with dramatic ripples and shockwaves, complicated interference patterns and fine details over a large spatial extent. The

standard approach is to use a large and fine-grained *grid*. However, this quickly becomes unfeasible: For even a small molecule like water, the exponential cost implies that a coarse description will require more bytes than the number of electrons in the universe!

An approach to circumvent the enormous cost of a grid is to instead use *linear combinations of complex gaussians*, often called *explicitly correlated gaussians* (ECGs). A gaussian wavefunction is partially localized and can therefore be used like LEGO bricks. Given enough such gaussians distributed in space, any kind of wavefunction Ψ can be produced to arbitrarily high accuracy. In Figure 1, the principle is illustrated in a single spatial dimension for clarity.

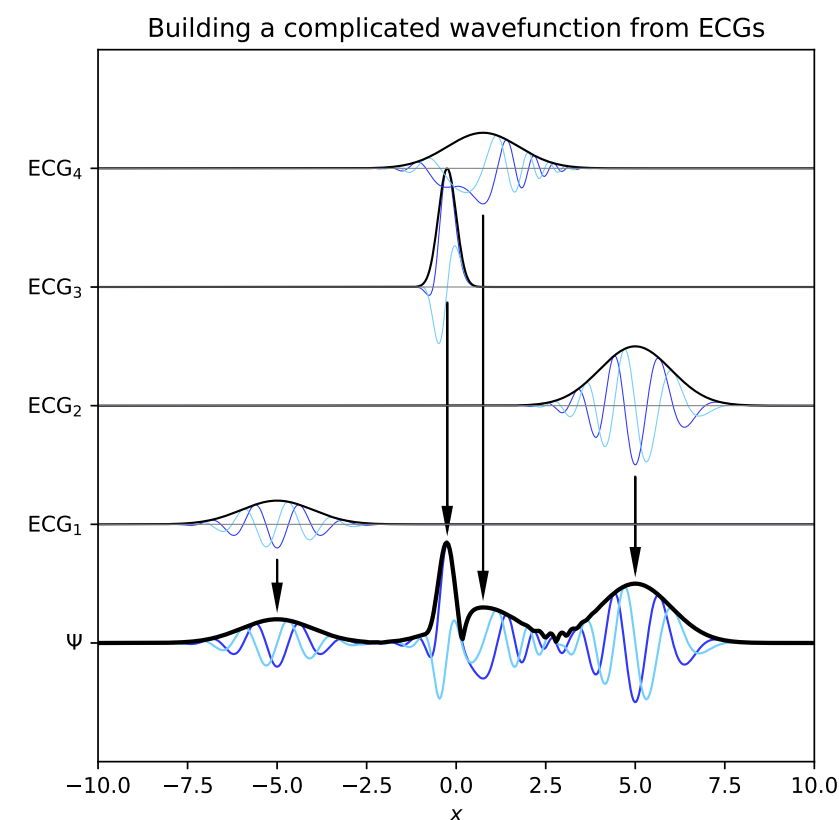


Fig. 1: Illustration of how complicated a complex-valued wavefunction can be built using explicitly correlated gaussians (ECGs). Each component ECGi is summed to yield the total wavefunction Ψ . This sum can have arbitrarily high level of detail. The more gaussians are used, the more accurate the wavefunction has potential to become. Illustration: Simen Kvaal.

Using ECGs in quantum chemistry is not a new idea, with a whole community devoted to extreme high accuracy calculations of atomic and molecular properties using such functions. The results are impressive, and in many cases at a resolution rivaling experiments [3]. The goal has, however, mainly been the determination of the *spectra* of the systems under study, as opposed to the time-resolved dynamics.

Unfortunately, it turns out that *moving* the ECGs in space is exceedingly difficult. Indeed, it turns out that the more malleable the component functions are, the more difficult it is to find their positions as function of time. The classical approach to moving ECGs around is by means of the *Dirac-Frenkel variational principle* [2, 4, 5], which translates the

Schrödinger equation into a low-dimensional but extremely stiff (i.e., hard to solve) coupled set of ordinary differential equations for the positions, widths and other aspects of the ECGs [5, 6]. Our approach is instead to use *Rothe's method*, named after German mathematician Erich Rothe, who in 1930 [7] proposed to solve evolution equations in a radical way: instead of choosing a spatial representation and finding a time-continuous evolution, one should *first* choose a discrete set of points in time and instead try to find the best possible space-discrete approximation [8]. In the case of the time-dependent Schrödinger equation, *time stepping is transformed into an optimization problem*. Indeed, it turns out that Rothe's method works surprisingly well for the ECG representation of Ψ . The procedure is adaptive, and ECGs

may be added or removed whenever needed.

In [9], A. Wozniak, L. Adamowicz, S. Kvaal, and T.B. Pedersen performed a study of the representational power of ECGs. In this paper, it is demonstrated that as little as 36 ECGs is sufficient for a very accurate description of the dynamics of a 2d hydrogen atom model with an extremely strong laser pulse added. While encouraging, there is no guarantee that this impressive compression of the dynamical wavefunction is transferrable to more realistic systems.

In [10], Rothe's method for ECGs was applied to a realistic simulation of high-harmonic generation spectra of the hydrogen atom in 3d. *High-harmonic generation*, or HHG, refers to the process where an

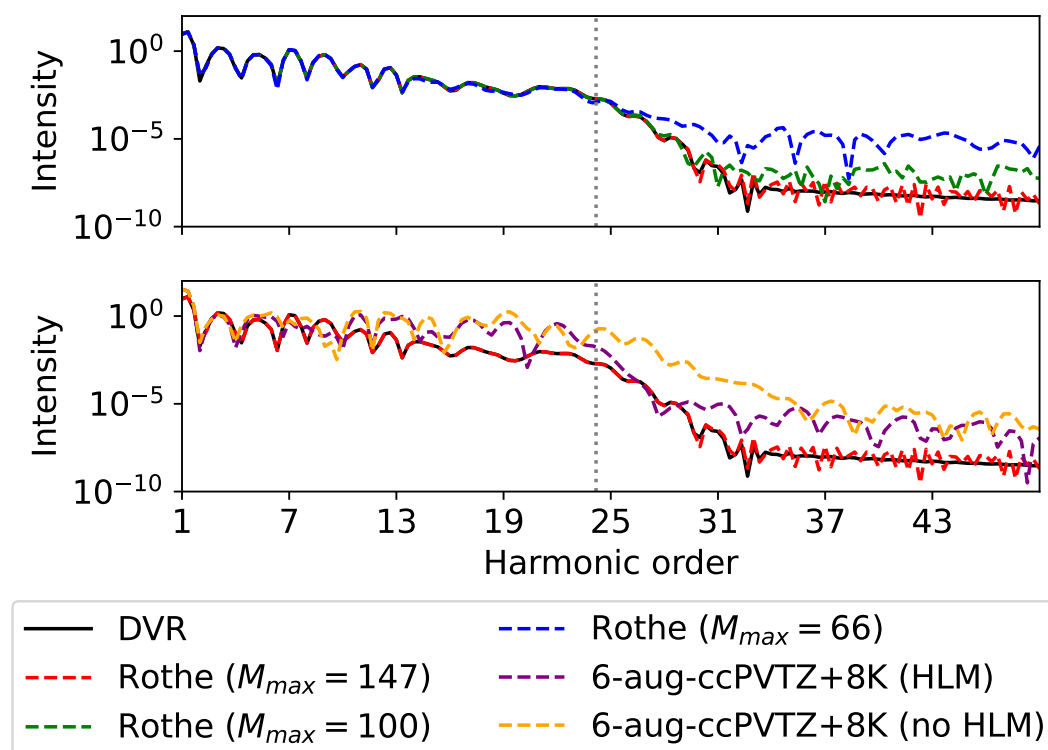


Fig. 2: Comparison of HHG for the hydrogen atom. The spectra are computed using a high-resolution discrete-variable representation (DVR) grid method, Rothe's method, and finally fixed gaussian basis sets (6-aug-ccPVTZ+8K). The fixed gaussian basis is the classical quantum chemist's approach and does not produce a high-quality spectrum. This is due to the lack of the ability to describe highly oscillatory components far away from the atomic nucleus. On the other hand, the Rothe approach gives much more accurate results, and as the number of ECG functions is increased, the calculation approaches the grid calculation, which is essentially exact in this case. *Reproduced with permission from J. Chem. Phys.* 161, 044105 (2024).

atom or molecule is subject to an ultrafast femtosecond laser pulse, resulting in complicated electronic accelerated motion and subsequent emission of photons in the form of attosecond pulses or trains of pulses. These photons can have very much larger energy than the impinging photons of the driving laser, i.e., the outgoing photons are high harmonics. In Figure 2, the HHG spectra from various simulations of the same instance of hydrogen plus laser are shown. The reference calculation, performed on a large grid, is shown as a black solid line, while the highest quality Rothe calculation, using at most 147 component ECGs, is shown as a red dashed line. Further details are given in the caption of Figure 2. The calculation using Rothe's method achieves virtually identical results as the grid calculation, but with a much more compact description of the wavefunction.

These results indicate that using the simple ECG functions do indeed also work in 3d, with a much-reduced cost compared to a grid calculation.

Even if the wavefunction is compactly represented, the calculations are comparatively expensive. Each time step requires the approximate solution of a nonlinear optimization problem, where the objective function is an intricate combination of a many analytical gaussian integrals and their derivatives. However, especially in higher dimensions, the expense may be well justified, if the efficiency of the ECG wavefunction representation is equally good as for the examples seen so far.

Our next study, accepted for publication in December 2024, was the dynamics of the Henon-Heiles model [11], a tradition-

al test model for nuclear vibrational dynamics. The model exhibits chaotic behavior in the classical regime, and quantum dynamics becomes very complicated. This is therefore an excellent challenge for Rothe's method with ECGs. We computed the dynamics of 2d, 3d, and 4d versions of the model, and computed the autocorrelation spectra. We compared with grid calculations using a DVR method, and in 4d, these reference calculations are indeed quite expensive. In Figure 3, snapshots of the 2d simulation are shown, exhibiting the extremely complicated wavefunctions of the Henon-Heiles model. In 3d and 4d, these wavefunctions are harder to visualize. We instead turn to the computed autocorrelation spectrum. In Figure 4, the spectrum for the 4d Rothe calculation is shown, for an increasing number of ECGs. The convergence is clear, and im-

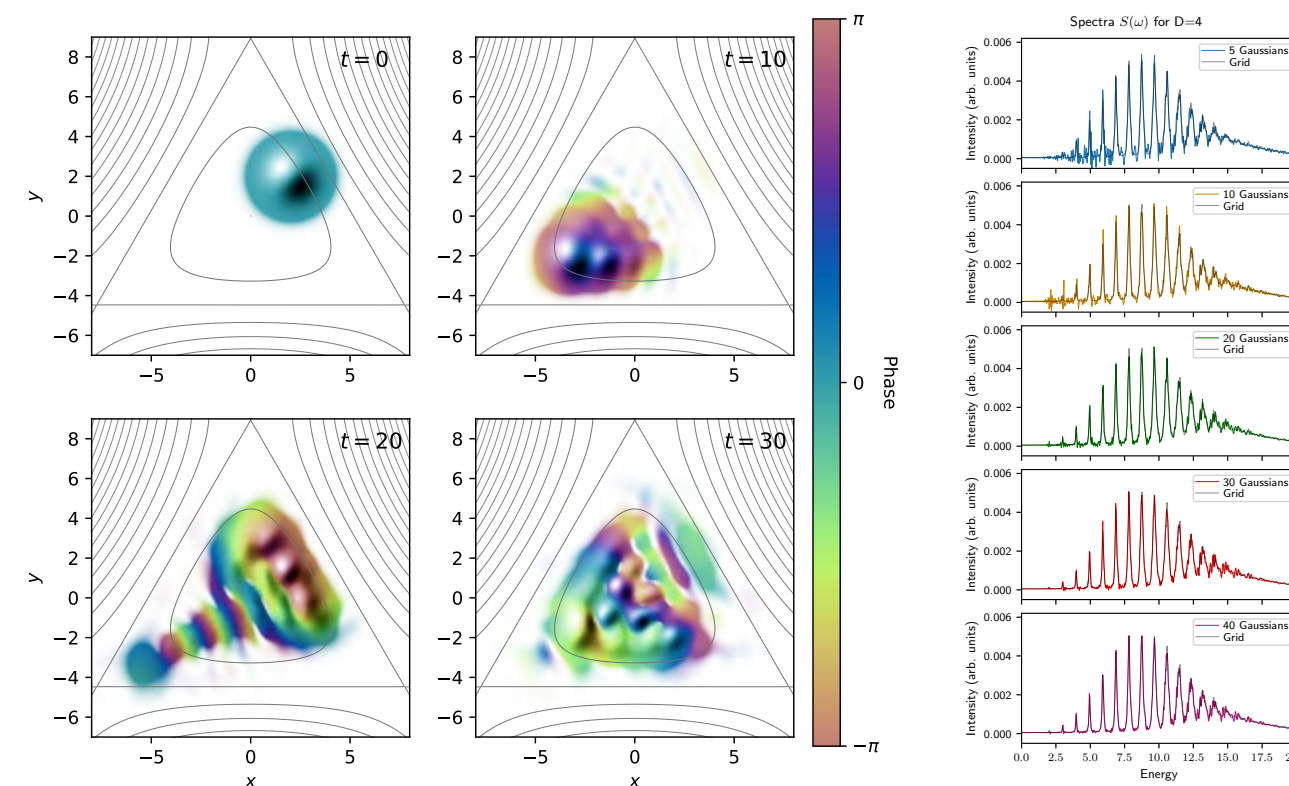


Fig. 3: Snapshots of a 2d simulation of the Henon-Heiles model. The potential-energy surface is visualized by contour lines, and the wavefunction is visualized by shaded and colored plots. Where the wavefunction is very small, the wavefunction is completely transparent. The colors correspond to the phase of the complex-valued wavefunction. The dynamics of the wavefunction is seen to be highly complicated, with a striking variation in structure and level of detail. *Reproduced with permission from J. Chem. Phys.* 162, 024109 (2025).

Fig. 4: The autocorrelation spectrum of the 4d Henon-Heiles model. The wavefunction is much too complicated to be visualized directly. The spectrum becomes increasingly more accurate as more gaussian functions are added to the wavefunction. *Reproduced with permission from J. Chem. Phys.* 162, 024109 (2025).

pressively, merely 40 gaussians give a virtually exact spectrum.

Our research demonstrates that Rothe's method can propagate wavefunctions built with ECGs, i.e., complex-valued gaussian functions. Our method is computationally intensive, but robust, and easily rivals the most accurate traditional grid calculations. The representational power of the ECGs is impressive, and a striking observation is that this does not seem to bate with increasing dimension. In fact, Rothe's method seems to handle higher dimensions very well, with very accurate results. Our next step is to tackle multielectron dynamics using time-dependent Hartree-Fock and density-functional theory, as well as realistic nuclear dynamics simulations using realistic *ab initio* potential energy surfaces.

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Ning Cao and Ainara Nova

Copper (II)-Oxyl Formation in a Biomimetic Complex Activated by Hydrogen Peroxide

Lytic polysaccharide monooxygenases (LPMOs) are important enzymes for the natural recycling of carbon. The knowledge of their structure has motivated the synthesis of catalysts that mimic their active sites. In 2024, we have investigated the reactivity of one of these systems in which Cu was anchored in a metal organic framework (MOF) by a histidine brace.

The mechanism for the oxidation of a bioinspired Cu(I) complex mimicking the active sites of LPMOs using hydrogen peroxide was investigated by Ning Cao and Ainara Nova, together with Abril Castro, David Balcells and Unni Olsbye. In these enzymes, hydrogen peroxide reacts with a Cu(I) center to eventually generate a highly reactive Cu(II)-oxyl species, which is capable of effectively oxidizing C(sp³)-H bonds. The N,N,N tri-dentate Cu complex, containing a histidine brace, was synthesized and installed into UiO-67 MOFs [1], see Figure 1.

However, this Cu-MOF did not behave as expected; instead of oxidizing the substrate, the ligand was oxidized, and the Cu was released into the solution. To rationalize these results, static den-

sity functional theory (DFT) calculations alongside ab initio molecular dynamics (AIMD) simulations were employed to elucidate the reaction mechanism [2]. The results indicate that the flexible coordination environment around copper strongly influences the nature of the oxidized species.

To reduce computational cost, the reaction mechanism was modeled using a tridentate Cu complex corresponding to the Cu site within the MOF. Initially, H₂O₂ coordinates to the Cu(I) center, leading to O-O bond cleavage and the formation of a cis Cu(II)-(OH)₂ intermediate. AIMD simulations reveal that this intermediate rapidly isomerizes to a more stable trans configuration. This rearrangement has significant consequences for reactivity: the trans isomer

hinders the hydrogen atom abstraction necessary for forming the Cu(II)-oxyl species, thereby favoring an alternative intramolecular oxidation pathway, specifically, the oxidation of a secondary amine ligand to an imine, which aligns with experimental observations.

The study also explores solvent effects by introducing water molecules and acetonitrile. With one water molecule, the formation of the Cu(II)-oxyl species is concerted, while the presence of two water molecules stabilizes the cis hydroxo arrangement, preventing the trans isomerization. Acetonitrile preferentially binds to the Cu(I) complex, and its coordination also leads to the formation of the cis Cu(II)-(OH)₂ intermediate upon O-O cleavage. Building on the large flexibility of the Cu coordi-

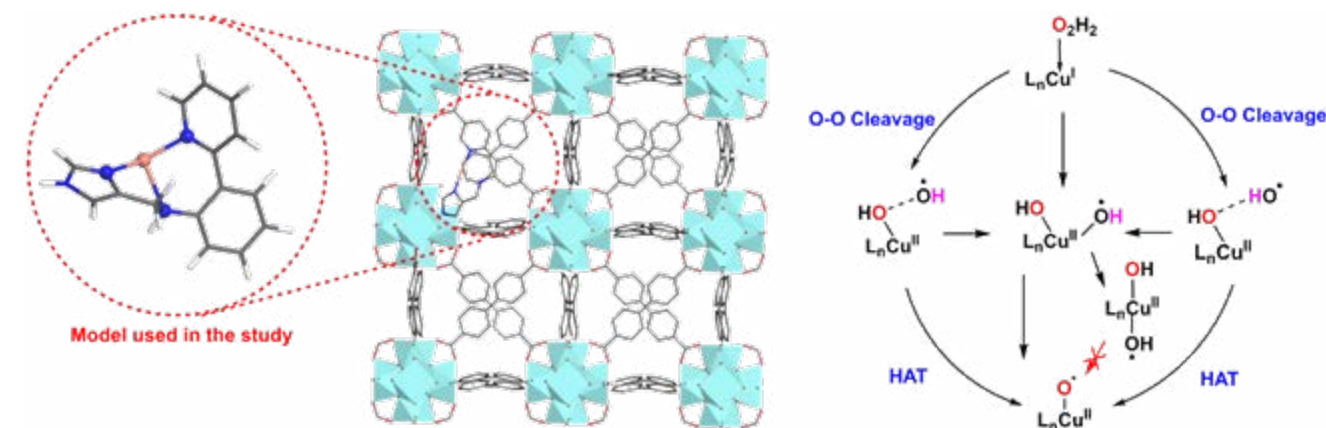


Fig. 1: Schematic representation of the Cu-MOF studied in this work and the resulting reaction mechanism. Illustration: Ning Cao.

nation sphere observed with AIMD, a CREST conformational search was conducted in several reaction intermediates, followed by DFT optimization. This effort uncovered a new intermediate in which the two hydroxo ligands, along with the N_{IM} and N_{MeCN} groups, are arranged trans to each other, while the N_{amine} and N_{py} ligands dissociate from copper. Since copper remains bound solely through the Cu-NIM bond, this species is predicted to be unstable within the MOF, which is consistent with the experimentally observed copper leaching during the reaction.

Overall, the findings of this work underscore that subtle changes in the copper coordination sphere. In particular, the isomerization from cis- to trans-Cu(II)-(OH)₂ can profoundly affect the reaction

pathway by determining whether the reactive Cu(II)-oxyl intermediate forms. This mechanistic insight is crucial for designing more efficient bioinspired copper catalysts for C-H oxidation and offers valuable perspectives on similar processes in natural enzyme systems.

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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.

Previous Almlöf-Gropen Lecturers

2008 Prof. Björn Roos

University of Lund, Sweden
Multiconfigurational quantum chemical methods and heavy element chemistry

2009 Prof. Tom Ziegler

University of Calgary, Canada
Analyzing complex electronic structure calculations on large molecules in simple chemical terms

2010 Prof. Michele Parrinello

ETH Zürich, Switzerland
Through mountains and valleys with metadynamics

2011 Prof. Pekka Pyykkö

University of Helsinki, Finland
Relativity and chemistry: some recent results

2012 Prof. Harry B. Gray

California Institute of Technology, USA
The 21st century solar army

2013 Prof. Henry F. Schaefer

University of Georgia, Athens, USA
From donor-acceptor complexes to Gallium Nitride nanorods

2014 Prof. Leo Radom

University of Sydney, Australia
Adventures in free radical chemistry: a computational approach

2015 Prof. Arie Warshel

University of Southern California, USA
How to model the action of complex biological systems on a molecular level

2016 Prof. Emily Carter

Princeton University, USA
Quantum solutions for a sustainable energy future

2017 Prof. Jack Simons

University of Utah, USA
The wonderful world of molecular anions

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. Clemence 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

Almlöf-Gropen Lecturer 2024

Professor Fernanda Duarte

Professor Fernanda Duarte
University of Oxford, United Kingdom

Exploring chemical reactivity in the age of
automation and machine learning

September 17, 2024, University of Oslo
September 19, 2024, UiT – The Arctic
University of Norway



Prof. Fernanda Duarte, University of Oxford,
United Kingdom.

Fernanda Duarte was born in Santiago, Chile. She completed undergraduate and graduate studies at Pontificia Universidad Católica de Chile (PUC). Her PhD research focused on the formulation of theoretical frameworks for characterising chemical processes employing Density Functional Theory (DFT) and hybrid Quantum Mechanics/Molecular Mechanics (QM/MM) approaches. After graduation, she joined the Department of Cell and Molecular Biology at Uppsala University, Sweden, where she pur-

sued training in biomolecular modelling. In 2015, she moved to the University of Oxford with a Royal Society Newton Fellowship, working in the area of computational organic chemistry. She then joined the School of Chemistry at Edinburgh with a Chancellor's Fellowship before returning to Oxford in 2018 as an Associate Professor in Chemistry. Throughout her career, Fernanda has received various accolades, including the L'Oreal-UNESCO Women in Science award (2009), Pre-doctoral Fulbright scholarship (2010), Marie Curie Career Grant (2015, decline in lieu of the Newton Fellowship), MGMS Frank Blaney Award (2020), OpenEye Outstanding Junior Faculty Award (2021), Harrison-Meldola Memorial Prize (2021), Novartis Early Career Award in Chemistry (2022) and Finalist in Chemical Sciences for the 2024 Blavatnik Awards for Young Scientists in the UK. Her team develops computational methods to understand (bio)chemical reactivity and guide molecular design.

In her Almlöf-Gropen lecture, Duarte discussed one of the *Grand Challenges* in computational chemistry, namely the

efficient and accurate modelling of chemical reactions in the condensed phase. While characterizing reaction energy pathways has become routine, exploring these processes while accounting for solvent and dynamics effects remains a time-consuming and non-systematic endeavour, even for experienced computational chemists. Solvent effects significantly impact reaction rates, selectivity, and the reaction mechanism itself. Duarte presented her team's efforts to address these challenges through integration of automation and machine learning, demonstrating their potential for studying complex reaction mechanisms in the condensed phase. These efforts include the open-source software autoDE, which streamlines the characterisation of reaction pathways, requiring minimal user input and expertise and being compatible with several electronic-structure theory software packages. In addition, she discussed ongoing efforts to model reactions in solution using machine learning potentials (MLPs) as efficient surrogates for traditional *ab initio* methods. Finally, Duarte closed her lecture by discussing current challenges and opportunities within the field.

Almlöf-Gropen

Young Speakers 2024

Tonje Reinholdt Haugen, Hylleraas Centre,
UiT – The Arctic University of Norway



Investigating cyclic peptides interactions with
lipid bilayers using computational methods

Tonje Reinholdt Haugen is a PhD student at UiT – The Arctic University of Norway in Tromsø where she also obtained her master's in science degree (2021). She wrote her master thesis on small cyclic peptides and has continued this work in her PhD. Her focus is now on how these cyclic peptides interact with different lipid bilayers of different complexity and to increase our understanding of how they work as antimicrobial peptides.

Marinella de'Giovannetti,
Hylleraas Centre, University of Oslo



Grignard meets machine learning: cracking Grignard chemistry with neural network potentials

Marinella de'Giovannetti received her bachelor's degree in chemistry from the University of Pavia, Italy, in 2019. She then moved to the University of Copenhagen, Denmark, where she specialised in theoretical and computational Chemistry, with a focus on computational spectroscopy. She graduated with a master's degree in physical chemistry in 2021, and later that year she joined the Hylleraas Centre at the University of Oslo, Norway, for her PhD. Here, she is currently developing neural network potentials to study Grignard systems.

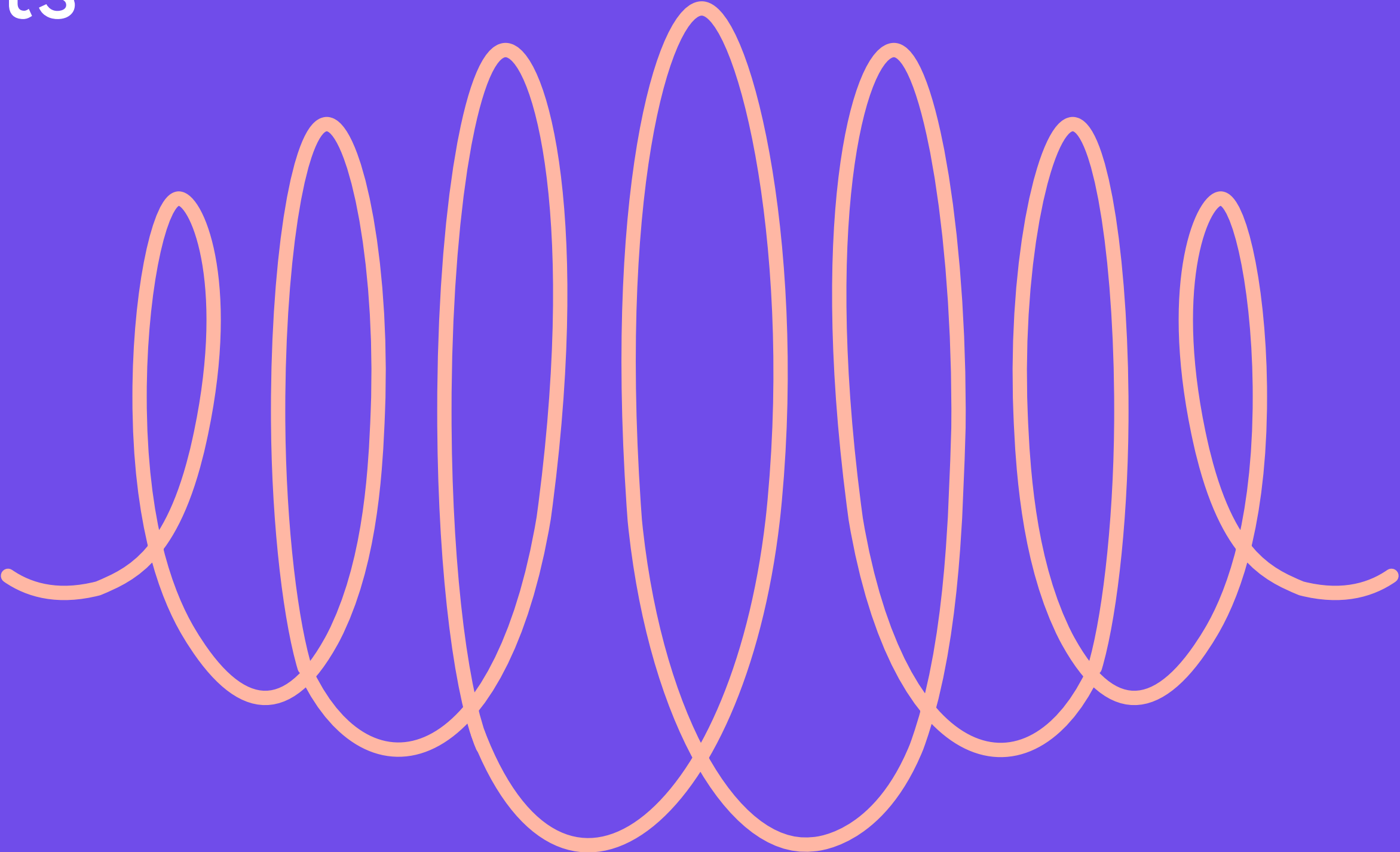


Daniel Schipper introduces Prof. Fernanda Duarte and Marinella de'Giovannetti to virtual reality in the context of molecular simulations at the Hylleraas Centre in Tromsø. Photo: Stig Eide.



Prof. Fernanda Duarte experimenting with virtual reality and molecular simulation during her visit in Tromsø. Photo: Stig Eide.

Meetings and events



Meetings and events



Participants at the 2024 Hylleraas School. Photo: Marco Bortoli.

Hylleraas School

Hotel Hadeland, Gran
January 9-12, 2024

The third edition of the Hylleraas School was held at Hotel Hadeland on January 9-12, 2024. 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 2024 Hylleraas School melded scientific education with social interaction, fostering new collaborations at Hotel Hadeland, with 57 participants. The scientific theme was electron dynamics and optical properties.

The 2024 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 with introductory lectures on spectroscopy and optical properties by Thomas Bondo Pedersen, followed by a lecture on experimental attosecond spectroscopy by Dr. Antoine Camper from the Section for High Energy Physics at the Department of Physics, University of Oslo. The second day had three lectures on response theory and NMR spectroscopy by Magnus Ringholm, Erik Tellgren, and Abril Castro, followed by computational exercises in the afternoon. The third day was dedicated to electron dynamics, with lectures by Simen Kvaal in the morning and computational exercises in the afternoon.

Regarding social activities, there was a festive banquet on Thursday night and "presentation karaoke" organized by the Young Researcher Parliament. In "presentation karaoke," participants are asked to give a five-minute presentation based on slides they have never seen before, followed by a question-and-answer session. 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 2025 edition.

Visit from Talentsenteret

Hylleraas Centre, Oslo
January 17, 2024

Talentsenteret is an initiative for senior high school students by Oslo Vitenstenter. Students who are particularly talented and interested in natural science can apply to participate. As part of that initiative, on January 17 twelve students and three accompanying staff visited the Centre. The visit was coordinated by Cathrine Strøm and planned by Erik Tellgren.

The program included an introductory lecture about quantum chemistry by Trygve Helgaker, smaller lectures and

Talentsenteret, an initiative for talented senior high school students, visited the Hylleraas Centre and got a peak into computational chemistry and experimental chemistry.

computer demonstrations of classical dynamics, quantum dynamics, and molecular orbital theory by Erik Tellgren and Hanan Gharayba. The students were introduced to computational chemistry using both simple, minimalistic programs for model systems as well as

through visualization of molecular orbitals, geometry, and vibrations using advanced software. The latter part benefitted from the Hylleraas Software Platform. In addition, the students visited Mauritz Rydberg for a demonstration of the mass spectrometry lab.



Visit from Talentsenteret on January 17, 2024. Master student Hanan Gharayba from the Hylleraas Centre in Oslo explains Euler's method for simulating classical motion. Photo: Erik Tellgren.

Participants at the Skibotn Hackathon 2024 attending the Alumni Talk of Dr. Hima Bindu Kolli on Zoom from Oslo. Photo: Inga Schmidtke.



Ainara Nova (left) with Aleix Comas-Vives (TU Wien, Austria) and Maren Podewitz (TU Wien, Austria) at the 18th International Congress on Catalysis in Lyon, France. Photo: Aleix Comas-Vives.

Skibotn Hackathon

Skibotn field station
April 22-26, 2024

Organized by Magnus Ringholm, the 2024 Skibotn Hackathon took place between April 22 and April 26 at the Skibotn field station of UiT – The Arctic University of Norway.

On April 22-26, 2024, 29 researchers spent the week Skibotn field station, working on their own projects or in collaboration with others. Most participants tend to come from the Hylleraas Centre itself, but participation is also open to external collaborators of Hylleraas members.

The Skibotn Hackathon offers participants the chance to stay at a relatively secluded location and spend both work and social time with other like-minded people away from many everyday con-

cerns. This year's event included an introduction to competitive programming, a science-oriented bingo game/quiz, and opportunities to explore the natural surroundings.

Session at the 18th International Congress on Catalysis

At the 18th International Congress on Catalysis, a major international event with more than 2200 participants, Ainara Nova co-organized the topical session Computational Approaches at the Atomic Scale of Catalysis – Unifying Concepts to Tackle Dynamics in Computational Catalysis on July 17, 2024.

Lyon Convention
Centre, Lyon, France
July 17, 2024

Ainara Nova, together with Aleix Comas-Vives (TU Wien, Austria), Nuria López (ICIQ, Spain), and Maren Podewitz (TU Wien, Austria), organized a topical session at the 18th International Congress on Catalysis, which had 2250 participants. Chaired by Ainara, the session was entitled “Computational Approach-

es at the Atomic Scale of Catalysis – Unifying Concepts to Tackle Dynamics in Computational Catalysis” and featured six lectures, including one given by Dr. Jordan Rio, Sorbonne University, Paris, France, who visited the Hylleraas Centre in Oslo in 2023 and who will join the Centre in 2025 as a postdoc.



Michele Cascella (left) and Trygve Helgaker (right) presenting at the 2024 Hylleraas Annual Meeting. Photo: Cathrine Strøm.



Dinner at Brasserie Coucou in Oslo. From left: Morten Ledum, Sigbjørn Løland Bore, Henrik Sveinsson, Anders Johansson, Boris Kozinsky, and Henrique Musseli Cezar. Photo: Sigbjørn Løland Bore.

Sigbjørn Løland Bore (left) and Anders Johansson at the Hylleraas Seminar on Friday August 30, 2024. Photo: Thomas Bondo Pedersen.

Hylleraas Annual Meeting

This year's annual meeting was hosted by the Oslo node and attended by 51 members of the Hylleraas Centre. Held at Sanner Hotel in Gran, the meeting was organized by the Young Researchers Parliament (YRP) representatives at UiO, Marinella de'Giovanetti and Oliver Macphail Bohle.

Sanner Hotel, Gran
August 19-21, 2024



Participants at the 2024 Hylleraas Annual Meeting. Photo: Cathrine Strøm.

This year the YRP representatives invited two external speakers. Asbjørge Dyveke Johnsen, research advisor at the University of Oslo) gave a talk on the practical side of grant proposal writing, while Per Magnus Kommandantvold, Special Adviser at the Research Council of Norway, gave an overview of the ERC, MSCA, and FRIPRO calls.

Simen Kvaal gave a very educational talk on the responsible use of generative AI in research, sharing his reflections on AI reliability. Michele Cascella presented a talk on the philosophical problem of knowledge, prompting some very interesting questions and discussions afterwards. Finally, Trygve Helgaker gave a concise account of his career as

a theoretical chemist, including valuable advice and tips for the young researchers in the audience.

It has become customary for the PhD and masters students attending the meeting to give a 5-minute presentation about their research project. While all speakers did a stellar job, PhD candidate Hannes Kneiding won the prize for the best presentation, with master student Hanan Gharayba and PhD candidates Aurore Denjean and Simon Elias Schrader in the shared second place.

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

Hylleraas Centre, Oslo
August 26-30, 2024

Organized by Sigbjørn Løland Bore, the second Young CAS meeting took place at the Hylleraas Centre with the primary objective of implementing the concepts discussed during the initial meeting. The key focus areas of included:

- Fine-tuning machine learning potentials
- Efficiently running ORCA 6.0 for dataset generation
- Developing machine learning algorithms for ice geometry generation

As part of his Young CAS project *Can ice be described from first principles?*, Sigbjørn Løland Bore organized a week-long workshop at the premises of the Hylleraas Centre in Oslo.

The working group was composed by Henrique Musseli Cezar and Morten Ledum from the Hylleraas Centre, and Anders Johansson from Harvard University, USA. Professor Boris Kozinsky, the PhD supervisor of Anders Johansson at Harvard University, made a surprise one-day visit. Professor Kozinsky delivered an insightful talk to a packed Hylleraas Lecture Room in Oslo, highlighting the work of his research group in the application of machine learning to computational chemistry. His presentation emphasized the integration

of machine learning with Density Functional Theory (DFT) and the group's advancements in developing machine learning potentials. The first day concluded with a delightful dinner at Brasserie Coucou. On Friday, Anders Johansson gave the Hylleraas Seminar of the week.

Computational chemistry across scales and disciplines: celebrating the 60th birthday of Ursula Röthlisberger



Logo of the CECAM workshop co-organized by Michele Cascella in honor of Prof. Ursula Röthlisberger, member of the Hylleraas Scientific Advisory Committee 2017-2023. Credit: CECAM.



Group work during the KUPP3 workshop on October 29. Photo: Frithjof Bringager.



Trygve Helgaker and Olaug Kristine Bringager at work during a break at the KUPP3 workshop on October 29. Photo: Frithjof Bringager.



Panel discussion closing the KUPP3 workshop on October 29. Photo: Frithjof Bringager.

CECAM workshop: Computational chemistry across scales and disciplines

CECAM Headquarters,
EPFL, Lausanne,
Switzerland
October 1–3, 2024

To celebrate the 60th birthday of Prof. Ursula Röthlisberger, EPFL, Switzerland, the workshop *Computational chemistry across scales and disciplines* was organized under the auspices of the CECAM network.

Co-organized by Michele Cascella, the three-day event – one of the CECAM Flagship Workshops of 2024 – was attended by 55 scientists. The workshop featured lectures by world-leading researchers in the field of ab-initio and multiscale modelling applied to a large field of disciplines, including chemistry, materials science, condensed-matter physics, biology, and medicine. Several

of the speakers were alumni of Ursula Röthlisberger with successful careers in science.

KUPP3 – Workshop on career development for young researchers

Norwegian Academy
of Science and
Letters, Oslo
October 29, 2024

More than 60 people from the Centres of Excellence at the University of Oslo gathered on October 29 at the Norwegian Academy of Science and Letters in Oslo. This was the third workshop on career development, KUPP3, organized by the Hylleraas Centre.

KUPP3 was organized by Trygve Helgaker, Thomas Bondo Pedersen, Olaug Kristine Bringager, and Jan Ingar Johnsen from the Hylleraas Centre with assistance from Ragnhild Eskeland from CanCell, Ragnhild Brøvig from RITMO, and Else-Marie Lingaas from the central administration at the University of Oslo.

Transfer of knowledge and sharing experiences were important components of the workshop, which had a balanced mixture of lectures and group work within and across the centres. A major component of KUPP3 was outgoing career support, which includes identification of transferable skills. Based on the work-

shop, a report will be worked out and published on the Hylleraas web page.

In addition to the organizers, Manuela Leal Nader, Luca Frediani, David Balcells, and Jan Ingar Johnsen participated from the Hylleraas Centre.



Trygve Helgaker (left) chairing a session at the Royal Swedish Academy of Sciences on November 7, here directing the discussions following the talk of Prof. Andreas Savin (right). Photo: Screenshot from the video published at the YouTube channel of the Royal Swedish Academy of Sciences.

DFT in chemistry – dispute at inception and rise to prominence

Royal Swedish Academy of Sciences,
Stockholm, Sweden
November 7-8, 2024

On November 7-8, 2024, the seminar *DFT in Chemistry – Dispute at Inception and Rise to Prominence* was held at the Royal Swedish Academy of Sciences, with many prominent speakers. The meeting was organized by Sture Nordholm and Trygve Helgaker, both members of the Swedish Academy.

Today, Kohn-Sham density-functional theory (DFT) is the workhorse of computational electronic-structure theory. However, for a long time, the development of modern DFT within the field of physics was met with skepticism by most chemists, who preferred the rigor of wave-function methods in quantum mechanics. By the 1990s, however, the approximations within DFT had improved sufficiently to capture the interest of leading quantum chemists, sparking a period of rapid development and widespread application of DFT in chemical research. The significance of this

shift was underscored in 1998 when the Nobel Prize in Chemistry was awarded to Walter Kohn and John Pople, with the incorporation of DFT into chemistry cited as a key motivation.

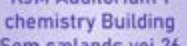
The purpose of the symposium, after an additional 25 years of DFT's evolution, was to reflect on this critical development. The speakers addressed the limitations that initially hindered DFT's acceptance, the innovative approximations that eventually garnered the respect of the chemistry community, and the key figures who drove these breakthroughs.

The list of speakers consisted of sixteen leading international experts on DFT, all of whom were either present at the theory's challenging inception or contributed to its rise to prominence. In order of appearance: Evert Jan Baerends, Dennis Salahub, Weitao Yang, Robert O. Jones, Peter Gill, Andreas Savin, John Perdew, Axel Becke, Kieron Burke, Trygve Helgaker, Erin Johnson, Stefan Grimme, David Tozer, Martin Head-Gordon, Paola Gori-Giorgi, and Gustavo Scuseria.

NordCO₂ Symposium on Sustainable Chemistry
Friday December 13th 2024, 09:00-16:00 CET

Session I chair: Annette Bayer 09:00 CET	 Facilitating Nordic research collaboration for a sustainable future Siri Jorgensen Bjarnar, Chief Operating Officer, NordForsk  Chemical Technologies for Recycling Plastics Designed to Last Troels Skrydstrup, Professor, Aarhus University
Session II chair: Sascha Ott 10:40 CET	 Recycling noble metals Timo Repo, Professor Helsinki University  Towards stereoselective carboxylation with CO ₂ Annette Bayer, Professor, UiT The Arctic University of Norway
Session III chair: Troels Skrydstrup 14:00 CET	 Understanding redox catalysis in metal-organic frameworks Sascha Ott, Professor, Uppsala University  From CO ₂ to methanol: What have we learnt Ainara Nova, Senior Researcher, University of Oslo



Register here! 

Poster advertising the symposium on December 13, 2024.

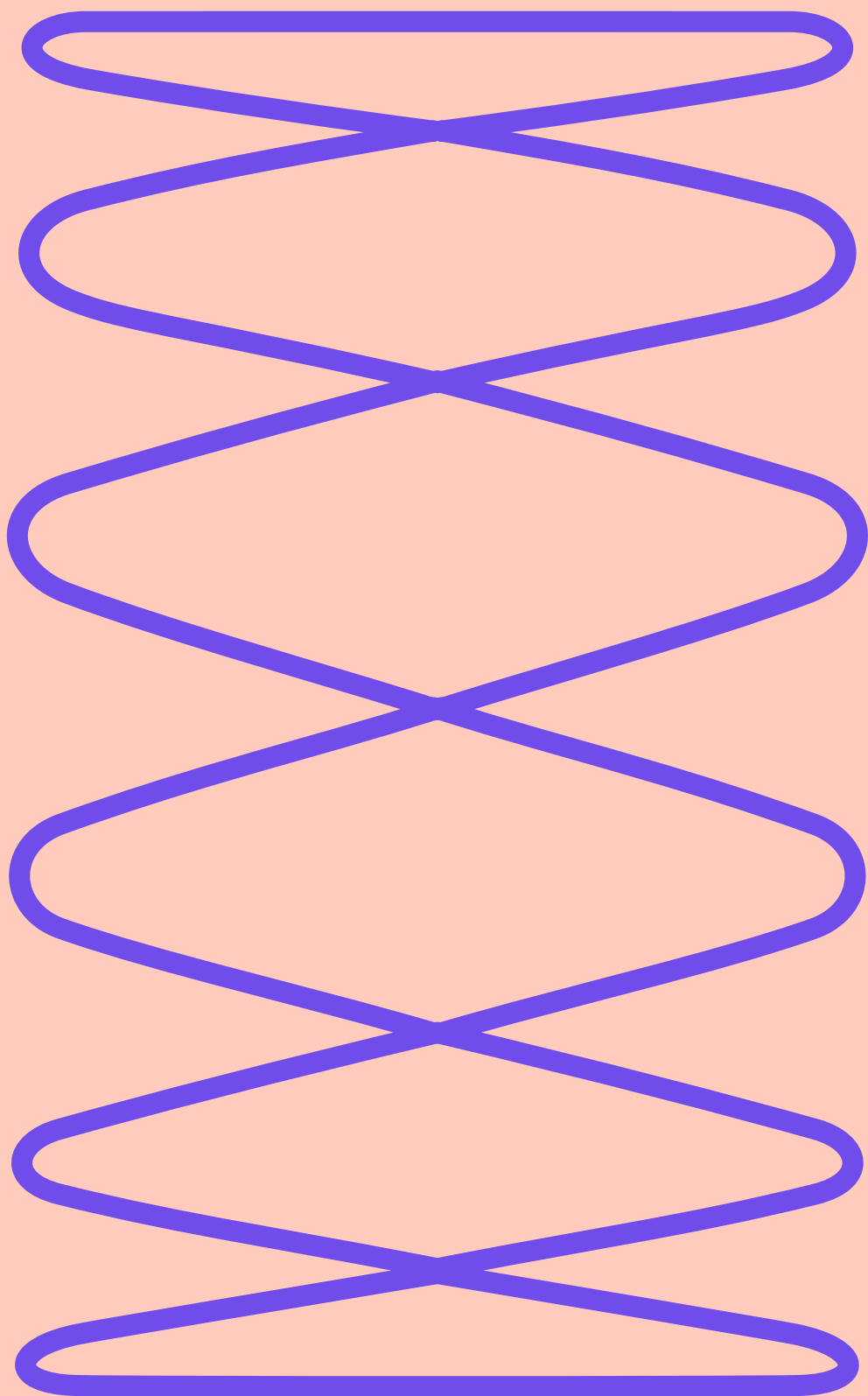
NordCO₂ symposium on sustainable chemistry

Department of Chemistry,
University of Oslo
December 13, 2024

Marking the end of the Nordforsk-funded project *Nordic Consortium for CO₂ Conversion (NordCO₂)*, Ainara Nova organized a one-day symposium at the Department of Chemistry, University of Oslo.

The NordCO₂ symposium on sustainable chemistry was organized by Ainara Nova and held at the Department of Chemistry, University of Oslo, on December 13, 2024. The symposium was free of charge and open to everyone interested, an opportunity exploited by many Hylleraas members and scientists in Oslo. At the symposium, leading scientists from the NordCO₂ consortium presented their research, discussing sustainable strategies explored in the Nordic region for plastic

and noble metals recycling, stereoselective carboxylation reactions using CO₂, redox catalysis in metal-organic frameworks, and the CO₂ conversion to methanol.



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. Two seminars were scheduled in 2024, one in April by Dr. Hima Bindu Kolli and another in November 2024 which, unfortunately, had to be cancelled at the last minute.

Alumni talks

Dr. Hima Bindu Kolli

Researcher, Rutherford Appleton Laboratory, UK

Multiscale Simulation Scattering Intensity Calculator (MuSSIC): Validation and Application to Soft-Matter Systems

Online seminar from the Hylleraas Centre, University of Oslo. April 26, 2024



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. Two seminars were scheduled in 2024, one in April by Dr. Hima Bindu Kolli and another in November 2024 which, unfortunately, had to be cancelled at the last minute.

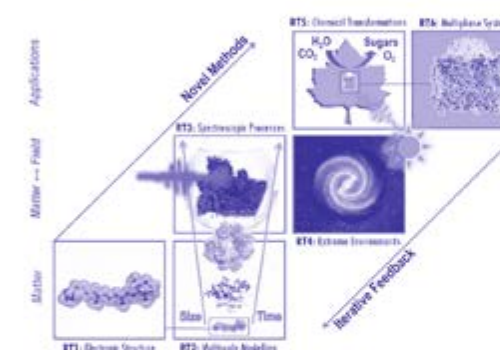
On Wednesday April 26, Hylleraas Alumnus Dr. Hima Bindu Kolli visited the Hylleraas Centre in Oslo and delivered

her seminar on *Multiscale Simulation Scattering Intensity Calculator (MuSSIC): Validation and Application to Soft-Matter Systems*, commenting on her path from an MSCA postdoctoral fellowship at the Hylleraas Centre in Oslo to her current position. During her time in Oslo, she worked on the development of hybrid particle-field molecular dynamics under the supervision of Michele Cascella.

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 molekylær 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 størrelsskalaer, 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 tidssavhengige Schrödingerlikningen for molekyler på datamaskinen, utforske kvante- og grenseland 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

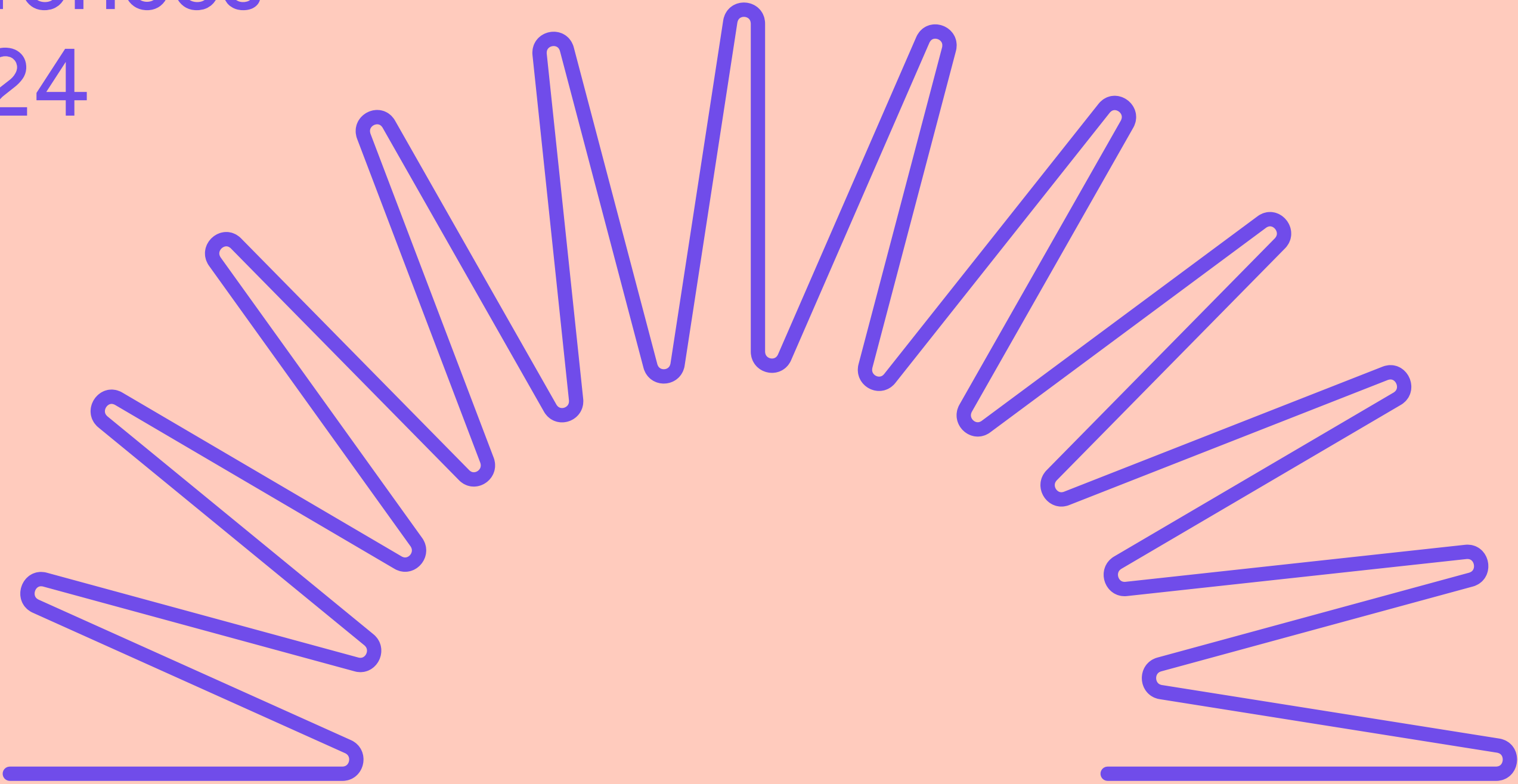
Sammen med **Abril Castro** vil du lære hvordan du simulerer strukturelle, elektroniske og spektroskopiske egenskaper. Mulige emner er modellering av NMR-egenskaper for å forutsi og tolke eksperimenter, analyse av kjemiske bindinger i løsnings- og faststoffsystemer, og studier av molekyler som inneholder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



← Besøk vår nettside



PhD Defences 2024



PhD Defences 2024

Education and training of the next generation of scientists is a key goal of the Hylleraas Centre. During 2024, seven young researchers defended their PhD theses at the Hylleraas Centre.



Candidate: Mahika Luthra

University: University of Oslo
Date: January 26, 2024
Thesis: *Computational Study on the Electrochemical Reduction of CO₂ using Transition Metal catalysts with Pendant Amines*
Trial Lecture: *Transition state theory and its limitations in light of experiments and calculations*
Supervisors: Research Prof. Ainara Nova, University of Oslo
 Research Prof. David Balcells, University of Oslo
 Prof. Michele Cascella, University of Oslo
 Research and Development Director Espen Taarning, Topsoe A/S, Denmark
Committee: Prof. Feliu Maseras, ICIQ, Spain
 Assistant Prof. Maren Podewitz, TU Wien, Austria
 Prof. Truls Norby, University of Oslo
Chair: Prof. Harald Walderhaug, University of Oslo
Format: Physical



Candidate: Ryan Scott Wilkins

University: UiT – The Arctic University of Norway
Date: February 26, 2024
Thesis: *Mechanisms of enzyme adaptation to extreme environments: The rational design of a thermophilic chorismate mutase*
Trial Lecture: *Protein engineering and design: from early beginnings to now*
Supervisors: Prof. Bjørn Olav Brandsdal, UiT – The Arctic University of Norway
 Project Manager Geir Villy Isaksen, Helse Nord IKT
 Postdoc Bjarne Aarmo Lund, UiT – The Arctic University of Norway
Committee: Prof. Fahmi Himo, Stockholm University, Sweden
 Prof. Ute Krengel, University of Oslo
 Prof. Luca Frediani, UiT – The Arctic University of Norway
Chair: Prof. John Sigurd Mjøen Svendsen, UiT – The Arctic University of Norway
Format: Physical



Candidate: Magnar Bjørgve

University: UiT – The Arctic University of Norway
Date: April 4, 2024
Thesis: *Unleashing the VAMPyR. A Python Journey into the Realm of Multiwavelets and Quantum Chemistry*
Trial Lecture: *The roles of theory and simulation in chemical discovery and design*
Supervisors: Prof. Luca Frediani, UiT – The Arctic University of Norway
 Researcher Stig Rune Jensen, UiT – The Arctic University of Norway
 Prof. Tor Flå, UiT – The Arctic University of Norway
Committee: Prof. Robert Harrison, Stony Brooke University, USA
 Assoc. Prof. Sarai Dery Folkestad, Norwegian University of Science and Technology, Researcher Bin Gao, UiT – The Arctic University of Norway
Chair: Prof. Peik Haugen, UiT – The Arctic University of Norway
Format: Physical



Candidate: Lin Xue

University: University of Oslo
Date: April 19, 2024
Thesis: *Communication and interaction among surface-adhered membranous protocells*
Trial Lecture: *Necessary molecules for protocell formation in the prebiotic era, like water, (phospho-)lipids, RNA, etc: What do we know about their origin?*
Supervisors: Prof. Michele Cascella, University of Oslo
 Prof. Reidar Lund, University of Oslo
Committee: Prof. Marie Skepö, Lund University, Sweden
 Prof. Marit Sletmoen, Inland University of Applied Sciences
 Prof. Harald Walderhaug, University of Oslo
Chair: Prof. Ola Nilsen, University of Oslo
Format: Physical



Candidate: Hannes Kneiding

University: University of Oslo
Date: September 27, 2024
Thesis: *Complex Learning – Machine learning approaches for transition metal complexes*
Trial Lecture: *Large language models for chemistry – Passing fad or transformative tool?*
Supervisors: Research Prof. David Balcells, University of Oslo
 Prof. Thomas Bondo Pedersen, University of Oslo
 Prof. Riccardo De Bin, University of Oslo
Committee: Prof. Kim Jelfs, Imperial College London, UK
 Prof. Kjell Jorner, ETH Zürich, Switzerland
 Prof. Reidar Lund, University of Oslo
Chair: Prof. Truls Norby, University of Oslo
Format: Physical



Hannes Kneiding with supervisors and committee members after his successful PhD defense on September 27, 2024, in Oslo. From left: Riccardo De Bin, Reidar Lund, Kjell Jorner, Kim Jelfs, Hannes Kneiding, David Balcells, Thomas Bondo Pedersen, and Truls Norby. Photo: Marco Bortoli.



Candidate: Sahil Gahlawat

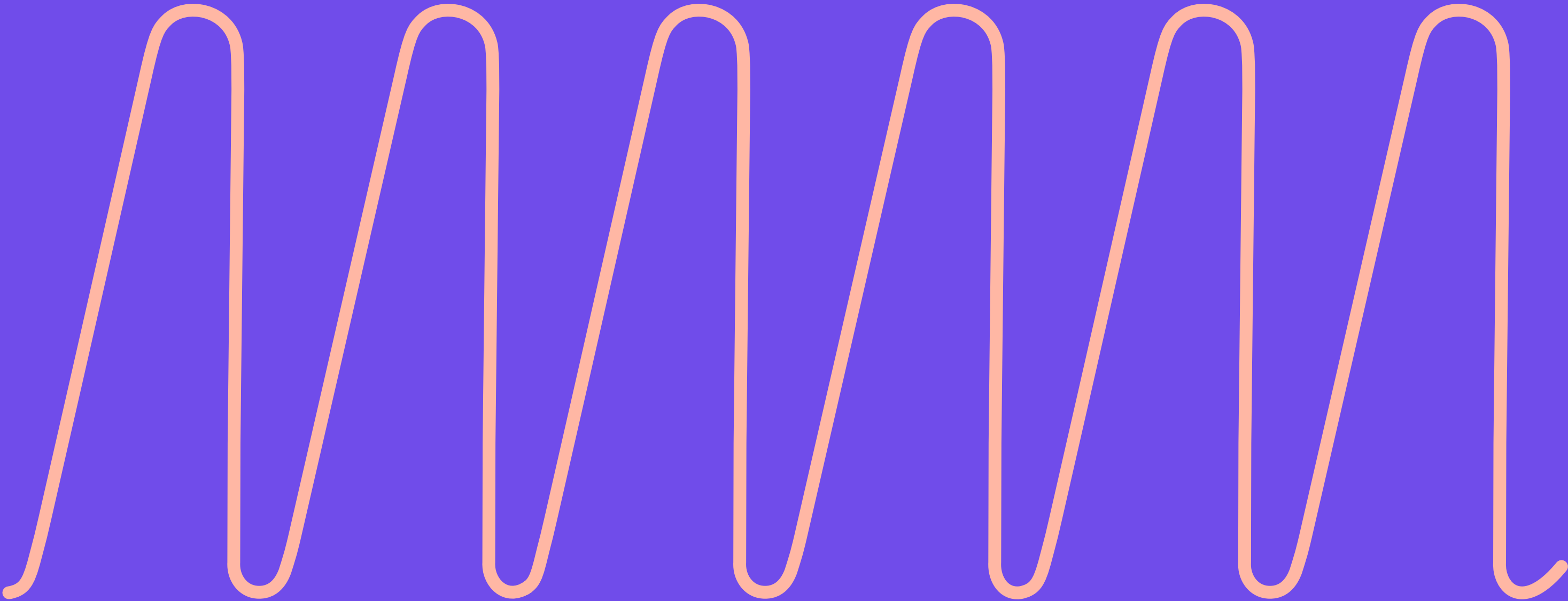
University: UiT – The Arctic University of Norway
Date: October 25, 2024
Thesis: *Computational Approach to Molecular Reactivity of Transition Metal Complexes*
Trial Lecture: *In Silico Catalyst Design: History, State of the Art, and Perspectives*
Supervisors: Prof. Kathrin H. Hopmann, UiT – The Arctic University of Norway
 Researcher Abril Castro, University of Oslo
 Principal Scientist Per-Ola Norrby, AstraZenca
Committee: Prof. Vidar Remi Jensen, University of Bergen
 Researcher Cristina Trujillo, University of Manchester, UK
 Researcher Bin Gao, UiT – The Arctic University of Norway
Chair: Pro-Dean, Prof. Cordian Riener, UiT – The Arctic University of Norway
Format: Physical



Candidate: Marinella de'Giovanetti

University: University of Oslo
Date: December 6, 2024
Thesis: *The multifaceted nature of lithium derivatives, and its implications for Grignard chemistry – A computational study from first-principles to machine learning*
Trial Lecture: *How are artificial intelligence methods currently applied in chemistry and how will they change research in this domain?*
Supervisors: Prof. Michele Cascella, University of Oslo
 Prof. Odile Eisenstein, University of Montpellier, France
 Research Prof. Ainara Nova, University of Oslo
Committee: Prof. Hélène Gérard, Sorbonne Université, France
 Prof. Evert Jan Meijer, University of Amsterdam, The Netherlands
 Assoc. Prof. Håvard Jenssen, University of Oslo
Chair: Prof. Harald Walderhaug, University of Oslo
Format: Physical

Visits and mobility



Interview
with visiting researcher:

Gabriela Garcia

Gabriela Garcia is a PhD candidate at the University of São Paulo in Brazil. From December 2023 to November 2024, she visited the Hylleraas Centre in Oslo to work with Ainara Nova on a C-C coupling reaction using an Mn electrocatalyst.



Gabriela Garcia's PhD research focuses on the investigation of CO₂ reduction mechanisms, particularly on homogeneous electrochemical systems. She is a member of Prof. Ataulpa Braga's research group, which applies theoretical chemistry methods to study catalytic processes.

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

My main supervisor in Brazil worked together with Ainara Nova some years ago, so they work in correlated areas. Yet, our laboratory had only recently initiated its first project on electrochemistry, and we lacked experience in this field. While studying the subject, I came across her work, which motivated me to go on a research visit at Hylleraas.

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

My research developed a lot after learning electrochemical theoretical treatments from Ainara's expertise. It was a great opportunity given the limited number of specialists in this area. The members of the theoretical catalysis group are very supportive, so interacting with them allowed me to improve my skills. Additionally, the center's computational resources and office structure led to a much faster progress of the work.

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

During my one-year stay in Norway, I had the chance to explore a lot of the country and fell in love with its stunning

landscapes. Thanks to events organized by the Hylleraas Centre, I also visited Tromsø and Oslo's surroundings. I particularly loved Oslo's outdoor lifestyle – it's incredibly accessible due to the city's structure and the culture of its residents. I arrived in winter, which was initially challenging since I had never seen snow before. However, I quickly adapted and discovered fun activities that were new to me, like skiing and witnessing the northern lights. And as summer approaches, we are allowed to engage in many other activities, like hiking into the woods, camping, cycling and enjoying the beaches and islands.



Interview
with visiting researcher:

Luis Miguel Varela Cabo

Dr. Luis Miguel Varela Cabo is a professor of condensed matter physics at the Department of Particle Physics, University of Santiago de Compostela, Spain. He visited the Hylleraas Centre in Tromsø for a week in October 2024, establishing new collaborations with Luca Frediani on modelling interfaces between materials.



Prof. Luis Miguel Varela Cabo from the University of Santiago de Compostela, Spain, during his visit at the Hylleraas Centre in Tromsø.

Hylleraas Centre for Quantum Molecular Sciences

Luis Miguel Varela (Lugo, 1972) graduated in Physics at the University of Santiago in 1995 and in Law at the Open University (UNED) in 2000. He got his PhD in Physics (with Honors) from the University of Santiago de Compostela, where he is currently full professor in its department of Particle Physics (Condensed Matter division). His teaching has focused on thermodynamics, statistical mechanics, and statistical data analysis, as well as on Econophysics and on the thermodynamics of Renewable Energies. His research interests focus on the statistical mechanics of complex systems, especially complex charged fluids, and more specifically on ionic liquids, and on complex networks. He has also made contributions in the field of thermal energy storage and thermal fluids. He is the author or co-author of more than 160 articles, chapters, and monographs in these fields, and more than 120 conference communications,

having directed 17 doctoral theses and more than forty graduate and master's theses, and coordinated regional, national, and European projects, as well as research contracts with industries and with the Public Administration. In addition, he is the inventor of several patents in the field of energy harvesting devices and materials for energy applications. He has been Dean of the Faculty of Physics at the University of Santiago de Compostela from 2010 to 2018 and has coordinated its Master's in Physics and Master's in Renewable Energies and Energy Sustainability programs at USC, as well as its Doctoral program in Renewable Energies and Energy Sustainability.

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

My major interest was to get in touch with the Theoretical and Computational Chemistry Group of prof. Frediani, whose activity in the field of computational modelling of solvation and metal-ligand interactions I was previously aware of by the literature, and which are very well aligned with the theoretical research we are currently doing in my Nanomaterials, Photonics and Soft Matter group at USC in ionic liquids for energy applications. I found that some aspects of the recent research of Prof. Frediani's group could be of much interest for our coming research in the formation and composition of the solid electrolyte interface at the electrolyte-electrode interface of ionic-liquid based devices, and I asked for a visit. Of course, the well-known international reputation of the Hylleraas center, for Quantum Chemistry was also a major component of my choice.

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

The visit to the centre and to the city of Tromsø was truly a great experience. I was very well received not only by Luca and his team, but also by Stig Eide, a very pleasant member of staff with whom I had very pleasant chats with a cup of tea. As for the city I must say that it was surprising to find such a large bunch of interesting places to visit including museums like the Polar Museum, and the Arctic cathedral, as well as its livable and warm atmosphere. Moreover, for a Southerner it is always amazing to see the magnificence of the breathtaking polar landscapes of its surroundings and its Northern lights (I was lucky), and to bathe in the frozen waters of the city port sauna facilities. I had a memorable time, undoubtedly, and I am looking forward to go back.

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

During the visit I had great scientific discussions with Luca Frediani and members of his group. Specifically, we discussed a toy computational framework for ionizing molecules at interfaces in inhomogeneous dielectric media, agreeing to develop further collaborative research to upgrade the model to describe redox processes of ionic liquids in contact with electrified solid electrodes. These computational efforts for modelling ionized molecules at atomistic interfaces are really promising to advance in the description of SEI formation in battery cells, which is currently, and will be in the future, an important part of our research at USC.

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

I confirmed once more my previous opinions (based on previous visits to Oslo) that the Norwegian is an ordered, community-based society with a slow but highly efficient way of living. People may seem cold on a first approach, but they very soon prove to be very friendly, collaborative people with high standards of living. I think I could very easily get accustomed to living there, specifically to Tromsø, even when getting accustomed to the long winter Arctic night -with all its amazing beauty- would be challenging for a Southerner like me!

Incoming Visits

There were in total 25 visits and 24 unique visitors to the Hylleraas Centre in 2024.

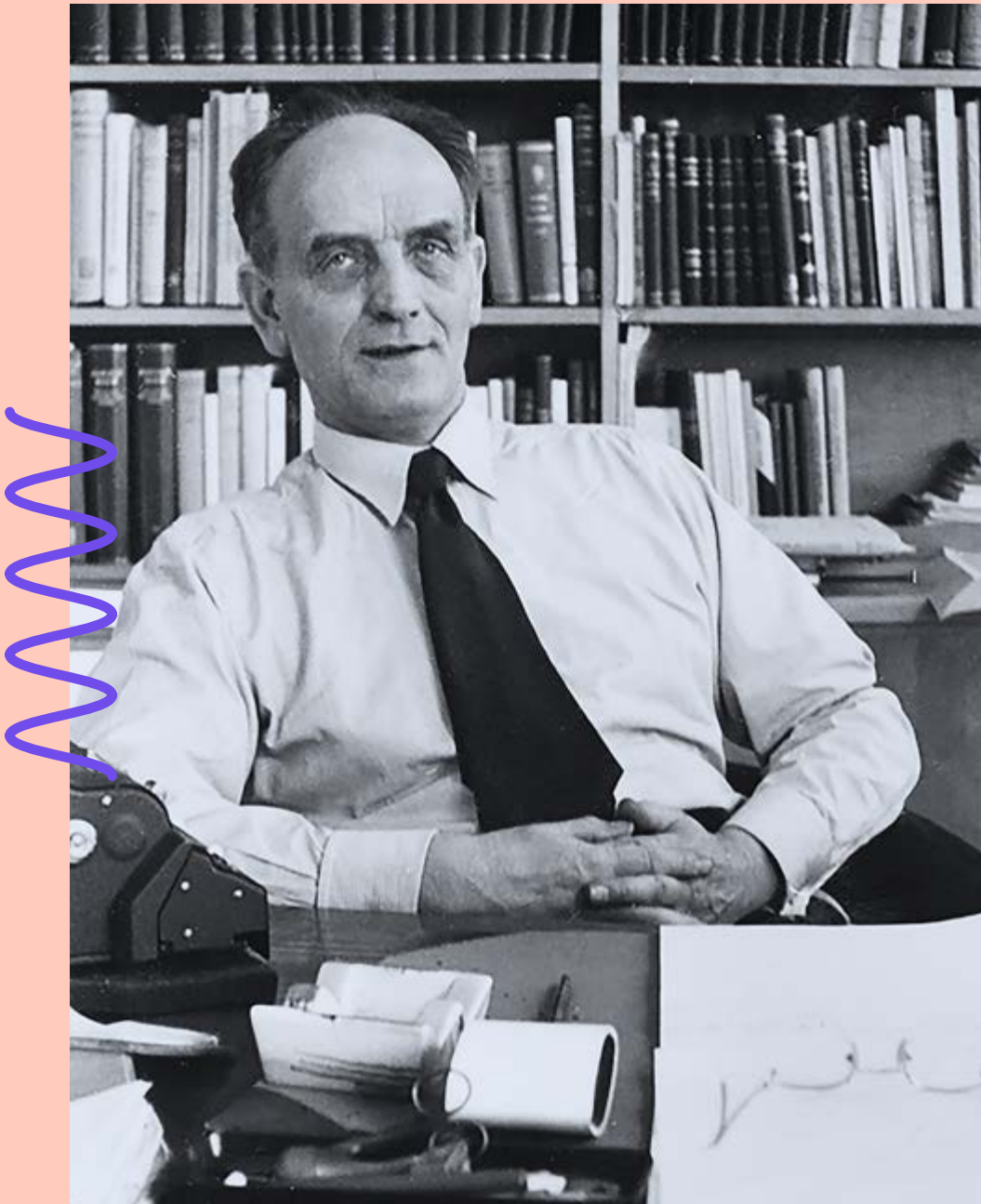
Visitors to Oslo

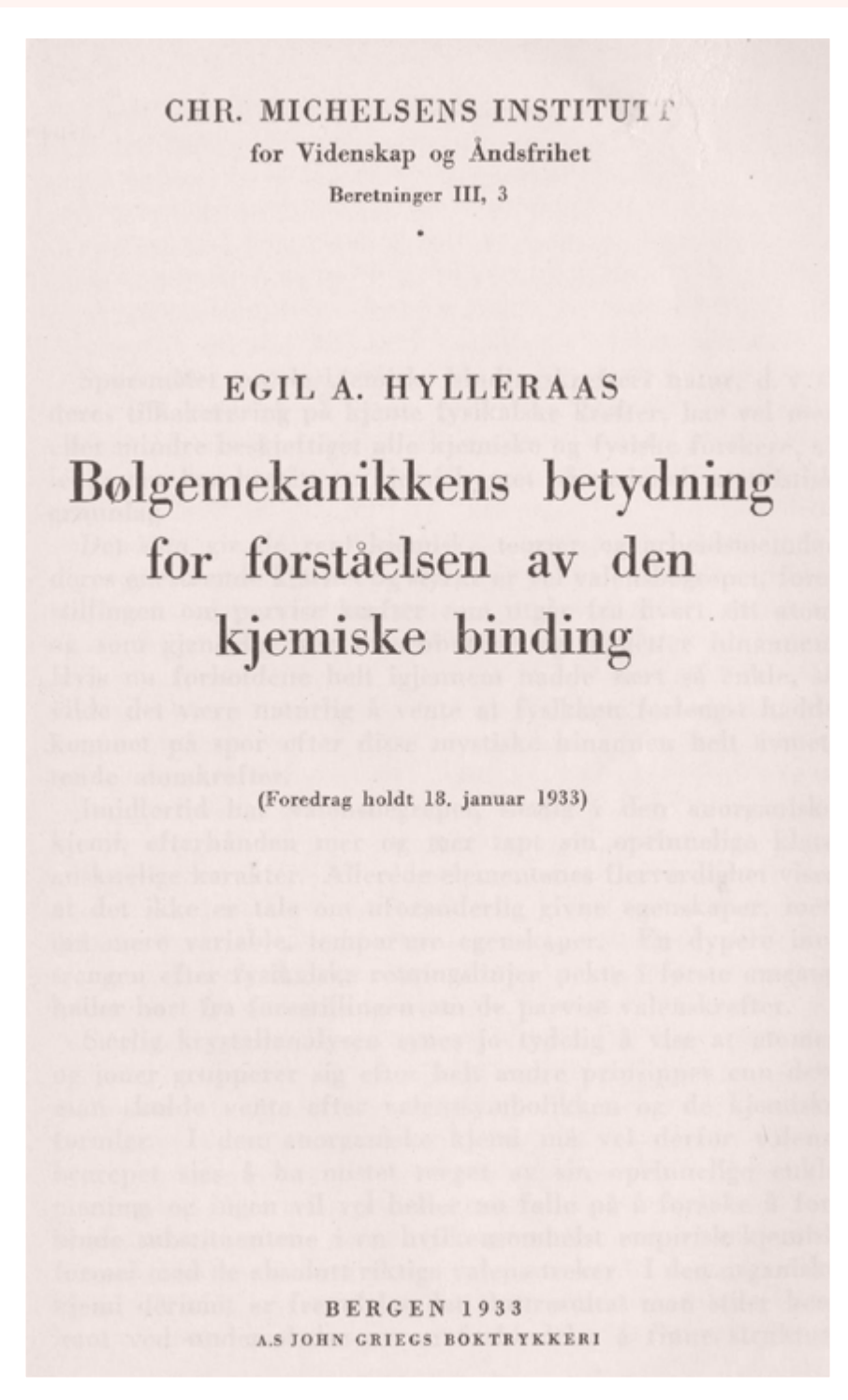
MSc Gabriela Garcia	University of São Paulo, Brazil	Jan 1 – Nov 1
Assoc Prof Chao Zhang	Uppsala University, Sweden	Feb 15 – Feb 17
MSc Jordi Buils	Institute of Chemical Research of Catalonia, Spain	Feb 26 – May 27
Prof Ludwik Adamowicz	University of Arizona, USA	Mar 1 – Jun 30
MSc Judit Gálvez	University of Girona, Spain	Mar 1 – May 31
MSc Ronghui Lu	Aarhus University, Denmark	Mar 5 – May 31
MSc Joel Ormala	Finland	Mar 6 – Dec 31
Assoc Prof Riccardo Capelli	University of Milan, Italy	Mar 13 – Mar 16
MSc Gonzalo Darío Nuñez	University Rovira iVirgili, Spain	Apr 3 – Jun 28
Dr Hima Bindu Kolli	Rutherford Appleton Lab, UK	Apr 25 – Apr 25
Assoc Prof Ivan Rivalta	University of Bologna, Italy	May 29 – May 31
Prof Rinaldo Poli	CNRS Toulouse, France	Jun 16 – Jun 19
MSc Alejandra Pita	University of Sevilla, Spain	Aug 12 – Nov 12
Dr Elisa Rebolini	Institut Laue-Langevin, France	Aug 23 – Aug 27
Prof Fernanda Duarte	University of Oxford, UK	Sep 16 – Sep 18
MSc Jonas Elenius Skovly Mikkelsen	Aarhus University, Denmark	Oct 1 – Dec 31
Dr Mauricio Portiolli Franco	University of Campinas, Brazil	Oct 1 – Dec 31
MSc Sophia Burger	University of Mainz, Germany	Oct 27 – Nov 26
MSc Vinicius Firmino dos Santos	University of São Paulo, Brazil	Nov 21 – Dec 31

Visitors to Tromsø

BSc Niklas Göllmann	University of Münster, Germany	Mar 3 – July 6
MSc Moritz Gubler	University of Basel, Switzerland	Apr 5 – May 3
MSc Josefine Hvarregaard Andersen	KTH Stockholm, Sweden	Jun 4 – Jun 6
Prof Fernanda Duarte	University of Oxford, UK	Sep 18 – Sep 20
MSc Klaus Schleich	Goethe University, Frankfurt, Germany	Sep 23 – Dec 22
Prof Luis Miguel Varela Cabo	University of Santiago de Compostela, Spain	Oct 26 – Oct 31

Egil A. Hylleraas





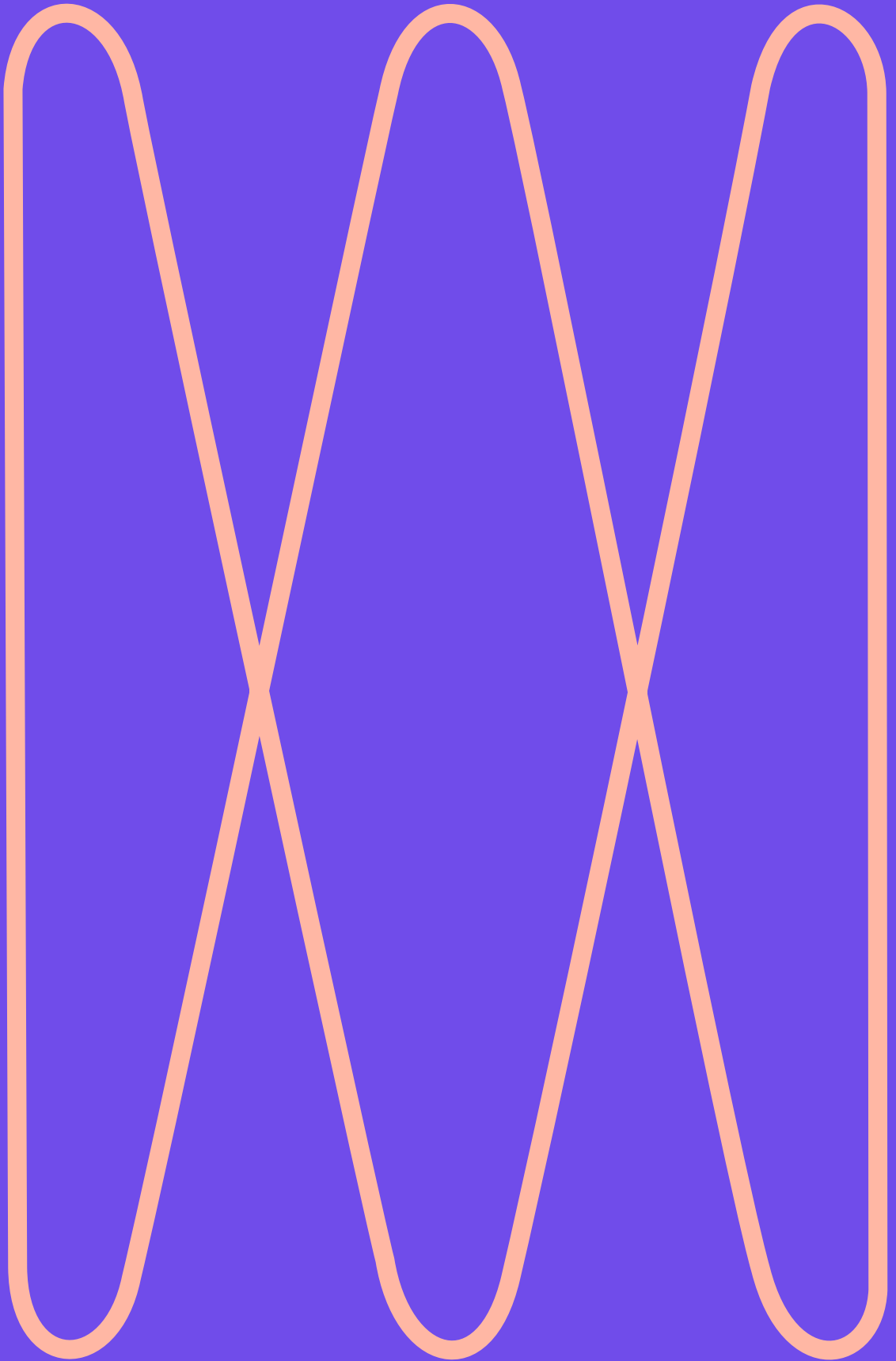
Egil A. Hylleraas

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, LiH (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 nu foreligger ganske vidtrekkende muligheter for å bygge op 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)



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 2024. Progress in these projects will in the future be reported as part of the activities of the research themes in the coming years.

CLIMB: Complex lipid membranes for science and technology

Starting in March 2025, CLIMB (Complex Lipid Membranes for science and technology) will be a doctoral network funded by the EU Horizon Europe Framework. The programme will involve leading European lipid-research laboratories with strong complementarity in expertise and training capabilities.

Prof. Michele Cascella (UiO)
Prof. Reidar Lund (UiO)

EU Horizon Europe – Marie Skłodowska
Curie Doctoral Network
2025–2029

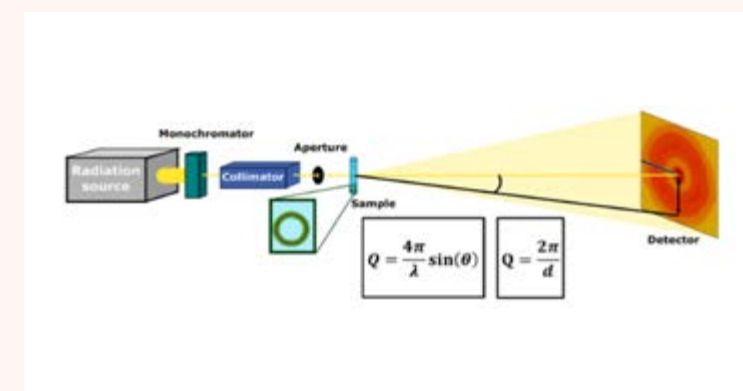
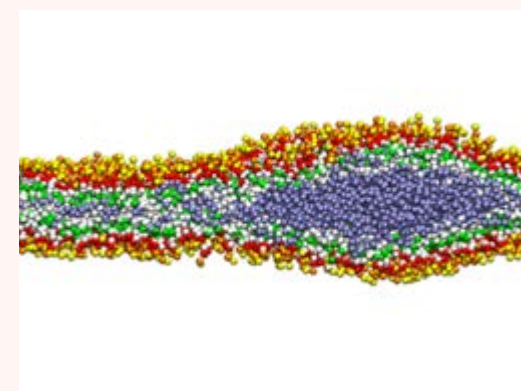


Prof. Michele Cascella



Prof. Reidar Lund

«Development and characterization of novel lipid mixtures including natural extracts and novel protective polymer-based coatings»



CLIMB will focus on the exploration of structural properties and of membrane driven interactions, that are key to the development of complex lipid-based nanostructures that mimic the cellular environment and function as high-performance sustainable materials.

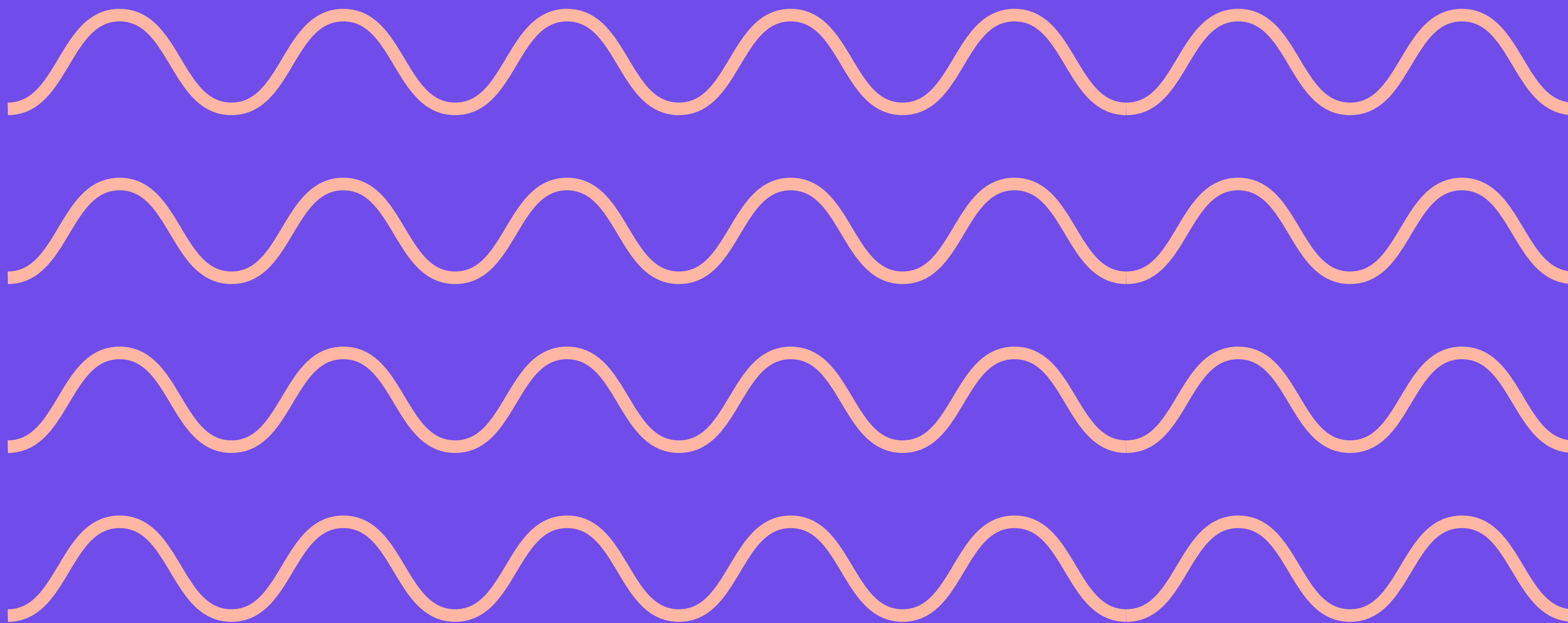
CLIMB will focus on the development and characterization of novel lipid mixtures including natural extracts and novel protective polymer-based coatings. The UiO node of CLIMB is coordinated by Prof. Reidar Lund together with Prof. Michele Cascella. They will provide expertise for:

- time resolved small angle X-ray/ neutron scattering techniques for the investigation of kinetic processes and interactions in lipid vesicles,
- computational multi-scale modeling and simulations of self-assembly dynamics, integrating all-atom and coarse-grained resolutions with data driven enhanced sampling approaches.

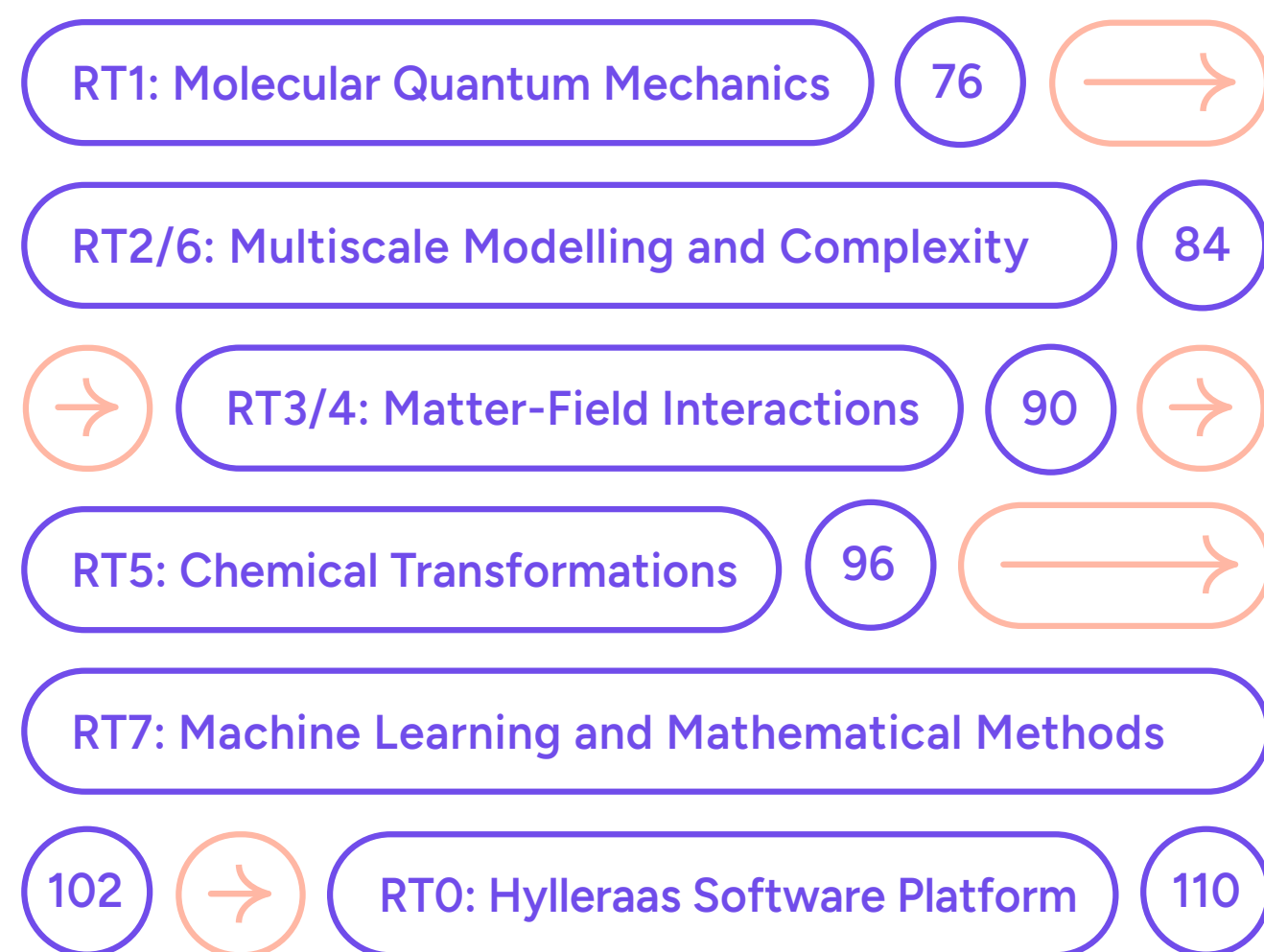
During the CLIMB project, the UiO node will be primarily responsible for one PhD student, host students for secondments, and organize training activities.

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



Research Themes:



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 2024 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 Frediani



Prof. Thomas Bondo Pedersen



Prof. Luca Frediani

«Our preliminary investigations indicate that multiphoton ionization peaks from positronium chloride are well isolated from those of positronium, thus providing a route to spectroscopic identification of this mixed matter-anti-matter system at CERN»

Non-Born-Oppenheimer methods

While exceedingly accurate calculations of the low-lying bound (“rovibrational”) quantum-mechanical states of small molecules can be performed without assuming the ubiquitous Born-Oppenheimer approximation, simulations of molecular quantum dynamics driven by ultrashort and intense laser pulses is significantly more challenging. For stationary states, the full molecular wave function can be expressed as linear combinations of explicitly correlated Gaussians with proper symmetry adaptation with respect to particle permutations. Propagating this wave function in time under the influence of an ultrashort intense laser pulse is considerably more challenging, however. Based on pioneering work initiated during the CAS project *Attosecond quantum dynamics beyond the Born-Oppenheimer approximation* led by Simen Kvaal and Thomas Bondo Pedersen from 2021 to 2023, we have in 2024 continued our investigations of Rothe’s method for solving the molecular time-dependent Schrödinger equation [1,2,3]. This is a close collaboration with RT7 and we refer to the RT7 activity report and to the Research Highlight by Simen Kvaal for more detailed information.

Coupled-cluster theory

Within the Born-Oppenheimer approximation, coupled-cluster (CC) theory stands out as the most accurate and reliable electronic-structure theory around. Starting in 2018, we have over the past years extended CC theory to the time domain, aiming at accurate simulations of attosecond many-electron dynamics with two main goals. The first goal is to reliably interpret and predict attosecond spectroscopic experiments on small molecular systems. The second goal is to investigate whether such ultrashort laser pulses can be used to control the quantum-mechanical motion of molecules, essentially allowing us to control their behavior, including their chemical reactivity. These are monumental challenges for several reasons. One reason is the nonvariational character of CC theory, which makes it hard to interpret CC simulations in ordinary quantum-mechanical terms – i.e., in terms of probability amplitudes and interferences among them. To address this issue, we have in 2024 worked on a novel approach to the quantum-mechanical interpretation of CC states and properties.

The concept of configuration weight plays a central role in molecular electronic-structure theory where it explicitly reveals the single- or multi-reference character of a given configuration-interaction wave function. In ref. [4], Håkon Emil Kristiansen and co-workers propose to compute weights as expectation values of projection operators within a bivariational framework that guarantees the validity of the Hellmann-Feynman theorem (Figure 1). This definition of weights can be applied to any CC model, including those based on perturbation theory for the energy. Notably, it can be used to compute weights within the CC singles-and-doubles with perturbative connected triples (CCSD(T)) model, often referred to as the “Gold Standard” of quantum chemistry. This allows computational chemists to analyze CC calculations in the same manner as configuration-interaction-based wave functions such as those obtained from complete active space self-consistent field (CASSCF) calculations.

A related CC interpretation issue arises in simulations of laser-driven many-electron quantum dynamics. Once the time-dependent CC equations are solved, it is straightforward to compute observ-

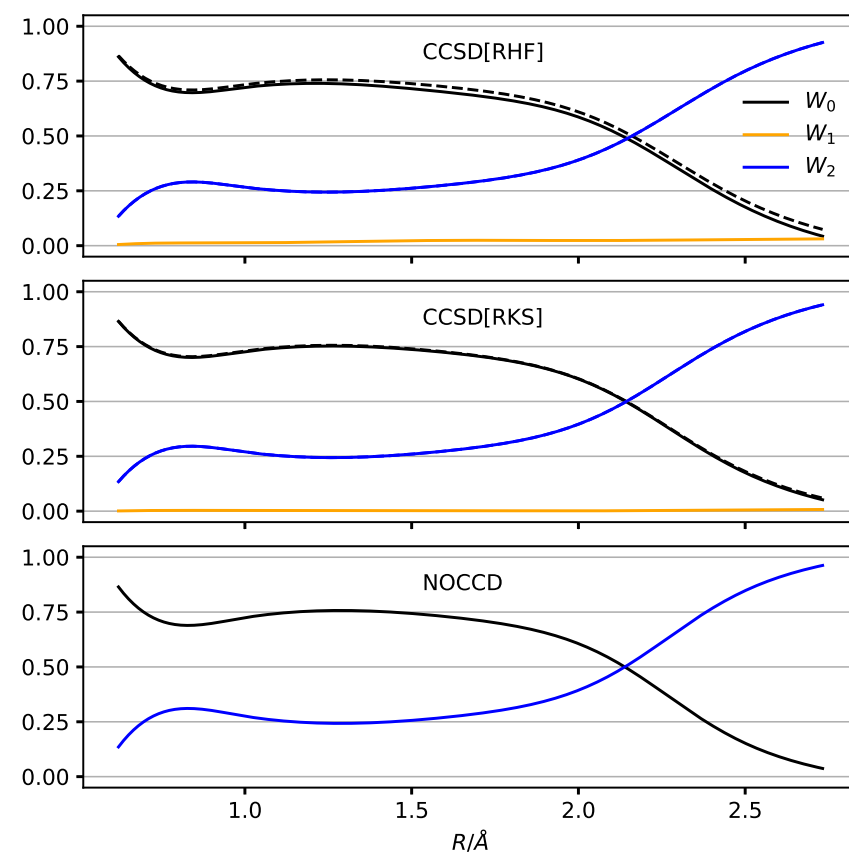


Figure 1: Weights of the reference (W_0), single-excited (W_1), and double-excited determinants (W_2) obtained with the CC singles-and-doubles (CCSD) method and the cc-pVTZ basis set using either the restricted Hartree-Fock (RHF) or restricted Kohn-Sham (RKS) ground state as reference determinant for the C_2 molecule at different bond distances (R). Also shown are the weights obtained with the nonorthogonal orbital-optimized CC doubles (NOCCD) model. The dashed lines indicate weights of the T_2 -transformed determinants. The T_2 -transformed reference weights do not depend on the choice of RHF or RKS determinant and, furthermore, are the same as the reference weight obtained with the NOCCD method, which optimizes the orbitals in concert with the correlating amplitudes. This clearly exhibits the approximate orbital invariance of CC theory. Reproduced from ref. [4] under CC-BY 4.0 license.

able quantities as expectation values of Hermitian operators. One example is the induced time-dependent electric-dipole moment whose Fourier transform is related to the absorption spectrum. Unfortunately, the correlated description provided by the cluster amplitudes impedes assignments of the computed spectral lines to elementary orbital transitions. So, while the complete absorption spectrum can be generated by a single CC simulation, including absorption lines in the x-ray spectral region (core excitations), one cannot assign and thus in-

terpret the spectrum. During 2024, we have generalized the CC weights concept to the time-dependent domain and developed an automatic but approximate assignment algorithm (Figure 2). This work is still in progress and will be published in collaboration with the group of Prof. T. Daniel Crawford at Virginia Tech, USA, in 2025.

Another collaboration with the group of Prof. Crawford was completed in 2024. In ref. [5], we present the first Gaussian-based implementation of

time-dependent CCSD theory with approximate triples corrections, the CC3 model. In this paper, we use the quadratic ramped continuous wave approach proposed by Ofstad et al. [6] to compute (hyper-)polarizabilities, magnetic optical rotation tensors, and Cauchy moments from real-time CC3 simulations (Figure 3). A remarkable conclusion from this work is that single-precision arithmetic yields sufficient accuracy, paving the way for faster calculations on central processing units (CPUs) and, in particular, on graphical processing units (GPUs).

An alternative method for extracting molecular electromagnetic properties such as hyperpolarizabilities from CC simulations is to use the so-called pulsed-wave approach. In ref. [6], Ofstad et al. showed that the pulsed-wave approach converges systematically but slowly to the correct results. In 2024, MSc student Derya Aricigil has developed an extrapolation scheme that circumvents the slow convergence. Supervised by Thomas Bondo Pedersen, her findings will be reported in her master's thesis in 2025.

PhD student Jonas Elenius Skovly Mikkelsen from Aarhus University, Denmark, visited the Hylleraas Centre in Oslo for three months in the fall of 2024. Collaborating with Thomas Bondo Pedersen and RTo PI Simen Reine, Mikkelsen worked on atomic decompositions of polarizabilities and Cauchy moments at all levels of theory implemented in the Dalton quantum chemistry package, from Hartree-Fock and density-functional theory to CC response theory. The long-term goal of the project, which is led by Mikkelsen's supervisor in Aarhus, Prof. Frank Jensen, is to develop reliable polarizable and reactive force fields from first principles for molecular dynamics simulations.

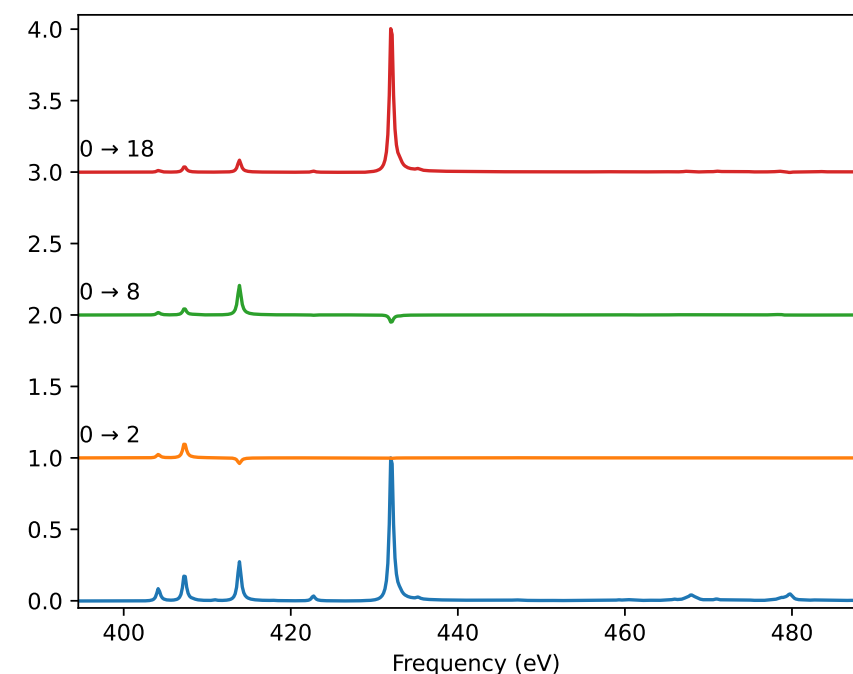


Figure 2: Core excitation spectrum of the ammonia molecule obtained by Fourier transformation of the induced time-dependent electric-dipole moment computed at the CCSD level of theory with the aug-cc-pVDZ basis set. The blue line at the bottom shows the full nitrogen K-edge spectrum, while the red, green, and orange lines on top show the contributions from individual orbital transitions, with 0 denoting the nitrogen 1s orbital and the integer n to the right denotes the virtual LUMO+ n orbital. Illustration: Thomas Bondo Pedersen.

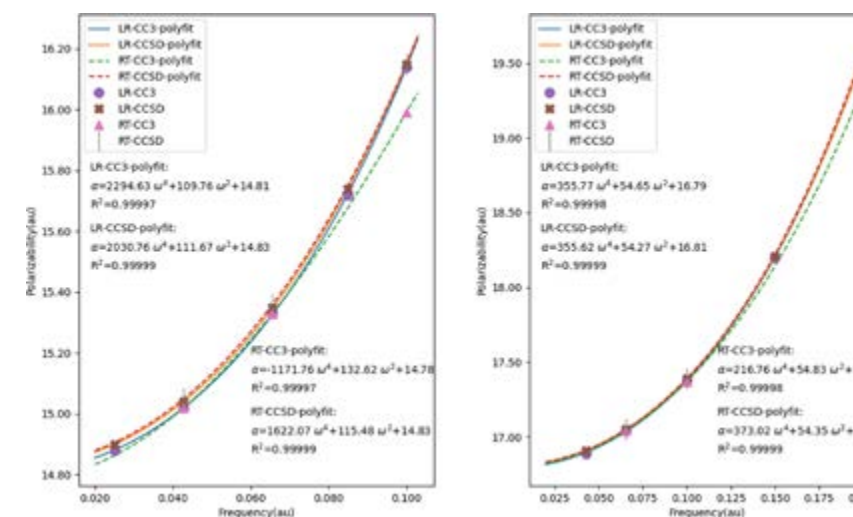


Figure 3: Dispersion of $\alpha_{||}$ for ammonia (left) and polarizabilities for methane (right), calculated using the time-dependent CCSD and CC3 methods. Reproduced from ref. [5] under CC-BY 4.0 license.

Grid methods

Since 2023, Postdoc Håkon Emil Kristiansen and PhD candidate Einar Aurbakken have developed a software framework for grid-based simulations of quantum dynamics, with special emphasis on the discrete variable representation (DVR). While computationally expensive, such grid-based methods yield superior results compared with atom-centered Gaussian basis function, partly because continuum states are automatically included in the description. This is of the utmost importance to attosecond laser-driven quantum dynamics where ionization processes are unavoidable. Hence, grid-based results have been used as benchmarks for the development of the Rothe propagation scheme discussed above and in the activity report of RT7.

Another application area is to short-lived matter-antimatter “molecules” such as PsCl. Here, Ps denotes positronium which is a hydrogen-like system composed of an electron and its antiparticle, the positron. The lifetime of such molecule-like systems is a few nanoseconds, which leaves ample time to conduct attosecond spectroscopic experiments. In a collaboration with Dr. Antoine Camper from the Department of Physics at the University of Oslo, Aurbakken, Kristiansen, Kvaal, and Pedersen have worked on an implementation of DVR-based time-dependent Hartree-Fock theory for mixed electron-positron systems. Camper is also associated with the AEgIS collaboration at CERN and the goal of the project is to predict the attosecond spectroscopic properties of PsCl with sufficient accuracy to aid the planning of future experiments at CERN. One example is the prediction of photoelectron spectra (the antiparticle analog of photoelectron spectra) such as above threshold ionization (ATI) spectra (Figure 4). In an experimental setup, there will be tiny amounts of PsCl “molecules” present in a sample which will instead be dominated by Ps “atoms”. Hence,

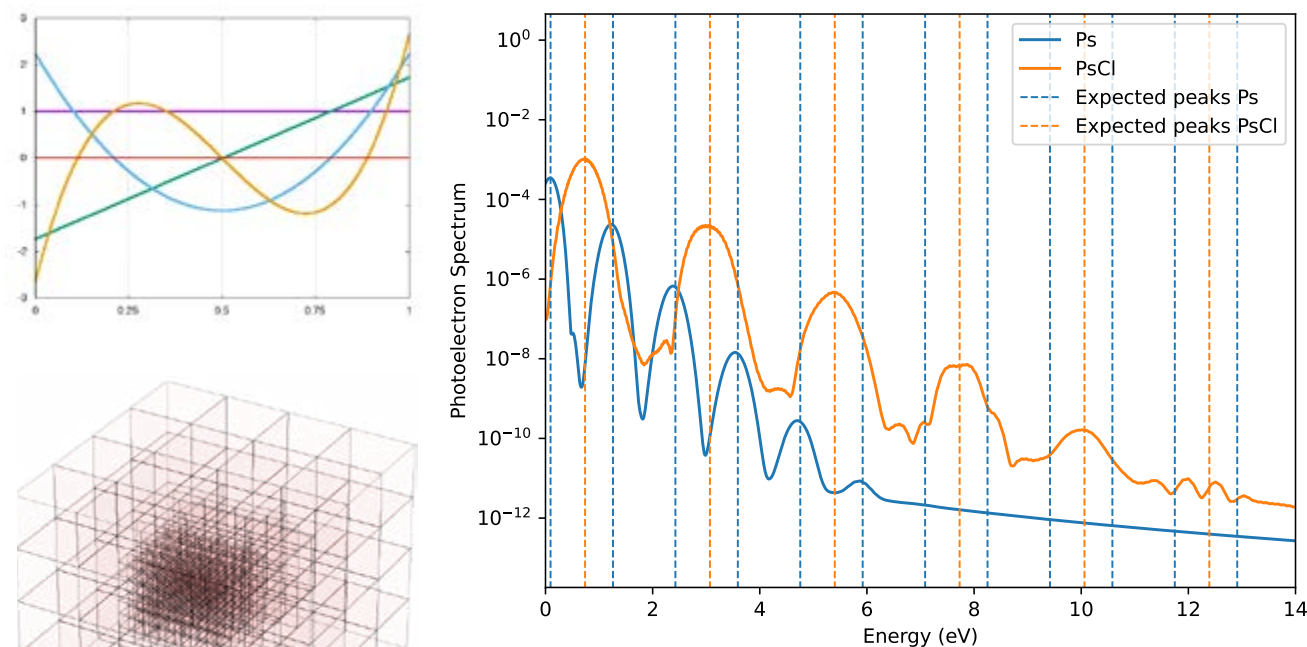


Figure 4: Photo-positron ATI spectra of Ps and PsCl computed from time-dependent Hartree-Fock simulations using the Discrete Variable Representation. Illustration: Einar Aurbakken.

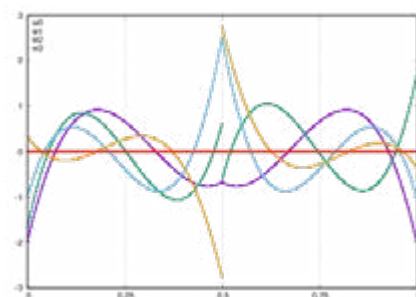


Figure 5: Top panel: scaling functions of order $k = 3$ defined in the interval $[0,1]$ are simple polynomials. Mid panel: the corresponding wavelet functions are piece-wise polynomials with four vanishing moments (orthogonal to polynomials up to the cubic one). Bottom panel: adaptive grids are constructed on demand to minimize storage and meet precision requirements. Reproduced from ref. [7] under CC-BY 4.0 license.

spectral signatures of PsCl must be well isolated from those of Ps to be detected. As seen in Fig. 4, our preliminary investigations indicate that multiphoton ionization peaks from PsCl are well isolated from those of Ps, thus providing a route to spectroscopic identification of PsCl. A manuscript is in preparation and will be submitted for publication in 2025. The project work of BSc student Catherine Hughes is based on pseudo-spectral methods and focuses on atomic and molecular stabilization in super-intense high-frequency laser fields. As new experimental laser facilities become available for the generation of such strong laser fields, theoretical predictions are indispensable to correctly interpret new observations. Since high-frequency radiation is ionizing, one would intuitively expect that complete ionization results from increasing the intensity. As it turns out, however, the opposite happens with significant

probability: Above a certain intensity-frequency ratio, the ionization probability drops, and the atomic or molecular system exists in an exotic state created by the presence of the laser field. The BSc project of Catherine Hughes aims to develop computational tools to accurately model such states using low-order Floquet theory.

Multiwavelets

Wavelets are special types of functions which have been introduced around 40 years ago. They found immediate application in the processing of signals e.g. for noise filtering and data compression. From a mathematical point of view, a key-feature is their localization both in real space and in Fourier space. This makes them very attractive to achieve efficient numerical implementations. One family of Wavelets is called Multiwavelets. They are derived by taking a set of polynomials on an

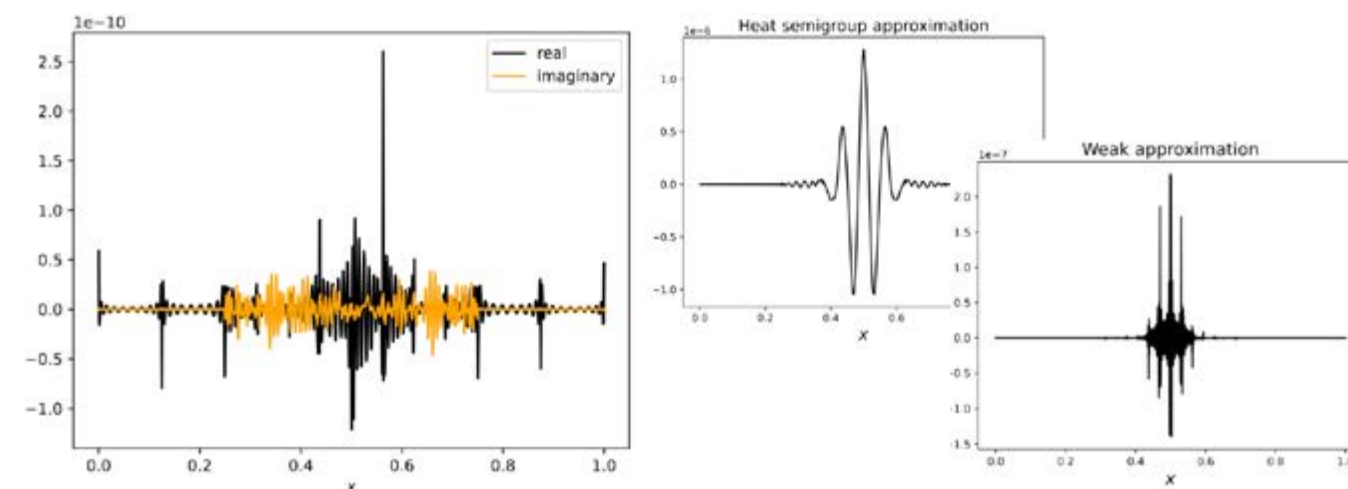


Figure 6: Left panel: Error in the real and imaginary part of a 1d harmonic oscillator wave functions after applying the time-evolution operator derived in [8,9]. Right panel: error obtained when the Laplacian operator is applied according to the new method proposed by E. Dinvaay and the original one based on the weak definition of the derivative operator. Although the old method is slightly more precise, it is visibly "noisier", which prevents successive applications, such as those required in a time propagation algorithm. Adapted from ref. [9] under CC-BY 4.0 license and from ref. [10] under CC0 1.0 license.

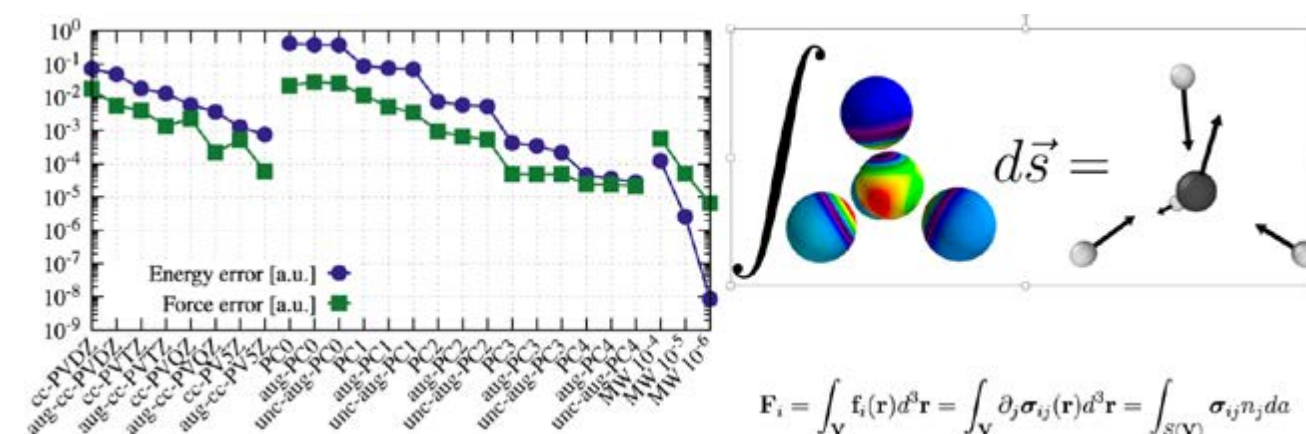


Figure 7 (above): Left panel: Benchmarking gradients and energies obtained with different methods: cc-pVXZ bases, PCX bases, MWX bases. Right panel: a cartoonish representation of the concept which was developed in ref. [11]. Gradients are obtained by integrating the stress tensor density over a surface enclosing a nucleus. Adapted from ref. [11] under CC-BY 4.0 license.

interval. Successive refinements of the interval lead to an adaptive grid supporting functions which are increasingly compressed and hence able to represent precisely very detailed features of, e.g., orbitals and the electronic density (Figure 5). They can achieve a precision which is not attainable for traditional basis sets and are well poised to take full advantage of modern High Performance Computing architectures.

One of the most active areas of research in 2024 has been the development of methods to treat time-dependent problems using multiwavelets. This is a hot research area which on the one hand connect to other activities of RT1 in Oslo, and on the other hand is linked to applications in attosecond spectroscopy. Postdoc Evgueni Dinvaay found two distinct methods to overcome the difficulties of applying a time propagator within the Multiwavelet framework. This operator is challenging because its repre-

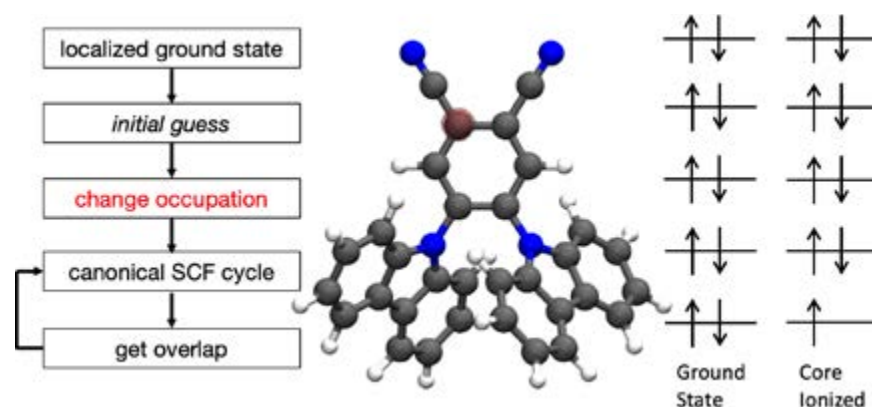


Figure 8: Combining MOM and MWs, it has been possible to obtain all-electron calculations of core excitations using MRChem. The protocol consists of a calculation of the ground state with localized orbitals, followed by a calculation of the ionized state with canonical orbitals and MOM. Illustration: Niklas Göllmann.

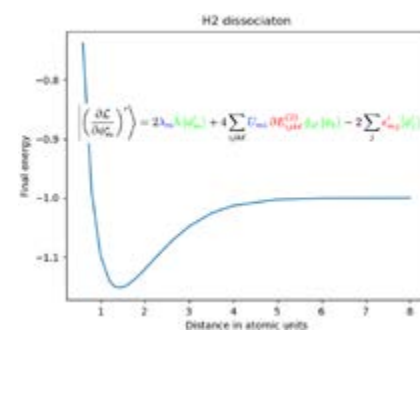


Figure 9: The first proof-of-principle DMRG/MW calculation of the dissociation of a hydrogen molecule. The red terms in the equation are obtained using the DMRG code chemtenor, whereas the right terms are represented using MWs. Illustration: Martina Nibbi.

sensation is difficult to compute and use due to its highly oscillatory behavior and because its representation is rather different from the diagonally dominated operators which MRChem has been dealing with so far. The first method relies on integration in the complex plane to make numerically feasible the calculation of the time evolution operator [8,9], whereas the second one is derived from the heat equation, and it achieves a direct representation of the Laplacian operator from the Taylor expansion of its exponential [10] (Figure 6). Another challenging issue for Multiwavelets is the computation of nuclear gradients (Figure 7). Although MWs can directly make use of the Hellman-Feynman theorem, computing gradients is numerically unstable because it basically relies on computing a function value (the electrostatic potential from the electronic density) at the nuclear position. PhD student Moritz Gubler, who was visiting us from the University of Basel, Switzerland, found out that a different strategy, based on surface integration could be employed, reducing the error by almost an order of magnitude, which makes the computation of nuclear gradients practical even at moderate precision (the previous implementation required rather high precision to achieve the same result) [11].

A third area of application has been the computation of X-Ray photoemission spectra with a DeltaSCF method combined with the Maximum Overlap Method (Figure 8). Computing X-Ray spectra is challenging because they require a very precise description of the electronic density in the nuclear core region, which can be challenging to achieve with Atomic Orbitals (AOs). On the other hand the lack of atom-based functions, makes it technically complicated to use MWs when an electron is removed: the “hole” would delocalize and the optimization would move it towards the valence region making the result unusable. A possible solution relies on using pseudopotentials on all but one atom. We adopted a different strategy based on the Maximum Overlap Method (MOM) which constrains the singly occupied orbital to have the maximum possible overlap with the original orbital from the neutral system. This strategy has been successfully implemented by Master Student Niklas Göllmann who was visiting from the University of Münster, Germany, in collaboration with adjunct professor Laura Ratcliff.

A new collaboration with the group of Professor Christian Mendl from the Technical University of Munich, Germany, started in 2024. The main goal of the project is to combine MWs with

the Density Matrix Renormalization Group (DMRG). The project is led by PhD student Martina Nibbi in Prof. Mendl’s group. Here we combine their expertise on DMRG methods with our MW code to obtain the first DMRG implementation at the Complete Basis Set limit (Figure 9).

The extension to the relativistic regime is progressing. The paper outlining the implementation of the full Breit-Pauli Hamiltonian in 4C has been published [12]. Researcher Peter Wind has extended the mrcpp library to deal natively with complex numbers, which is an important steppingstone in achieving an efficient four-component implementation. PhD candidate Quentin Pitteloud is currently working on a two-component implementation in Python, and Researcher Christian Tantardini in collaboration with adjunct professor Roberto Di Remigio Eikås have been working on an alternative approach to solve the Dirac equation which makes use of the square of the Dirac operator to achieve higher precision [13].

PhD student Magnar Bjørgve successfully defended his PhD thesis on April 4th with a thesis entitled: “Unleashing the VAMPyR. A Python Journey into the Realm of Multiwavelets and Quantum

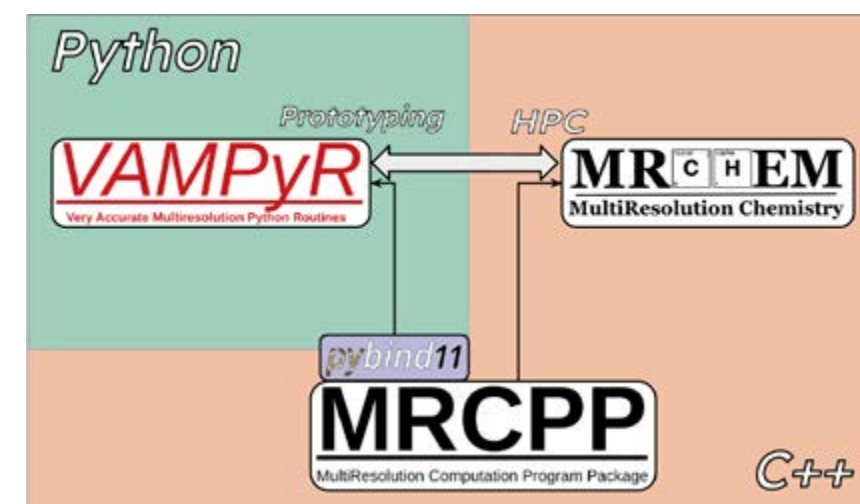


Figure 10: Logical structure of the coding environment to use Multiwavelets. The core library mrcpp contains all the low-level functionality to represent functions, apply operators and perform all algebraic operations. MRChem uses mrcpp to perform production quantum chemistry calculations. VAMPyR is a python library which was the centerpiece of Dr. Bjørgve’s PhD work. It exposes the MW functionality of mrcpp in an efficient and user-friendly way for prototyping. VAMPyR has for example been extensively used by Evgueni Dinvoy to develop the time-evolution operators and by Martina Nibbi for the DMRG calculations.

Chemistry”. The centerpiece of Dr. Bjørgve’s thesis was the implementation of the VAMPyR library (Figure 10). VAMPyR provides a user-friendly interface to the mrcpp library for MWs calculations. It has been instrumental in several works that document pilot implementations of Quantum Chemistry methods in different directions both for pedagogic purposes (it makes it very easy for a student to write their own SCF code, for example) and for research application (relativistic methods and solvent effect have been the most significant applications in the last few years). The work has also been summarized in a paper which has been published a few weeks after Dr. Bjørgve’s defense [14].

PhD student Gabriel Gerez has been working on the implementation of the Poisson-Boltzmann operator for solvent-effect calculations in ionic media, and he is expected to defend his thesis during 2025.

In the fall of 2024, Klaus Schleich visited our group as exchange student to work on a project to test different integration schemes for the time-dependent Schrödinger equation, under the supervision of Dr. Evgueni Dinvoy.

Two additional members joined the group in the fall of 2024: PhD student Ylva Os, and MSc student Julio Maximiliano Ramirez Oyhanarte. The former will work on implementing new functionality in MRChem and performing the corresponding benchmark calculations, whereas the latter will work on a project to extend solvent effect calculations to challenging environments such as high-pressure conditions or interfaces.

External Funding

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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



Prof. Michele Cascella



Prof. Bjørn Olav Brandsdal

«We have pushed the development of multi-scale models toward computational strategies incorporating physics-based approaches with data-driven protocols»

In 2024, we pushed the development of multi-scale models toward computational strategies incorporating physics-based approaches with data-driven protocols. These lines branch according to the choice of bottom-up or top-down strategies. In the first case, data from high-level calculations (i.e., electronic structure calculations) are used to establish molecular potentials, for example, in the form of neural networks. In the second case, experimental data are used either to calibrate molecular potentials or to drive the molecular simulations through Bayesian inference. These projects are in collaboration with RT7 and RTo.

Bottom-up models

Machine learning potentials (MLPs) 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 studying large systems over extended timescales, such as microseconds, as for supercooled water in ref. [1].

Developing MLPs presents challenges, especially concerning reliability, with primary issues being simulation crashes and inaccurate thermodynamics. In

2024, significant effort was put on establishing robust workflows for active learning of MLPs and simulations. This included the development of a software tool called HyAL. HyAL automates the creation of MLPs by automating tasks such as sampling new training set geometries and training models and performing high-throughput electronic structure calculations. Its modular design allows for the seamless integration of new software as it emerges.

In 2025, the focus will shift from pure development to application of HyAL. Specifically, we aim to publish a method paper on active learning algorithms, a software paper on HyAL, and two application papers examining ice friction and water in metal-organic frameworks (MOFs). These efforts align with the H₂O-MOF NFR, EuroHPC, and YoungCAS projects of Bore.

The structural nature of lithium halides (LiX, with X = Cl, Br, I) in organic solvents have been the subject of a wide scientific debate, and a large variety of forms has been isolated and characterized by X-ray diffraction. The identified molecular scaffolds for LiX, prominently by X-ray, are diverse, often built on (LiX)_n rings with a prevalence of rhomboidal arrangements and an appropriate number of solvent or Lewis base molecules coordinating the lithium ions.

Much less is known about the structures of LiX in solution, limiting the understanding of the synergistic role of LiX in reactions with various organometallic complexes, as prominently represented by the turbo Grignard reaction.

During 2024, PhD candidate Marinella de'Giovannetti, together with Postdoc Sondre H. Hopen Eliasson and Researcher Sigbjørn L. Bore, and by Cascella and Eisenstein, trained a machine learning potential on ab initio data (DFT/PBE) to explore the complex conformational landscape for systems comprising four LiX moieties in tetrahydrofuran (THF) [2]. The machine learning model revealed the presence of a diversity of scaffolds at thermally accessible free energy values. LiCl shows a preference for compact, pseudo-cubane Li₄Cl₄(THF)₄ structures, coexisting with open rings (Figure 1). At concentrations close to the solubility limit, LiCl forms hexagonal structures, in analogy with literature observations on pre-nucleating NaCl. LiBr tends to favour less compact, more solvated aggregates. LiI significantly differs from the two other cases, producing highly solvated, monomeric, dimeric, or linear structures. This study provides a comprehensive view of LiX in organic solvent, revealing dynamical polymorphism that is not easily observable experimentally. This project is in collaboration with RT5.

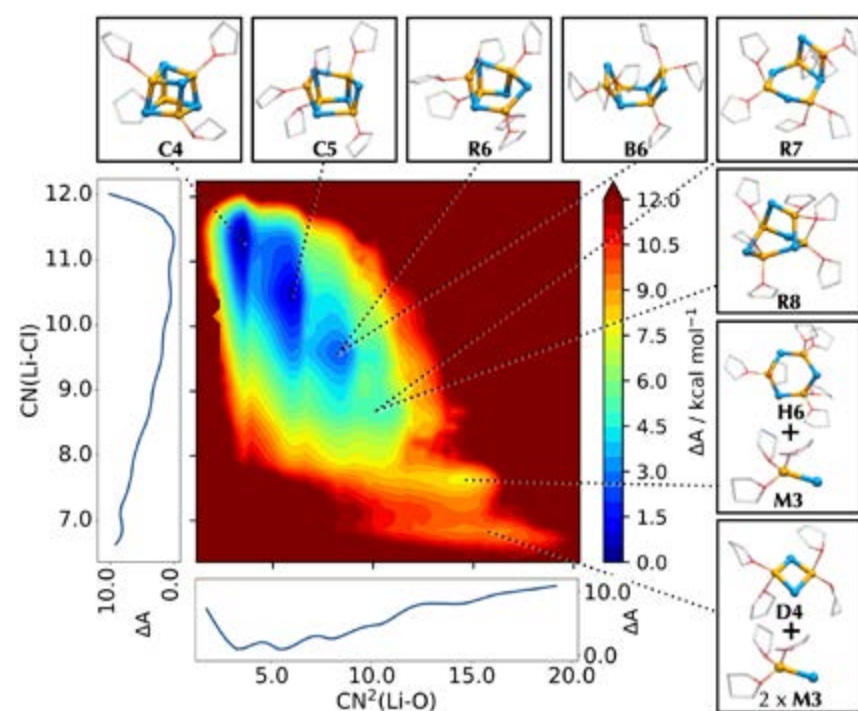


Figure 1: Helmholtz free energy surface of the conformational landscape of Li_4Cl_4 . The coordination number of Cl around Li, $\text{CN}(\text{Li-Cl})$, and the squared coordination number of O around Li, $\text{CN}^2(\text{Li-O})$, are used as collective variables for the free energy surface (FES). Side graphs report the projections of the FES onto the two respective axes. Representative structures corresponding to the basins of the FES are shown in balls-and-sticks (Li in yellow, Cl in cyan, and THF as transparent sticks). Figure from Ref. [2], under CC-BY 3.0 licence.

Top-down models

One of the major problems in calibrating coarse-grained models resides in the representation of the physics of the molecular objects of interest, and in its reduction into computationally efficient models employing, for example, two-body potentials over a minimal number of centroids representative of the structural moieties at play. This rather complicated conceptual issue often reduces to pragmatic solutions aiming at obtaining parameters that provide minimal discrepancy with the experiment for relevant quantities of interest. In fact, any quantity measured at thermodynamic equilibrium is understood in terms of its expectation value over the relevant statistical ensemble, which can be estimated as time average over a molecular dynamics (MD) trajectory. Because any MD trajectory depends deterministically on the force-field parameters, the re-

lationship between parameters and predicted expectation values can also be back-traced. This protocol takes the name of *differentiable molecular dynamics*.

Over the year, PhD candidate Manuel Carrer, with the help of Postdoc Henrique M. Cezar, S. L. bore, and Software Engineer Morten Ledum, developed ∂ -HyMD, the differentiable version of the HyMD software, to exploit differentiable strategies for the parameterization of a transferable force-field library for phospholipids [3]. The study shows how the use of multiple short, parallel MD simulations produces more consistent convergence of the optimal parameters, avoiding notorious issues related to numerical instability and memory over usage (Figure 2).

Small-angle X-ray/neutron scattering (SAXS/SANS) techniques provide valu-

able nanostructural information of self-assembling molecules. However, extracting the information from these experiments can be a challenging task, usually relying on predetermined assumptions. Conventional models for surfactant micelles consider a core-shell structure with a hydrophobic tail encapsulated by the hydrophilic part. This approach is successful in many cases but can fail even for common surfactants such as Triton X-100 (TX-100). H. M. Cezar, in collaboration with Hylleraas affiliate Prof. Reidar Lund, employed SAXS and SANS measured in combination with MetaInference molecular dynamics simulations to investigate TX-100 assemblies. Through this approach, it was possible to reveal a much more complex picture, composed by micellar aggregates with diffuse core-shell boundaries, multilayered structures, and polydisperse sizes. Altogether, all these ingredients

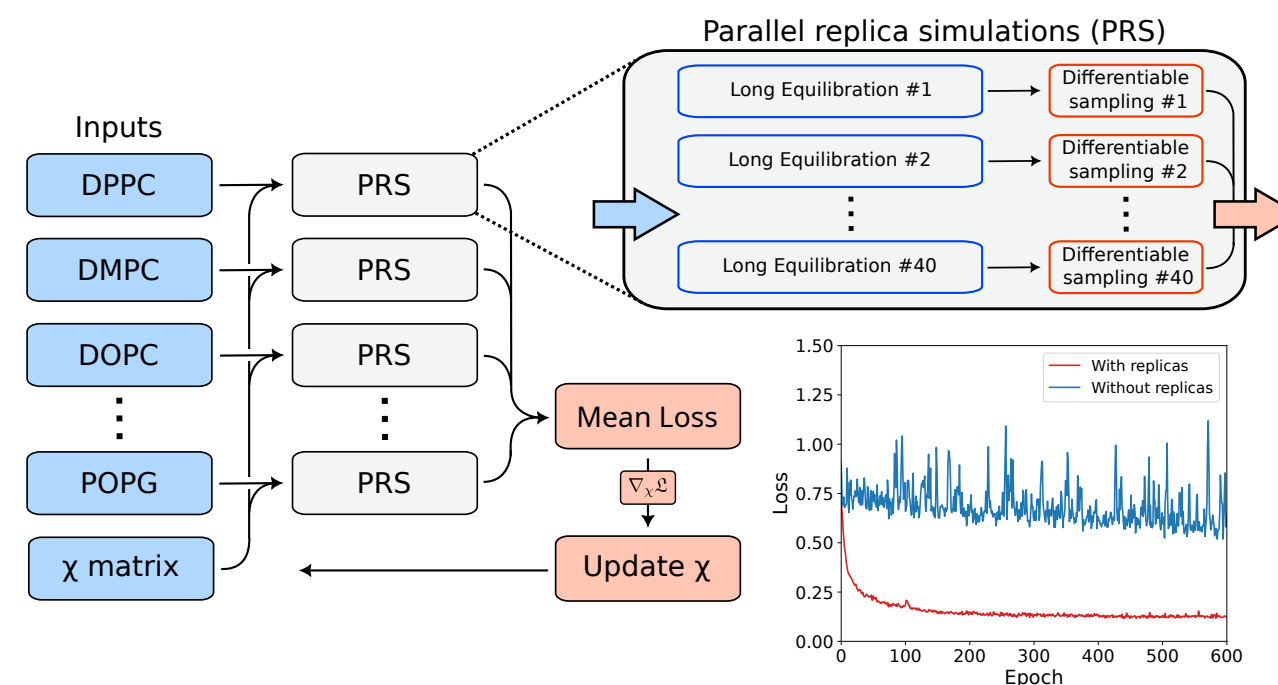


Figure 2: Differentiable MD protocol for the optimization of the lipid library. On the left is the overall training architecture, in which, for each lipid, we run a parallel replica simulation (PRS) without any communication. The results are combined to compute a mean loss function, which is the quantity effectively minimized. In the zoomed-in part at the top right, a single lipid optimization unit - PRS - which is composed of independent parallel simulations containing an equilibration followed by differentiable sampling. On the bottom right, comparison between the losses obtained from training a single DPPC membrane, with and without replicas. Figure from Ref. [3], under CC-BY 4.0 licence.

contribute to recomposing a quantitative agreement between the experimental data and the underlying molecular models (Figure 3). Comparison with the regular micelles formed by the chemically similar C12EO10 surfactant, it was possible to dissect the role of the hydrophobic core in micellization, finding that the relatively shorter and less hydrophobic tail of TX-100 favours polymorphism. This is the first work where MetaInference is simultaneously employed on SAXS and SANS data [4].

A final take on the physics of hybrid particle-field models

During 2024, we closed our work dissecting the physics of hybrid particle-field models (HhPF, see Hylleraas report 2023), demonstrating how it is possible to describe biphasic behaviour within the model, without the need of complicating the description of the functional and nu-

merical models. Specifically, by employing a linear combination of two Gaussians, we demonstrate that HhPF can generate potentials with attractive and steric components analogous to Lennard-Jones (LJ) potentials, which are crucial for modelling phase coexistence [5].

In the study, done by former Hylleraas members Samiran Sen and Xinneng Li, with the help of Cezar and Ledum, we compared the performance of the method with multi-Gaussian core models in simulating liquid-gas coexistence for a single-component system across various densities and temperatures (Figure 4). Our results show that HhPF effectively captures detailed information on phase coexistence and interfacial phenomena, including micro-configuration transitions and increased interfacial fluctuations at higher temperatures. Notably, the phase boundaries obtained from HhPF simu-

lations align more closely with those of standard Lennard-Jones systems compared to the multi-Gaussian core model.

Exploring Enzyme Adaptation to Extreme Environments using Empirical Valence Bond Simulations

Enzymes are highly effective biological catalysts with immense potential in industrial applications. However, the environmental conditions these systems are found in are often vastly different from optimal industrial conditions. Work on the CUBE3 project, led by Bjørn Olav Brandsdal, has made efforts to understand how to optimize enzymes to be better suited to industrial conditions using DFT, QM/MM, empirical valence bond (EVB) simulations, and molecular dynamics. These computational methods allow us to construct Arrhenius plots to help uncover enthalpic and entropic

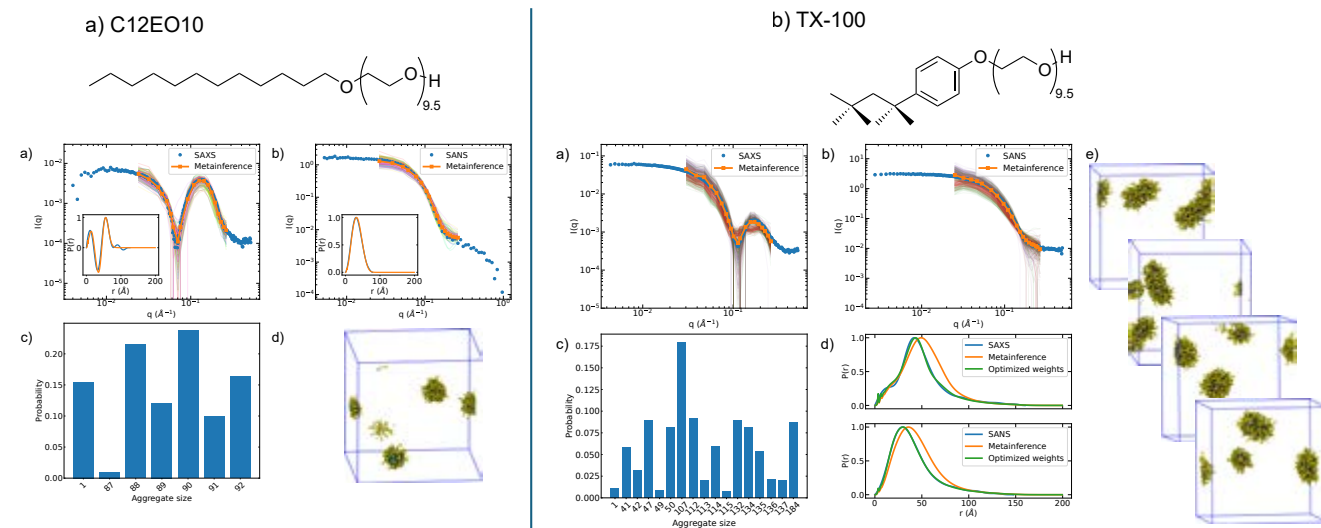


Figure 3: Left: C12EO10 Metainference results: a) SAXS curve in comparison with experiment and $P(r)$ in the inset; b) SANS curve in comparison with experiment and $P(r)$ in the inset; c) probability of observing a micelle of given size during the simulations; d) snapshot of the surfactants during the simulations (water beads were removed for clarity); Right: TX-100 Metainference results: a) SAXS curve in comparison with experiment and $P(r)$ in the inset; b) SANS curve in comparison with experiment and $P(r)$ in the inset; c) probability of picking an assembly of given size during the simulations; d) $P(r)$ for SAXS and SANS, obtained from the experiment, from the Metainference simulations and also from reweighing the contributions from each assembly to optimize the match with the experiment; e) snapshots of the four simulation boxes corresponding to the different replicas (water beads were removed for clarity). Figure elaborated from Ref. [4], under CC-BY 4.0 licence.

Figure 4 (below): Liquid-gas phase diagram from HhPF simulations of single bead systems. Simulations were conducted at various temperatures along five different densities. Each simulated case is represented by a point, with shape indicating the phase category and color showing the detailed micro-configuration. Snapshots illustrate different microconfigurations on the right side. The shaded zones correspond to the transition region between homogeneous and coexistence phases. The gray zone represents the results of the MGCM simulations. Figure from Ref. [5] under CC-BY 4.0 licence.

contributions to the free energy of the reactions being catalyzed.

There are a variety of enzymes being worked on in this project by various group members, all at different stages. A mesophilic chorismate mutase, being investigated by Postdoc Ryan Scott Wilkins, has been tested with several mutations which show promising results for thermophilic behavior and are awaiting experimental testing [6,7]. Former centre Postdoc Bjarte Aarmo Lund, who before his departure had begun studying a proline racemase, which helps the parasite *T. cruzi* evade detection from the immune system (Figure 5). His initial DFT results helped establish a mechanism for the reaction, which is being looked into with more detail via QM/MM and EVB by PhD students Bente Barge and Helena Hradiská. Hradiská is also currently in the initial stages of exploring the potential applications of laccase, a multicopper oxidase enzyme which may

help with bioremediation. Finally, PhD student Daniel Schipper is further exploring the details of *Mall*, an α -glucosidase which catalyzes the decomposition of various maltose substrates. Contrary to many other enzymes, *Mall* exhibits non-linear Arrhenius behavior and uncovering the “why” is the primary focus of Schipper’s work (Figure 6). In addition to this, he has also been focusing on enabling EVB simulations to be performed within GROMACS rather than software written by our external collaborators, which would vastly improve the accessibility of EVB.

Tackling antimicrobial resistance through molecular simulations

Overuse of antibiotics has led to antimicrobial resistance being one of the leading health problems of the 21st century. Unless better measures are taken and new antibiotics are developed, the World Health Organization expects antimicrobial resistance to be directly

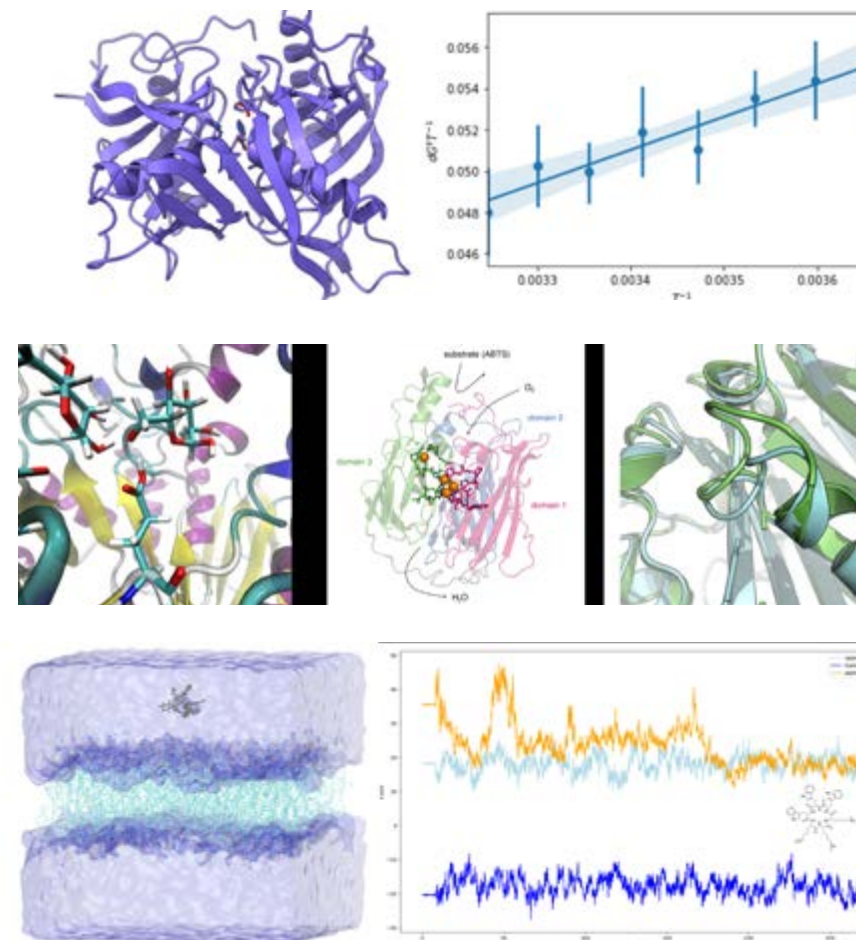
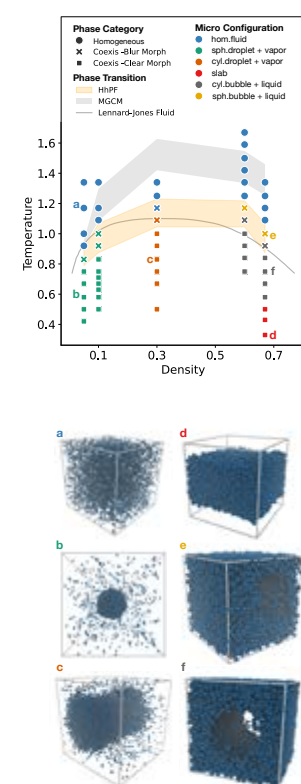


Figure 5: Structure and Arrhenius plot of activation free energies for the conversion between stereoisomers L- and D-proline in *T. cruzi*. Illustration: Bjarte Aarmo Lund.

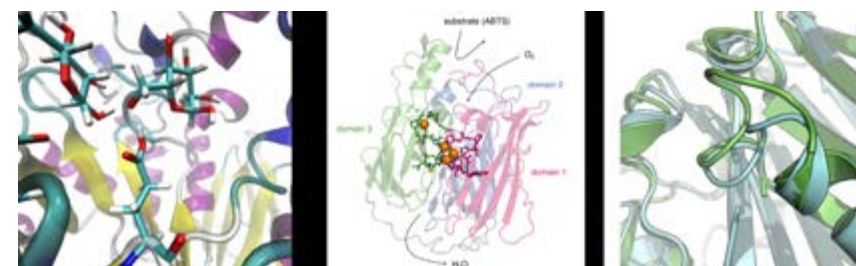


Figure 6: *Mall*, laccase, and chorismate mutase – three enzymes being investigated by members within the CUBE3 Project. *Mall* is a notable enzyme in that it exhibits non-linear Arrhenius behavior, which is being explored by Daniel Schipper (left). Laccase, being studied by Helena Hradiská, harnesses copper to serve as a useful biocatalyst for industrial bioremediation (middle). Mesophilic (green) and thermophilic (blue) variants of chorismate mutase are highly similar enzymes, yet have a small loop region displaying different flexibilities which can offer insight into their differences in behavior, which is being investigated by Ryan Scott Wilkins. Illustrations (left to right): Daniel Schipper, Helena Hradiská, Ryan Scott Wilkins

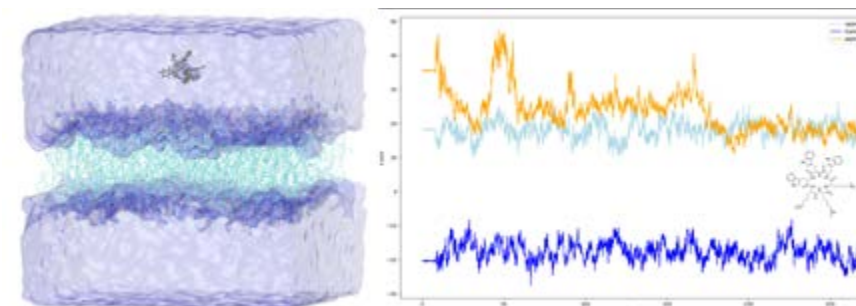


Figure 7: A cyclohexapeptide c(RRRWWW) in the process of interacting with a model bacterial membrane (left). Such cAMPs form clusters with other like molecules, which show strong susceptibility to interact with the outer membrane of a model bacterial lipid membrane. Upon insertion of the cAMP clusters into a membrane, the membrane will proceed to break apart, thus killing the bacteria. Illustration: Tonje Reinholdt Haugen.

responsible for up to 10 million deaths annually by 2050. PhD candidates Laura Ernstsén and Tonje Reinholdt Haugen are aiming to help find new candidates as potential antibiotics using molecular dynamics simulations. They are working on this project with experimental collaborators at UiT, who have developed a library of amphipathic barbiturates and cyclic antimicrobial peptides (cAMPs). Using molecular simulations has enabled them to test the abilities of these potential drug candidates to form clusters, which bind to bacterial membranes and cause them to rupture. Ongoing work in this study involves

testing which candidates are best able to inhibit bacterial membranes and understanding the mechanisms in which they do so (Figure 7).

During 2024, PhD candidate Tonje Reinholdt Haugen has also started applying her cAMPs to more complex systems. During a visit to the University of Oxford, she collaborated with Prof. Syma Khalid to study the effects of the cyclic hexapeptides in membranes containing aquaporins, a channel protein responsible for transporting water molecules through cell membranes.

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RT3/4: Matter-Field Interactions

Matter-field interactions are central to the Hylleraas Centre and RT3/4 is closely connected to research in other RTs, especially RT1 and RT7. Density-functional theory is a cornerstone of RT3/4 with applications to chemistry in strong magnetic fields, relativistic effects, and time-resolved ultrafast spectroscopy.

Principal investigators:
Michal Repisky and Erik Tellgren



Michal Repisky



Erik Tellgren

«Our relativistic study provided a reliable theoretical estimate for the nuclear quadrupole moment of ^{209}Bi at $-428(17)$ mb, which aligned well with molecular and atomic data, and suggested the need to revisit experimental EFG measurements for several bismuth oxyhalides»

Relativistic Methods and Phenomena

In 2024, Marc Joosten, Michal Repisky, Marius Kadek, and Kenneth Ruud, in collaboration with Pekka Pyykkö from University of Helsinki, presented a first four-component relativistic DFT implementation of electric field gradients (EFGs) using Gaussian-type orbitals and periodic boundary conditions, which allowed for the variational inclusion of relativistic effects crucial for heavy-element compounds [1]. The all-electron approach accurately accounted for both core and valence orbitals, essential for EFG evaluation, while efficiency was achieved through density fitting, quaternion algebra, and restricted kinetic balance. The methodology was applied to arsenic, antimony, and bismuth halides and oxyhalides, examining the impact of relativistic effects in solids and comparing them with molecular data. This study provided a reliable estimate for the nuclear quadrupole moment of ^{209}Bi at $-428(17)$ mb, which aligned well with molecular and atomic data, and suggested the need to revisit experimental EFG measurements for several bismuth oxyhalides.

An accidental triplet-harvesting mechanism in donor-acceptor dyads with low spin-orbit coupling (SOC) was discovered

by Torsha Moitra and Kenneth Ruud, in collaboration with Pijush Karak and Swapan Chakrabarti from the University of Calcutta, and Ambar Banerjee from Uppsala University [2]. This study demonstrated that SOC between the lowest singlet excited state and higher-lying triplet states, combined with nuclear motion-driven coupling between triplet states during free rotation about a sigma bond, is a possible pathway to achieve the experimentally observed intersystem crossing (ISC) rate in a class of donor-acceptor photoredox catalysts. This mechanism was identified as the dominant contributor to the ISC process in a specific spirobis[anthracene]dione molecule, where the donor and acceptor moieties are interlocked close to the optimal dihedral angle, highlighting the potential effectiveness of the proposed mechanism. These findings are expected to open novel strategies for synthesizing new generations of triplet-harvesting organic molecules.

Building on previous work, Kenneth Ruud, in collaboration with Pijush Karak, Pradipta Manna, and Swapan Chakrabarti from the University of Calcutta, and Ambar Banerjee from Uppsala University, investigated the origin of the inverted singlet-triplet gap (INVEST)

and the slow variation in the reverse intersystem crossing (rISC) rate with temperature [3]. A Wigner phase-space analysis revealed that, although INVEST is observed at equilibrium geometry, variations in exchange interactions and double excitations for other geometries within the harmonic region lead to non-INVEST behavior. This underscores the critical role of nuclear degrees of freedom in the INVEST phenomenon, with geometric puckering of the studied molecule playing a key role in determining INVEST and the associated rISC dynamics.

The critical role of spin-orbit coupling (SOC) in photo-physical processes, particularly intersystem crossing (ISC) and reverse intersystem crossing (rISC), was detailed by Pijush Karak, Torsha Moitra, and Swapan Chakrabarti in a chapter of Comprehensive Computational Chemistry [4]. This book chapter examines spin-forbidden transitions in photo-physical processes driven by SOC, a relativistic phenomenon resulting from the interaction of an electron's magnetic moment with the internal magnetic field it experiences. These transitions are fundamental to various modern applications, including photoredox catalysis, imaging, and advanced display technol-

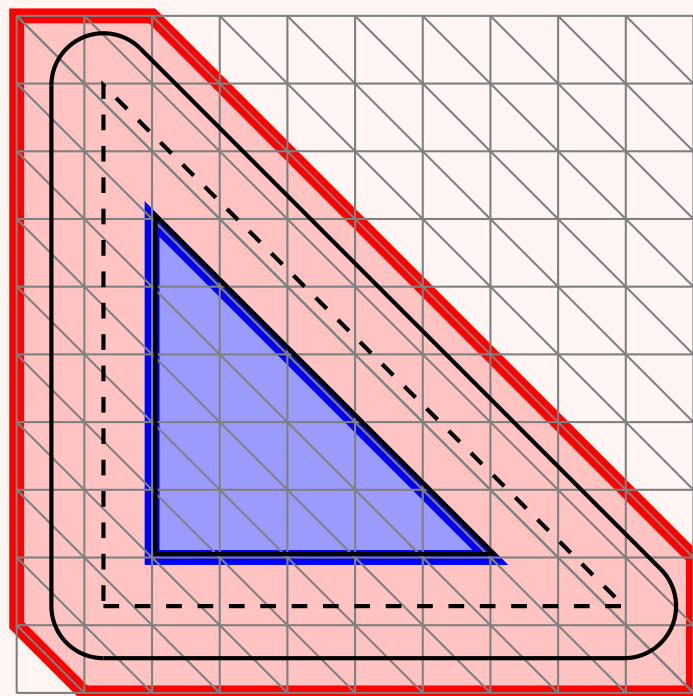


Figure 1: Schematic two-dimensional representation of the decomposition of the unit cube into 24 congruent tetrahedra used in the proof of the existence of the thermodynamic limit for an electron gas with uniform density and vorticity. The black line represents a large, smoothed "tetrahedron" without any sharp edges. Reproduced from Csirik et al. [9] under CC-BY 4.0 license.

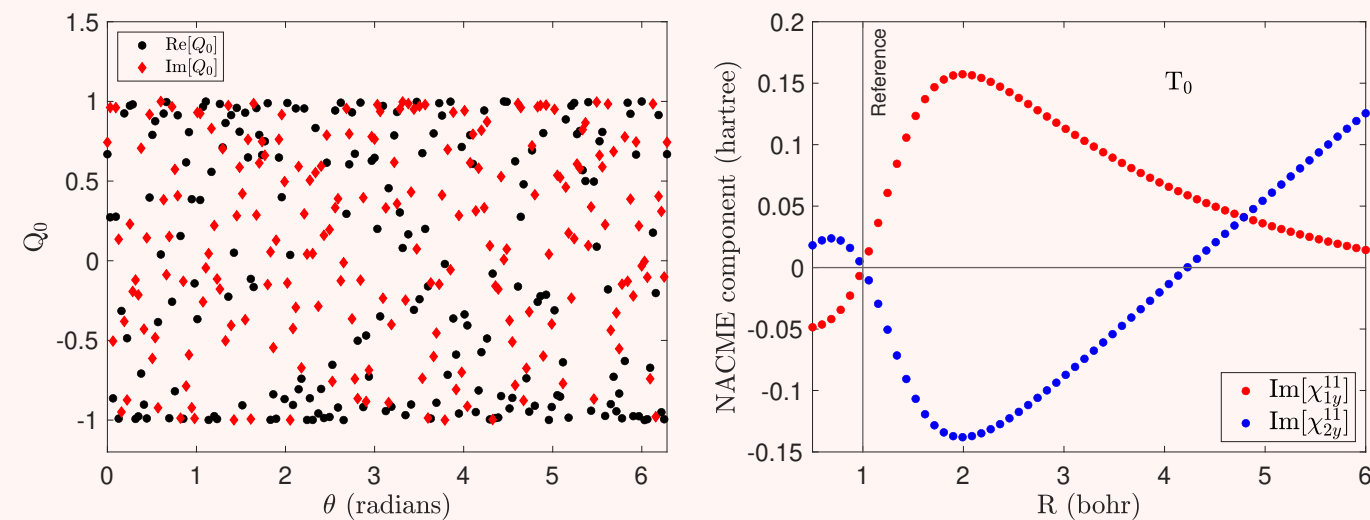


Figure 2: The figure on the left shows an absolute phase of a wave function for a hydrogen molecule as a function of the angle between the bond axis and the magnetic field; this is a non-physical quantity with an uncontrolled, erratic, and discontinuous behavior. The figure on the right illustrates that it is nonetheless possible to compute a continuous, well-behaved non-adiabatic coupling elements for excited states, here as a function of bond distance. Reproduced with permission from ref. [10].

ogies like organic light-emitting diodes (OLEDs). The authors provided an introduction to SOC theory, explored its impact on ISC and rISC dynamics, and discussed state-of-the-art computational methods, such as time-dependent generating function approaches, emphasizing both direct SOC and spin-vibronic mechanisms. The chapter also presents a wide range of applications for these methods.

Taking advantage of Cholesky decomposition to accelerate calculations, Hylleraas affiliate Stella Stopkowicz and coworkers devised and implemented relativistic coupled-cluster methods within the exact two-component frame-

work (X2C) [5]. The capabilities of the methods were demonstrated on uranium hexafluoride molecule (UF_6) and a solvated uranyl ion $\text{UO}_2^{2+}(\text{H}_2\text{O})_{12}$.

Recent advances in laser technology have enabled the observation of electronic motion on its natural timescale using ultrafast pulses, paving the way for attosecond and femtosecond spectroscopic experiments. Understanding these laser-driven processes—often involving non-linear light-matter interactions and non-equilibrium electron dynamics—remains a complex challenge, requiring collaboration between theory and experiment. In 2024, Marius Kadek, Lukas Konecny, and Michal Repisky published a book

chapter in Comprehensive Computational Chemistry, summarizing theoretical progress in simulating ultrafast laser experiments using relativistic real-time electron dynamics methods [6]. The chapter details the fundamental theory of relativistic particle-field interaction Hamiltonians and equations of motion for exact-state wave functions expressed through reduced density matrices. It then explores relativistic mean-field approaches to real-time electron dynamics, with a focus on Kohn-Sham Density-Functional Theory. The discussion transitions from four-component (Dirac) to two-component (Pauli) frameworks, incorporating modern exact two-component (X2C) Hamiltonians. Finally, the chapter high-

lights numerical techniques for real-time propagation and quantum signal processing, along with selected applications to frequency- and time-resolved spectroscopies.

Advances in Spectroscopic Techniques

In 2024, Monika Krupová, in collaboration with Patrycja Leszczenko and Ewa Sierka from Jagiellonian University in Krakow, and Sára Emma Hamplová, Blanka Klepetářová, Radek Pelc, and Valery Andrushchenko from Czech Academy of Sciences in Prague, conducted the first vibrational circular dichroism (VCD) study of adenosine crystals in the solid state [7]. Their research revealed that the highly ordered arrangement of

adenosine molecules in crystals leads to a significantly enhanced supramolecular VCD signal due to long-range vibrational coupling. Unlike guanosine crystals, adenosine crystals do not absorb atmospheric water. The study also identified scattering and orientational artifacts in the spectra due to the crystal's large size and proposed strategies to mitigate these effects. Additionally, unusual infrared absorption features were observed, attributed to the refractive properties of adenosine crystals.

Terahertz Stark spectroscopy

Hylleraas member Michele Cascella, former member Alex Borgoo, and collaborators have been able to model

Stark spectroscopy of molecules in solution, at the density-functional level of theory [8]. This involves strong electric fields oscillating on the THz scale, which is faster than the time scale for molecular rotation, offering time-resolved information from molecules that are always in motion in liquid solution. Spectra were obtained for two molecules, in either toluene or ethyl acetate solvents, in which relevant electronic excitations involve charge transfer, namely tetrathiafulvalene, benzothiadiazole, and anthanthrene, a conjugated molecule of interest as a semiconductor. The calculations assisted collaborators' interpretation of experimentally measured signals.

Strong magnetic fields, magnetic properties, and quantized electro-magnetic fields

The work by Hylleraas members Mihaely Csirik, André Laestadius, and Erik Tellgren [9] studied two fundamental mathematical issues connected to mathematical fields in density-functional theory (DFT). An novel N-representability result shows how to construct a quantum state that reproduces a given density and current density. Moreover a central model system in DFT, namely the uniform electron gas, was extended in a mathematically rigorous way to the magnetic case by requiring that also the vorticity is constant (Figure 1). This work combines the focus on strong magnetic fields in RT3/4 and on rigorous mathematical analysis in RT7.

The effect of the geometric phase on excited states in magnetic fields was studied in detail in work by Culpitt, Tellgren, Peters, and Helgaker [10]. The geometric phase is partly an expression of an ambiguity that appears when the electrons and nuclei in a molecule are treated on an unequal footing; e.g., a quantum mechanical description of the electrons and a classical description of the nuclei. However, it is partly a physical effect with consequences for the motion of the nuclei and resulting transitions between electronic states (Figure 2).

Hylleraas affiliate Stella Stopkowicz with co-workers have reported a variety of studies related to strong magnetic fields. Closed-shell paramagnetism, previously well-characterized when arises from p-orbitals, was studied for scandium and yttrium hydride, where it instead arises

due to the d-orbitals [11]. An investigation of methods to screen away small or negligible contributions in calculations of matrix elements for molecules in magnetic fields was also completed [12]. Another type of technique to improve the computational efficiency, namely Cholesky decomposition, was implemented and tested for coupled-cluster (CC) and equation-of-motion coupled-cluster (EOM-CC) methods [13] as well as for second-order derivatives [14]. Finally, the methods approximate coupled-cluster methods CC2 and CC3 were implemented for calculations of molecules in strong magnetic fields. It was found that CC2 may lead to unphysical result, while CC3 is a good approximation to the highly accurate CCSDT method [15].

The work by Monzel and Stopkowicz, the former a previous visitor to the Hylleraas center, presented a diagrammatic formalism for coupled-cluster ground and excited states in the presence of quantized electromagnetic fields, where the photon degrees of freedom are handled explicitly [16].

Software

In 2024, Bin Gao published an article in Journal of Computational Chemistry about his Tinned library—a C++ framework for symbolic differentiation and manipulation in response theory [17]. By identifying key components in density matrix-based and coupled-cluster response theories, the library implements corresponding symbolic classes for one- and two-electron operators, exchange-correlation energy and potential, and the coupled-cluster operator. This allows response theory formulas to be expressed

symbolically, with high-order perturbation derivatives easily computed and extracted for numerical evaluation. In summary, Tinned helps to streamline response theory development and provides a unified framework across different levels of electronic structure theory.

Personnel and Funding

Research in RT3/4 in 2024 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; RCN (Mobility) grant *Linear and Non-linear Response Properties and Spectroscopy of Solids from Relativistic TDDFT* led by Lukas Konecny.

In the Oslo node, currently E. Tellgren (researcher) is primarily active in RT3/4 and recruitment for a 2 year position supporting the work in the Oslo node has begun. Hylleraas members Pedersen (professor) and Laestadius (researcher) contribute partially to RT3/4.

Tromsø RT3/4 research team in 2024 consists of Kenneth Ruud (professor), Michal Repisky (researcher), Magnus Ringholm (researcher), Marius Kadek (postdoc), Lukas Konecny (postdoc), Monika Krupova (postdoc), Marc Joosten (PhD), Vanda Le (PhD), Torsha Moitra (postdoc), and Rasmus Vikhamar-Sandberg (PhD).

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

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RT5 – Chemical Transformations

In RT5 we apply computational methods to understand chemical reactions and develop more sustainable processes in collaboration with experimental groups. Our strategy combines the computational-assisted characterization of reaction intermediates with reactivity studies, including microkinetic models for reactions of high complexity.

Principal investigators:
Ainara Nova and Abril Castro



Ainara Nova



Abril Castro

«To develop a more sustainable catalysts with the same activity, a machine-learning approach is followed»

Hydrogenations and CO₂ conversion reactions

Three projects related to CO₂ conversion reactions were finalized in 2024: the EU ITN CO₂operate, the RCN FRIPRO CO₂pCat, and the NordCO₂ consortium.

One of the reactions studied under these projects is the hydrogenation of CO₂ to methanol with the Ru-MACHO catalyst. This work is being performed by the COMPSCI PhD student Mohamed E. A. Safy under the supervision of Nova and in collaboration with MSCA Raquel J. Rama. This study uses density-functional theory (DFT) and coupled-cluster (CC) methods to calculate free energy pathways. The resulting energies are then incorporated into microkinetic models (MKM) to evaluate the evolution of all reaction species over time, allowing the direct comparison of computational data with experimental observations. While MKMs have been highly applied to heterogeneous catalysis, they are less used in homogeneous catalysis. To change this trend, Rama and Nova published a review on the application of this methodology to reactions catalyzed by molecular organometallic complexes [1]. This work includes examples from the literature where MKMs are used to analyze complex reaction mechanisms and extract useful information for improving catalysis, such as identifying kinetically relevant steps and catalyst resting states. In addition, the challenges and limitations of this methodology when applied

to homogeneous catalysis are described, as well as ways to overcome them.

One of the interests of Ru-MACHO is its high efficiency in the hydrogenation of polar unsaturated bonds by promoting the heterolytic cleavage of hydrogen by the acid-base properties of the Ru-N functionality. To develop more sustainable catalysts with the same activity and higher robustness, a machine-learning approach is followed by PD Lucía Morán, under the CO₂pCat project led by Nova in collaboration with David Balcells in RT7. Another direction for this project is evaluating if highly polarized bimetallic complexes can perform similar chemistry. This work was started in 2024 by the MSc student Audun Uglenes, supervised by Nova in collaboration with the DStrain PD Miguel Angel Gaona Fernández. In addition, the MSc student Øystein Senstad Alve is determining potential correlations between the hydricity of molecular hydride complexes with ¹H NMR chemical shifts under the supervision of Castro and Nova.

One of the aims of these studies is to understand the optimal properties of the M-N and M1-M2 bonds that can be transferred to heterogeneous catalysis. In addition, we want to analyze whether heterogeneous catalysts could behave as homogeneous catalysts. This idea is being explored by the PhD student Aurore Denjean using N-doped graphene-based single-atom catalysts

(SAC). In her first work, supervised by Nova and Balcells, she studied a borrowing hydrogen reaction catalyzed by a Ni(II)-SAC (see Figure 1) [2]. Different models were formulated, including pyridinic (Py) and pyrrolic (Pyr) configurations with various charges and multiplicities. Subsequently, the free energies to add two H-atoms to these systems at Ni, N, or C were calculated using DFT methods (PBEo-D3BJ/def2-SVP/SMD). From the different possibilities, including NiH-NH, NH-CH, NH-NH_{cis}, and NH-NH_{trans}, the NH-NH_{cis} hydrogenation with the pyrrole model was preferred. Further, the complete free energy profiles for the borrowing hydrogen reaction with this system using high and low spin configurations and 0 and +2 charges were computed. This study showed important differences in reactivity between the Ni-N bond in graphene-based Ni-SACs and the Ru-N in Ru-MACHO complex, which will be further analyzed in future studies using different metals.

Another heterogeneous catalyst we have thoroughly investigated is the Pt-NP encapsulated in the UiO-67 MOF for CO₂ hydrogenation reactions [3,4]. This project has resulted in a long-term collaboration between Nova, Prof. Olsbye (Catalysis group, University of Oslo), and Skúlason (University of Iceland). Many of the results produced by this study were included in the PhD dissertations of Harsha Pulumati, Hylleraas visitor in 2019, 2020, and

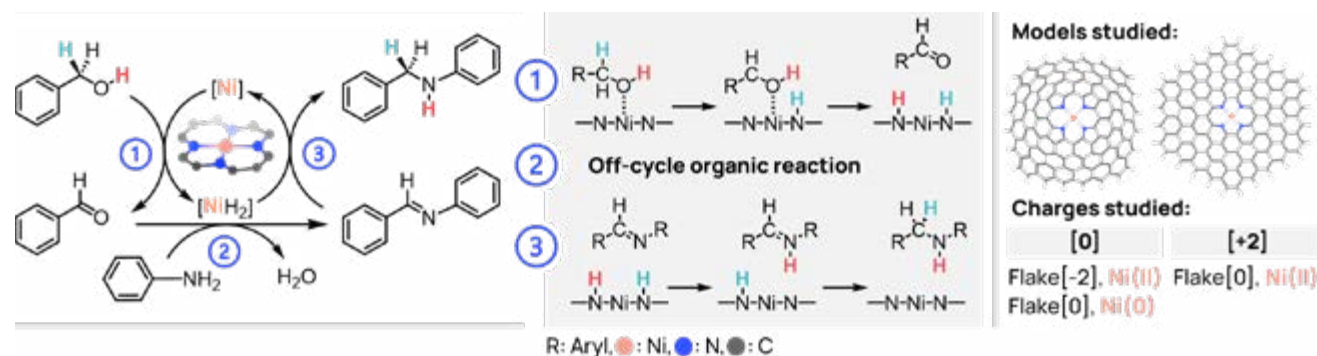


Figure 1: Borrowing hydrogen reaction studied using DFT methods. Illustration: Aurore Denjean.

2022, and Dag Sannes (experimental work) in 2024. That year, two publications appeared. The first describes the mechanism for the CO₂ hydrogenation reaction using different model systems (details of this work were provided in the Hylleraas annual report in 2023) [5]. The second one presents the reactivity of a similar system in which Zr atoms were replaced by Hf [6]. In this work, the adsorption energies of H₂O, methanol, and a mixture of both on a dehydrated and defective Hf SBU were determined by DFT methods. In addition, we built a microkinetic model to assess the species with the largest concentration at specific amounts of methanol and water. We found a higher affinity for water with Hf compared with Zr [4], which was used to explain the experimentally observed irreversible deactivation of the material in the presence of water.

In addition to the thermal hydrogenation of CO₂, we are interested in the electrochemical reduction of CO₂, ideally to methanol or C₂ products. Since amines play an essential role in the thermal reaction, we investigated systems using pendant amines. Dr. Mahika Luthra, who defended her PhD in January 2024 under the supervision of Nova, worked on this project. In her last publication [7], the influence of the metal on product selectivity was ex-

plored under the supervision of Castro, Balcells, and Nova. By using ab initio molecular dynamics (AIMD) to analyze the flexibility of the (bpy)Re(CO)₃ moiety and calculating free energy profiles for the formation of H₂, CO, and HCO₂H using the Re and Ru systems, we were able to explain the experimental observations. Our results suggest that the product selectivity changes from formic acid, with Mn, to CO, with Re and Ru, because each transition metal prefers a different reaction mechanism (Figure 2). As a continuation of this work, MSc Gabriela Garcia and Dr. Mauricio Portioli Franco from Brazil visited the Hylleraas Centre in 2024 to study the mechanism for the electrochemical reduction of CO₂ to C₂ products with M-corrole systems.

Another way to utilize CO₂ is through its co-polymerization with epoxides. Understanding the mechanism of this reaction using highly tunable ligands, such as N-heterocyclic carbenes (NHC), was one of the aims of the young talent of Nova. While this project was finalized in 2020, one publication appeared in 2024. This study, performed by Postdoc Torstein Fjermestad in collaboration with Prof. Erwan LeRoux (University of Bergen), investigated the mechanism of a CO₂ co-polymerization reaction catalyzed by the anionic [(κ³-O,C,O)-NHC)HfCl₃] complex using DFT methods

[8]. Interestingly, our results showed that the energy barrier for the CO₂ insertion into the *trans* Hf-O bond decreased after replacing two or three Hf-Cl bonds via epoxide ring opening. Only after this process occurred did the ring opening become the rate-limiting step, as observed experimentally.

Following our interest in hydrogenation reactions, Schmidtke has studied the reaction mechanism for ethylene hydrogenation with RhH(PPh₃)₃ in collaboration with Prof. Timo Repo (University of Helsinki). In this work, ³¹P NMR simulations, supervised by Castro, were used to assign one of the reaction products. In addition, the Hylleraas visitor, Dr. Gabriel M. Batista, from Aarhus University, studied the reaction mechanism for the C-O hydrogenolysis of an epoxy polymer using a (tripos)Ru complex and isopropanol as a hydrogen source [9]. The reaction mechanism was studied by combining experiments and DFT methods using a model system in which phenyl groups replaced the methyl bisphenol A substituents. The reaction pathway proposed was complex and unexpected. The reaction starts with the oxidation of the epoxy alcohol group, which has two effects: producing a Ru(II)-H and weakening the C-O bond in the beta-position. The final cleavage of this bond occurs by its oxidative addition into a Rh(o), which is

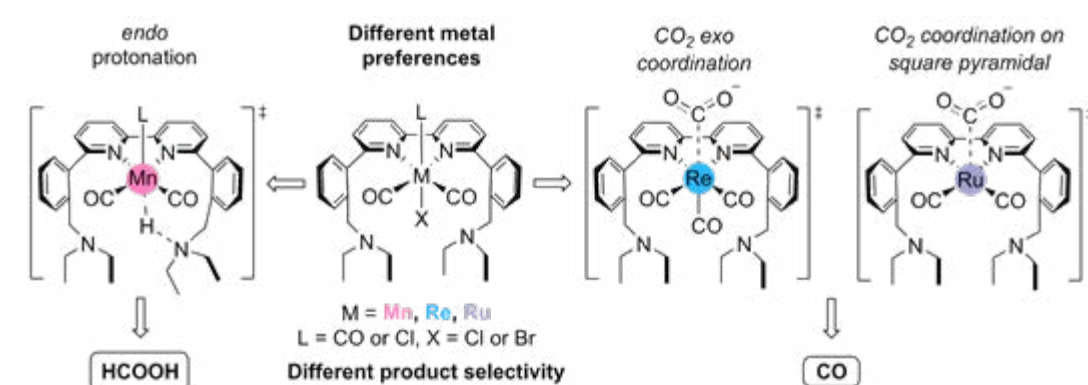


Figure 2: Critical steps defining product selectivity for Mn, Re, and Ru complexes. Illustration: Mahika Luthra.

produced by the reductive elimination of H₂. The additional hydride leading Rh(II)H₂ comes from the oxidation of isopropanol. The protons from the alcohol groups are used to protonate the Rh(II)-O and Rh(II)-C intermediates, liberating the final products.

C-H activation reactions

The selective activation of C-H bonds is a highly challenging reaction, particularly for unfunctionalized molecules like methane or cyclohexane. The oxidation of these substrates using hydrogen peroxide is one of the aims of the CUBE EU synergy grant project led by Olsbye from the catalysis group, which also involves the participation of Nova and Balcells. The mechanism for the reaction with cyclohexane using a Cu-NNN tridentate complex anchored into the UiO-67 MOF was studied by the PhD Ning Cao [10]. This system was modeled using periodic DFT calculations and AIMD simulations. Details of this work are described in the research highlight by Ainara Nova. In addition to reactivity studies, DFT methods were also used for the structural characterization of the Cu active site on a UiO-66 functionalized with histidine and Cu(II) ions [11]. This material was active in the aerobic oxidation of cyclohexene with tert-butyl hydroperoxide, yielding cyclohexenol and cyclohexanone. Starting from the optimized structure of

the pristine UiO-66, different models were built by replacing a linker with either histidine, a neutral hydrated Cu(II) species, or a histidine-Cu(OH) complex. The optimized structures were used to assist EXAFS fitting, which allowed us to conclude that most Cu atoms were located on the defective node. This result was also consistent with calculated thermodynamics using cluster models, showing that the Cu coordination to the Zr-node is more exergonic than to a histidine ligand.

Other catalytic C-H bond activation reactions studied are the coupling of methane and benzene using an Iridium complex and the coupling of aliphatic amines and organic halides using a Palladium complex. The first work was carried out by the PhD student Inga Lena Schmidtke, supervised by Nova, in collaboration with Prof. Pedro Perez (University of Huelva), and was submitted for publication in January 2025. The second work, published in 2024 [12], was performed by the Hylleraas visitor, Dr. Juliane Heitkämper, under the supervision of Nova and in collaboration with Bert Maes. In this study, DFT methods (Mo6-D3/def2-SVP/def2-TZVP, SMD) were used to determine the reaction mechanism for the formation of 3-(2-phenylethenyl)-N-picolinoylcyclohexanamine (3a in Figure 3). In this reaction, the oxidative addition of the

organobromide to Pd(II) was not found to be the rate-limiting step but rather γ-C(sp³)-H bond activation of the substrate. The Pd resting state was a Pd(II)-Br complex coordinated with the reaction product. The formation of this complex was prevented by using KOPiv as a co-catalyst, which allowed the bromide exchange by pivalate via precipitation of the KBr coproduct. In addition, the pivalate anion was found to facilitate the C(sp³)-H bond activation step via a concerted metalation deprotonation pathway.

Advancing ¹⁹F NMR prediction of metal-fluoride complexes in solution

Under the supervision of Castro and in collaboration with Kathrin Hopmann from the UiT – The Arctic University of Norway, significant efforts have been made to advance the prediction of ¹⁹F NMR chemical shifts in transition-metal complexes.

PhD candidate Sahil Gahlawat performed the computational work, employing state-of-the-art quantum chemistry methods to achieve accurate predictions of ¹⁹F NMR chemical shifts in square-planar nickel-fluoride complexes. This study highlights the crucial role of solvation effects in such calculations and was published in *The Journal of Physical Chemistry A* as part of the

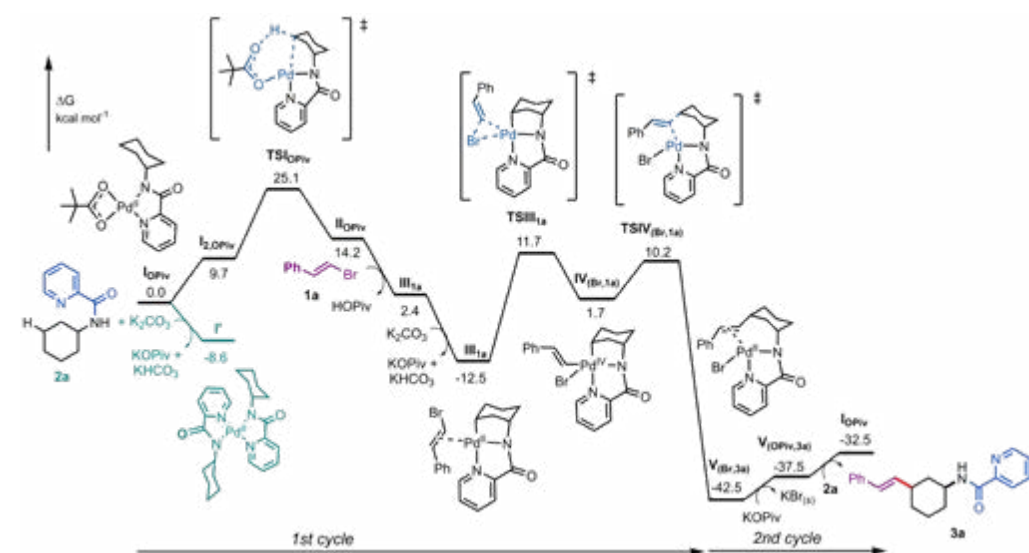


Figure 3: Free energy profile for the alkylation of *N*-picolinoylcyclohexanamine with (*E*)-β-bromostyrene. Adapted from ref. [12] under CC-BY 4.0 license.

virtual special issue “Trygve Helgaker Festschrift” [13].

The computational protocol used *ab initio* molecular dynamics (AIMD) simulations to capture the dynamic conformational flexibility of the square-planar $\text{trans}[\text{NiF}(\text{2,3,4,5-C}_6\text{F}_4\text{I})(\text{PEt}_3)_2]$ complex (Figure 4). This approach accounted for intramolecular interactions that implicit solvent models fail to capture, revealing effects that only become apparent with explicit solvation treatment.

Including dynamic averaging through AIMD simulations significantly improved the predicted ^{19}F NMR chemical shift of the nickel-bonded fluoride. This enhancement can be attributed to the considerable flexibility of both the phenyl group and the two $\text{P}(\text{Et})_3$ ligands, leading to pronounced non-covalent interactions around the fluoride ligand and the nickel center throughout the AIMD trajectory.

A relativistic approach for interpreting NMR chemical shifts on a molecular level

Accurate computational modeling of NMR chemical shifts in transition-metal complexes requires reliable treatment of relativistic effects, including scalar and spin-orbit (SO) coupling. These

effects are typically addressed using two-component (2c) or fully four-component (4c) relativistic approximations to the Dirac equation. While 2c methods, simplify calculations by separating wavefunction components, 4c methods offer higher accuracy, particularly for heavy-atoms systems.

Ramsey's approximation explains how paramagnetic contributions influence the NMR shielding tensor, with deshielding effects becoming more pronounced as the energy gap between interacting orbitals decreases. Deshielding of a nucleus is expected along the direction *i*, when an occupied orbital on this nucleus aligns with a vacant orbital on the same nucleus, rotated by 90° along the axis *i* (Figure 5).

The Natural Chemical Shift (NCS) analysis is widely used to interpret these paramagnetic contributions but is currently limited to non-relativistic and 2c methods, which may obscure spin-orbit coupling effects. To address this limitation, our project aims to develop a robust 4c-NCS methodology using relativistic 4c-DFT.

The key-point to enable the NCS analysis is to take advantage of the localized molecular orbitals (NLMOs) produced

during a Natural Bond Orbital (NBO) analysis calculation [14]. Hence, understanding how the NBO analysis transform the molecular orbitals is central to develop a method in a more general framework. The PhD candidate Alberto Guerrero is currently performing these studies under the supervision of Castro, Michal Repisky (RT3/4), and Simen Reine (RT0).

Personnel and Funding

RT5 received the visit of two PhD students and one PD in 2024. These were MSc. Gabriela Garcia from the University of São Paulo (Brazil), MSc. Ronghui Lu from Aarhus University (Denmark), and Dr. Mauricio Portioli Franco from the University of Campinas (Brazil). In addition, Prof. Rinaldo Poli, from the CNRS, Toulouse (France), visited the Hylleraas for a couple of days during the NKS National meeting organized in Oslo in June.

The mobility of PhD students and PD from RT5 has been mostly related to conferences. Inga Schmidtke and Jose Alberto Guerrero Cruz participated in the EuChemS Chemistry Congress in Dublin (Ireland) with oral and poster presentations, respectively. Inga Schmidtke and Aurore Denjean contributed to the 45th International Confer-

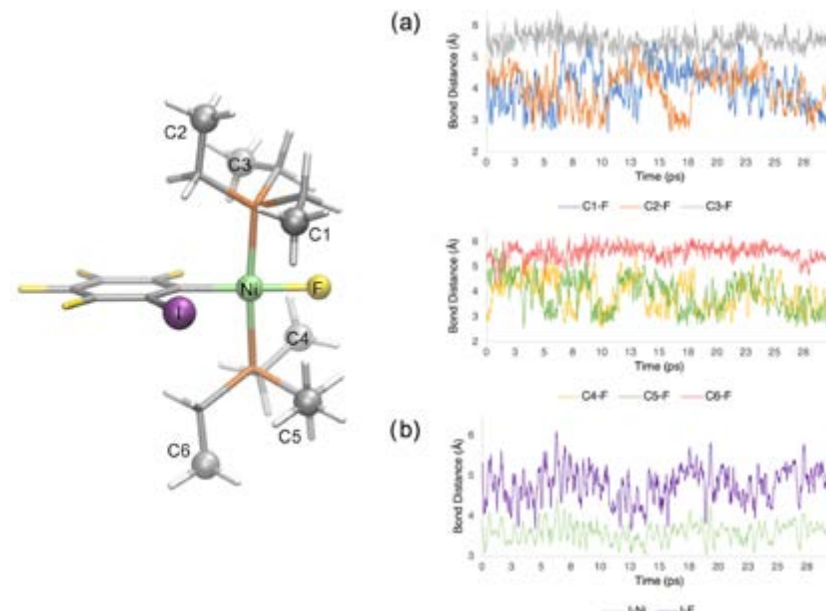


Figure 4: Evolution of distances between a) the fluoride ligand and the carbon atoms of the PET_3 ligands, and b) the iodine atom on the phenyl ligand with either the nickel metal or the fluoride ligand. Reproduced from ref. [13] under CC-BY 4.0 license.

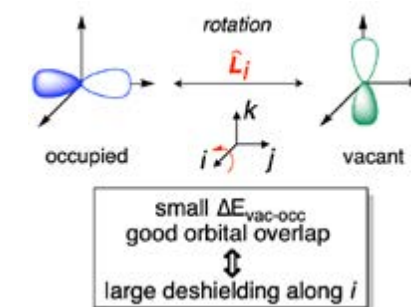


Figure 5: Magnetically induced coupling of occupied and vacant orbitals leading to a deshielding along the *i*-axis. Illustration: Abril Castro.

ence on Coordination Chemistry (ICCC) in Fort Collins, Colorado. Schmidtke won a poster prize at this conference, and Denjean contributed with an oral presentation. Schmidtke and Denjean also contributed with poster presentations to the Chemistry@Sete event in France to celebrate the 75th birthday of Prof Odile Eisenstein. Ning Cao gave an oral presentation at the International Conference on Theoretical Aspects of Catalysis in Seville, Spain. Mohamed Safy presented a poster at the ACS spring meeting in New Orleans, USA, while he was visiting Prof. Heather Kulik's group at MIT (US) for three months.

Nova was invited to give oral presentations at four international conferences in 2024: the “Molecular Heterogeneous Catalysis in Confined Geometries” symposium in Stuttgart (Germany), the Chemistry@Sette in Sete (France), a Sustainable Development Forum in Nanchang (China), and the ICC in Fort Collins (US). In addition, she contributed with an oral presentation at the Nordic Organometallic Meeting organized by the University of Helsinki (Finland) and co-organized the Symposium “Computational Approaches at the Atomic Scale of Catalysis – Unifying Concepts to Tackle Dynamics in Com-

putational Catalysis” at the 18th International Congress on Catalysis (ICC) that took place in Lyon, France. She also organized the NordCO₂ Symposium on Sustainable Chemistry in December at the University of Oslo.

As already mentioned, 2024 was the last year of three funded projects: the NordForsk NordCO₂, the EU-ITN CO₂-PERATE, and the FRIPRO CO₂pCat. The EU SyG CUBE project and FRIPRO-YT SpecTraM will last until 2026. In addition, in 2024, Castro, together with Profs. Petra Szilagyi and Unni Olsbye from the Catalysis group and F. Pourpoint from the University of Lille (France), received funding from the FRIPRO mobility program AURORA to promote the use of solid-state NMR of MOFs for CO₂ conversion reactions.

The PhD student Guerrero obtained a research mobility grant funded by the RCN to visit the Comenius University in Slovakia for five months to work on the project “4c-NCS – A Relativistic Approach for Interpreting NMR Chemical Shifts on a Molecular Level”. During his stay, he worked under the supervision of Michal Repisky.

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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



David Balcells



Simen Kvaal

«Hannes and David published a perspective in Chemical Science discussing the potential synergies between evolutionary and deep learning methods in the exploration of the chemical space»

Autocorrelations

This year we finished several projects that were initiated in 2023. These include the work on the atom-atom bond-bond bond-atom (AABBA) autocorrelations. AABBA is a set of functions that transform molecular graphs into a fixed-length vectors that, acting as fingerprints, reflect the topology and attribution of the graphs. The novelty of AABBA, compared to other autocorrelation transformations, is its ability to operate on both the node (i.e., atom) and edge (i.e., bond) properties of the graph. When tested in discriminative machine learning models like, for example, deep neural networks predicting energy barriers of metal-assisted reactions [1], AABBA clearly outperformed autocorrelations operating only on node properties. This work was done by Hylleraas members Lucía Morán-González, Jørn Eirik Betten, and Hannes Kneiding. Lucía was the main contributor, and she presented this work at the 2024 NKS Conference on theoretical chemistry in Trondheim (Norway). Jørn worked on dimensionality reduction with gradient boosting machines showing that both node- and edge-informed AABBA features are among the most relevant in the model predictions. After this work, Jørn moved to a PhD position at SIMULA in Oslo focused on the development of computer vision technologies. Hannes Kneiding contributed with the computation of the natural quantum graphs used as input [2] and Nishamol Kuriakose is currently leading the effort

to extend AABBA support to metal organic frameworks (MOFs), in the context of her HYSTRAM EU project. The work was supervised by David Balcells, and it was recently published in the special issue of the ACS Journal of Chemical Information and Modelling on the exploration of the chemical space [3].

Evolutionary multiobjective optimization

Another project from 2023 that was finished and extended during this year was the multiobjective optimization of metal complexes. Hannes Kneiding developed a genetic algorithm for this task with fine control over the direction and scope of the optimization, allowing for precisely selecting the region of the Pareto in which the solutions are evolved. David supervised the work and, together with Ainara Nova, contributed with a method for defining metal ligand charges from NBO analysis. The work was peer-reviewed and published in Nature Computational Science [4] and thereafter highlighted in Titan, the scientific Magazine of the University of Oslo [5]. This research was funded by the EU COFUND program (COMPS-CI project) and it was presented by Hannes at the AI for Chemistry conference (Figure 1) organized by the Royal Society of Chemistry at the University of Cambridge (UK), and by David at the Gordon Conference on Computational Chemistry in Portland (USA). In the second half of 2024, after successfully defending his PhD thesis, Hannes deve-

loped this method further for the optimization of three-dimensional problems, working together with Alejandra Pita, a visitor from the IIQ Centre in Sevilla (Spain), who also contributed to an extension of the code supporting execution in supercomputers. In relation to this work, Hannes and David published a perspective in Chemical Science discussing the potential synergies between evolutionary and deep learning methods in the exploration of the chemical space [6].

High-throughput virtual screening

Arron Burnage continued his work on high-throughput virtual screening. The focus was on metal-catalyzed cross-coupling reactions, considering three different variables: 1) oxidative addition barrier, 2) reductive elimination barrier, and 3) solvent coordination thermodynamics. The first and second variables are related to catalyst activity, quantifying the kinetics of the substrate-entry and product-exit to and from the catalytic cycle, whereas the third accounts for catalyst robustness, quantifying the in/off-cycle mass ratio of the catalyst. When screened over a chemical space containing hundreds of metal complexes, these variables provided a picture in which only a few of them were in the ideal region in which both barriers are low and solvent coordination is thermoneutral or endoergic (Figure 2). Interestingly, when further investigated through the Cambridge Structural Database, it was found that many of these complex-



Figure 1. Hannes Kneiding defended his thesis on September 27, 2024. Just ten days earlier, Hannes presented his latest work at the conference Artificial Intelligence for Chemistry which was organized by the Royal Society of Chemistry at the University of Cambridge, UK. Photo: Hannes Kneiding.

es identified as optimal had been already reported in the literature as active catalysts for cross-coupling reactions. Arron presented this work at the 2024 NKS Conference on theoretical chemistry in Trondheim (Norway). Hannes also contributed with the ligand library extracted from the tmQM dataset [7], and both Ainara and David contributed as supervisors. A first manuscript was drafted, and its peer-review is expected in 2025. The results of the screening shall inspire future work on active learning approaches to this chemical space based on similarity measures in the latent space of deep neural networks. This approach was also explored for CO₂ reduction catalysts in collaboration with RT5, and, connecting to both RT5 and RT2/6, Joel Ormala investigated the potential of using machine-learned interatomic potentials in the study of asymmetric catalysis.

Deep generative models

This year was also very active in the development of deep generative methods for transition metal complexes. Following the work done by Magnus Strandgaard, a visitor from Jan Halborg Jensen's group in the University of Copenhagen (Denmark), Trond Linjordet worked on the further extension of the junction tree variational autoencoder (JT-VAE), adding the conditional generation of metal ligands and improving the software engineering of the model. The JT-VAE is a complex method (Figure 3) in which a graph neural network (GNN) encoder maps molecular graphs into a latent space learned as a probability distribution. This distribution is thereafter decoded by a second GNN that tries to reconstruct the original graph. In order to augment the chemical validity of the output, graphs are encoded as junction trees which are coarsegrained representations in which

the nodes can be atoms, bonds, or rings. JT-VAEs are trained by minimizing a two-factor loss that includes a reconstruction term enforcing input = output, and a regularization term measuring the difference between the latent and normal distributions (Kullback-Leibler divergence). An auxiliary task can also be added to map the latent space into molecular properties, enabling generative tasks conditioned by a prompt expressing target values for those properties. The work done by Magnus and Trond delivered a JT-VAE that can do metal ligand and complex generation with high validity, uniqueness, and novelty, relative to the training data. Arron and Hannes were also part of the team, contributing to software engineering and chemical interpretation, respectively. Under the supervision of David, and in collaboration with Ainara and Jan, a manuscript was drafted and uploaded to the ChemRxiv

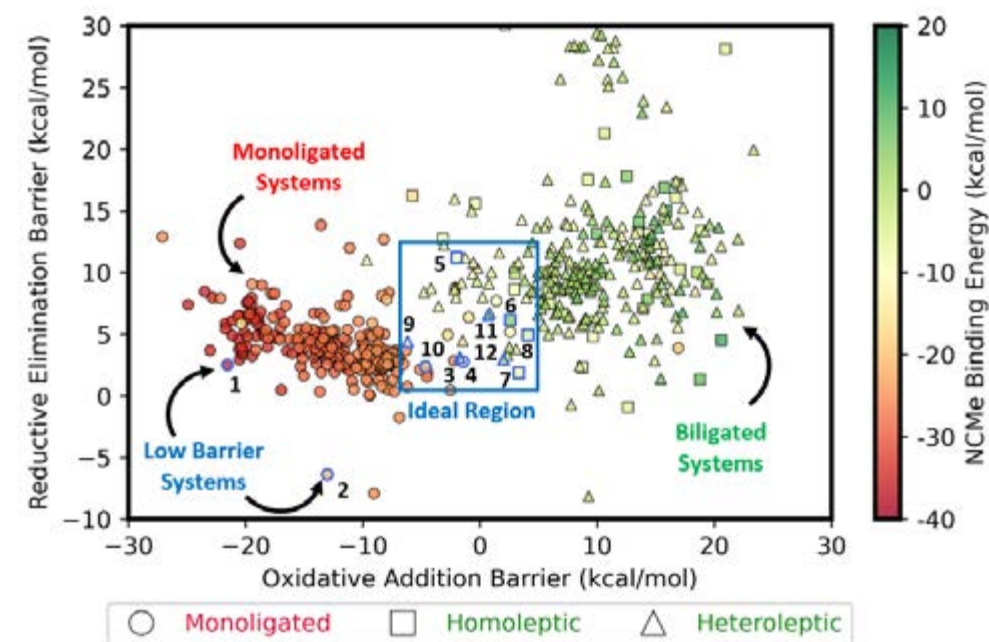


Figure 2. High-throughput virtual screening over three variables for metal complexes in cross-coupling reactions. Illustration: David Balcells.

preprint server [8]. This work was also presented by David in the Löwdin Symposium in Uppsala (Sweden) and the first edition of the Chemical Space Conference held in Heidelberg (Germany). David's CatLEGOS FRIPRO Grant for Ground-Breaking Research was the main funding source supporting this project. Also on the topic of generative AI, Trond started a project on diffusion models generating 3D geometries of metal complexes.

Coupled-cluster theory

The RCN project CCerror combines mathematics, physics, and chemistry and has been carried out at the Hylleraas Centre since December 2019. It directly involves PI Andre Laestadius and researcher Mihaly Csirik (both in adjunct positions). During 2024, the project work has continued addressing the mathematical aspects of coupled-cluster theory with the aim of generalizing results bey-

ond the strong monotonicity assumption, which are also applicable to excited states. Currently, the researchers of CC-error are collaborating with former Hylleraas member Fabian M. Faulstich and Aachen-based postdoc Mathias Oster.

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 (S. Kvaal), 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 (Figure 4). 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 are 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

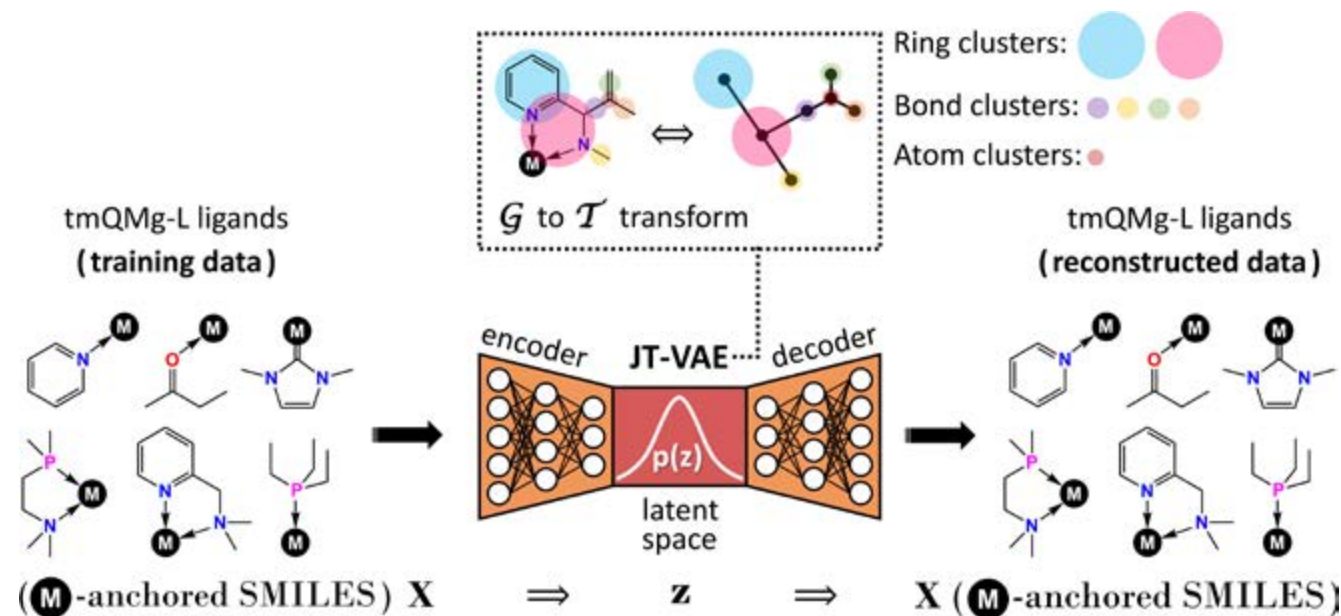


Figure 3. The JT-VAE method for metal ligand complexes. Illustration: David Balcells.

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 2024, the group is nearing the completion of a major mathematical study of error estimation in coupled-cluster theory.

Density-Functional Theory

A central research topic at the Hylleraas Centre is the mathematical development of density-functional 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. II Andre Laestadius (Associate Professor at OsloMet, 20 % at Hylleraas) aims to make MY-DFT a practical tool.

Laestadius, Csirik, Helgaker, and collaborators have published a study [9] extending our knowledge on exact behavior of the universal density functional. In [10], it is argued that a promising route towards accurate exchange-correlation energy approximations is via exact force expressions. These studies are very encouraging and may provide us with mathematical tools to obtain better functionals for practical DFT calculations.

Rothe's Method for Time Propagation

Electronic and molecular wavefunctions are highly complicated and their representation and time propagation repre-

sents enormous challenges. Since the AttoDyn CAS project (2021–23), we have been working on an adaptive scheme for propagating wavefunctions represented as linear combinations of *explicitly correlated gaussians* (ECGs). This adaptive scheme is called Rothe's Method, and our work is featured in this year's report in a Research Highlight authored by Simen Kvaal. The work crosses the boundaries of RT7 (Machine Learning and Mathematical Methods) and RT1 (Molecular Quantum Mechanics). The ECG wavefunction representations yield an enormous compression ratio compared to conventional grid or fixed-basis representations, as is conventional in quantum chemistry. In 2024, the group with collaborators have published 3 studies: In a collaboration with L. Adamowicz (Arizona) and A. Wozniak (War-



Figure 4 (above). The QOMBINE project anno 2023. Back row, second from right: PhD candidate Håkon R. Fredheim. Front row, from right to left: PhD candidate Snorre Bergan, Simen Kvaal, Nadia S. Larsen, and Sergiy Neshveyev. Photo: Elisabeth Seland.

saw) [11], the group produced a proof-of-concept study demonstrated that ECGs were able to accurately describe the complex dynamics of several two-dimensional model systems. PhD student S.E. Schrader has developed a general implementation of Rothe's method with ECGs using analytical integrals. In [12], the full 3d dynamics of the hydrogen atom was simulated, and high-harmonic spectra that rivals fully resolved grid time evolutions were obtained. A follow-up study [13] was accepted for publication in December 2024, showcasing highly accurate ECG calculations on the Henon-Heiles model in dimensions up to 4. Encouraged by these positive results, the group is pursuing Rothe's method also for more complicated many-body models such as time-dependent

Hartree-Fock and time-dependent density-functional theory.

Visitors and personnel

2024 was also a hectic year from the perspective of funding and visitors. David participated as a partner, in the role of PhD supervisor, in an EU Doctoral Network project that was granted. This project, DEMO, is a large international consortium focused on the development of C-H activation catalysts with nanoporous materials, including MOFs and zeolites inspired on enzymes, and using diverse experimental and computational tools, including machine learning algorithms. All PhD students in the network will aim at obtaining a PhD degree from two European Universities. At Hylleraas, DEMO will fund three PhD positions that started this year: one, Michael Augello,

in which UiO will be the main host, and two, Flavie Le Rai and Lucas Bitencourt Theodoroviez, in which UiO will be the secondary host. Miguel Ángel Gaona Fernández was hired as a postdoc in the DStrain project of the UiO, which was recently funded by the EU COFUND program. He will work under the supervision of David on frustrated Lewis pairs for CO₂ uptake and activation, combining DFT modeling with machine learning methods. Besides projects, David's group hosted three visitors from Spain in three-month PhD exchanges supported by their own funding: Jordi Buils, from ICIQ, Gonzalo Darío, from the University Ro-

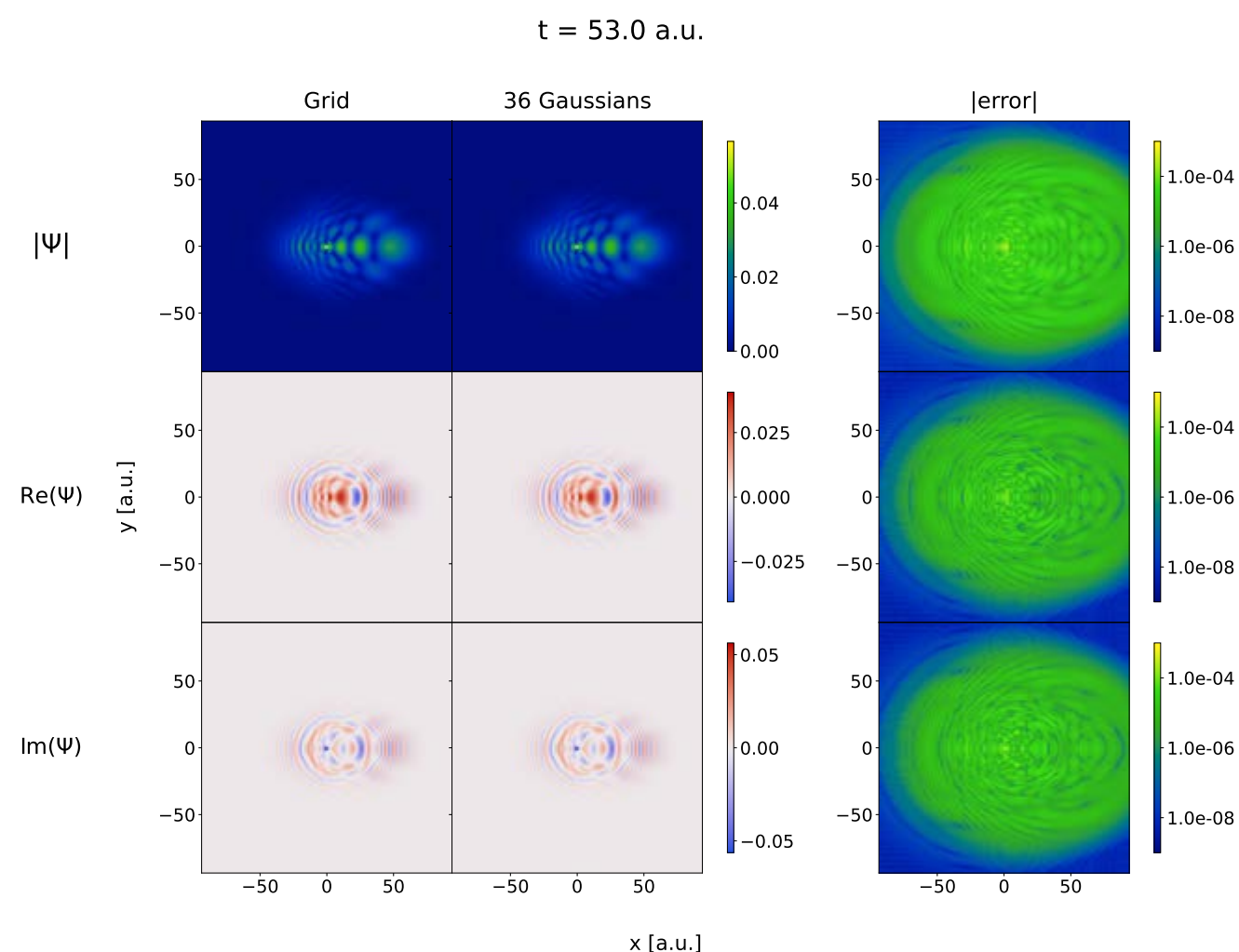


Figure 5. A snapshot of a simulation of a 2d hydrogen-like system subject to an extremely intense laser pulse. The figure shows a comparison of a virtually exact grid calculation, and the least-squares fit to a linear combination of 36 two-dimensional complex gaussian functions. On the right, the local error in space is plotted, showcasing the high accuracy obtainable by such a compact wavefunction representation. Reproduced from ref. [11] under CC-BY 4.0 license.

vira i Virgili, and Alejandra Pita, from IIQ. Sai Manoj, from the Tromsø node, visited Oslo for one month. Both Jordi and Gonzalo worked on molecular representations based on the quantum theories of atoms in molecules and natural bond orbitals. Sai worked in a training project on the topic of quantum-based machine learning, and Alejandra worked on three different projects: chemical space exploration of bimetallic complexes, graph neural networks predicting metal-ligand edges from point clouds, and three-objective optimization problems with genetic algorithms.

External Funding

catLEGOS FRIPRO, RCN, 2021-2025, 12 MNOK.
 DEMO Doctoral Network, EU, 2023-2027, 3.5 MEUR.
 HYSTRAM, EU, 2022-2025, 6.0 MEUR.
 QOMBINE, Fellesløft IV, RCN, 2022-2025, 3 MNOK share (25 MNOK total)

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RT0 – Hylleraas Software Platform

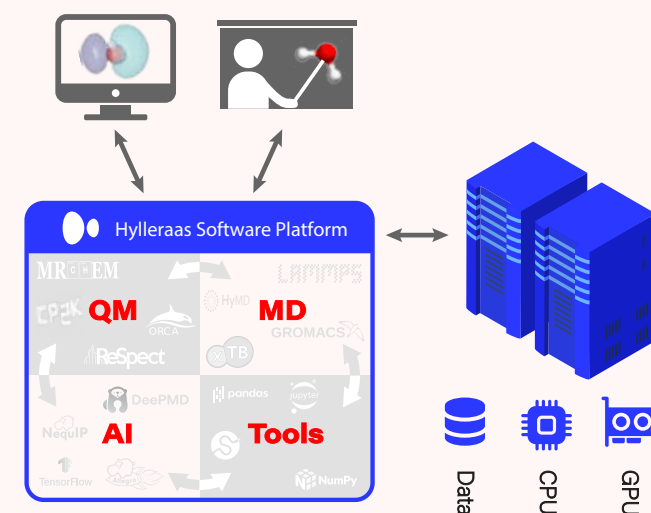


Figure 1. Illustration of the Hylleraas Software Platform and its current capabilities. Illustration by Morten Ledum.

«We have completed the active learning workflow, supporting usage of the Euro-HPC flagship super-computer LUMI.»

The year 2024 has been a highly productive and fruitful period for advancing the Hylleraas Software Platform for research and educational activities at the Centre.

Principal investigators:
Simen Reine and Bin Gao



Bin Gao



Simen Reine

This year, the Hylleraas Software Platform (HSP) team has focused on the application-driven development via internal and external collaborations, as well as education-oriented activities at the Centre (Figure 1). An important achievement is the completion of the active learning workflow, which is now in full production, involving, among other things, the usage of the EuroHPC flagship supercomputer LUMI. The workflow serves as a cornerstone for the active learning project in collaboration with Sigbjørn Løland Bore. The project began in 2023 with the aim to study complex scientific phenomena such as ion transfer processes, phase transitions, and chemical reactions. The HSP was integral to Bore's Centre for Advanced Study (CAS) workshop "Can Ice Be Described from First Principles?" in August 2024, where the focus was on automated machine-learning potential (MLP) generation for molecular dynamics studies of complex systems.

The team has also collaborated with RT3/4 and focused on the development of a flexible framework for studies of molecular properties using different electronic-structure approaches. A new member Gabriel Gerez, a Ph.D. Fellow

in theoretical chemistry at UiT and part of the HPC group at UiT, has joined the team this year and is dedicating 50% of his time to this project.

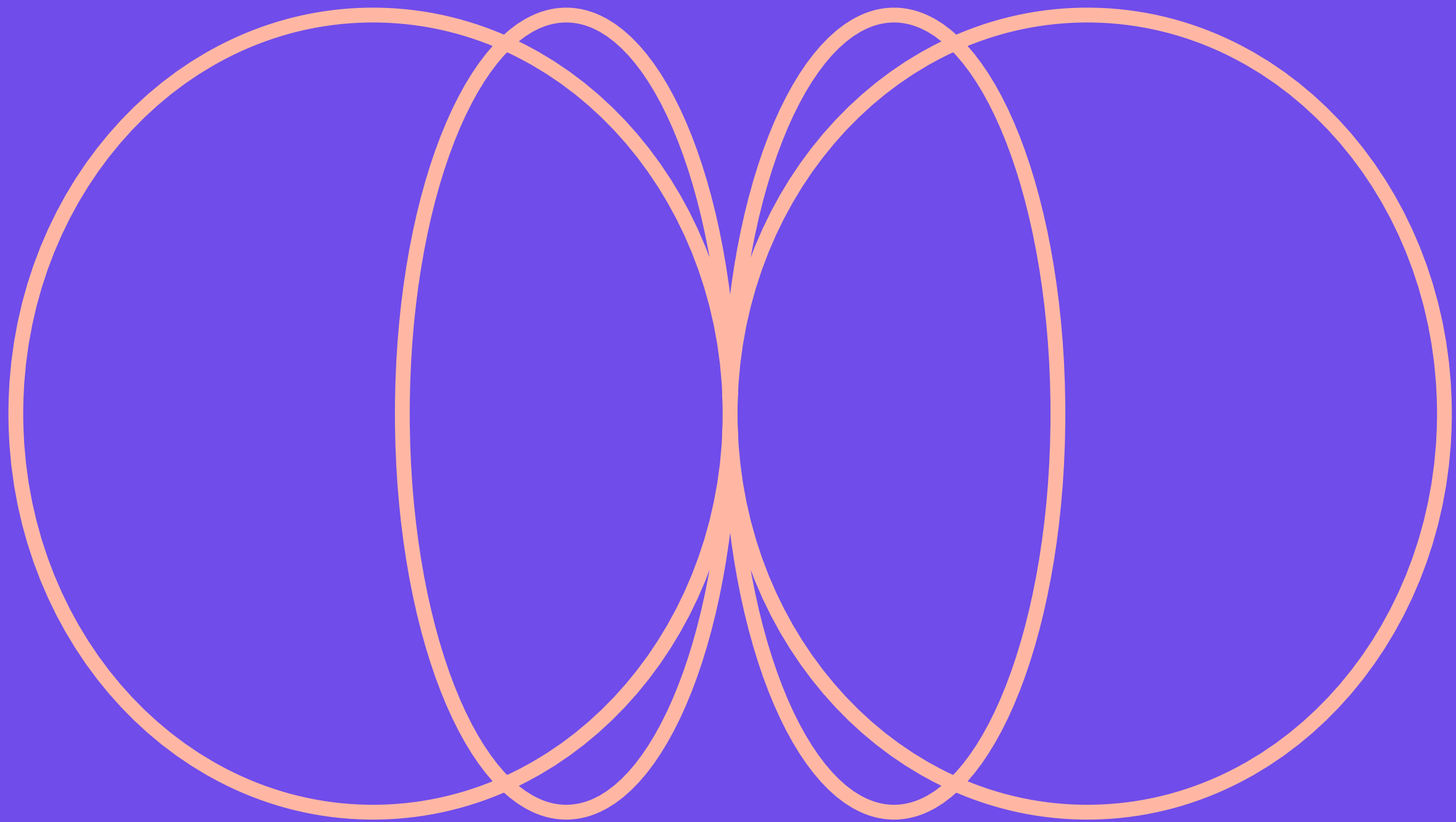
The Oslo-based team has also initiated a collaboration with Elisa Rebolini at the Institut Laue-Langevin (ILL) in Grenoble, France, to introduce HSP into the neutron experiment workflow for visiting scientists at ILL. The platform has been updated to support the local cluster at ILL in Grenoble. Team members Morten Ledum and Simen Reine spent one week in Grenoble in March, and Elisa visited Oslo in August. The next meeting of this ongoing collaboration is scheduled for February 2025.

A notable highlight of 2024 was the platform's involvement in pedagogical activities at the Centre. The platform was used for tutorials at the Hylleraas school 2024 (January 9th – January 12th), and for teaching visiting high school students in the Talentsenter with Erik Tellgren (January 17th) in Oslo. The platform was also used for an open introductory Python course for PhDs and other scientists affiliated with the Centre in December 2024, in connection with the upcoming 2025 Hylleraas school.

Furthermore, the team has worked on enhancing the platform's capabilities and user friendliness through a series of developments aimed at resolving various technical issues encountered by Centre members. An automated unit support system has been added, with built-in unit conversions, allowing for complex workflows involving programs with different internal unit definitions. Support for two-factor authentication (2FA) has also been implemented on the platform dispatcher, enabling the use of national HPC resources after the introduction of mandatory 2FA. Furthermore, the documentation of the platform has been thoroughly revised, with integrated and automated regression tests now running locally at UiO.

In summary, 2024 has been marked by an emphasis on the platform's application in both research and education at the Centre. The progress made significantly enhances the platform's capabilities as well as research flexibility within the Hylleraas community. External collaboration has also been initiated to expand the applicability of the platform across different research fields and to broaden its user base beyond the Centre.

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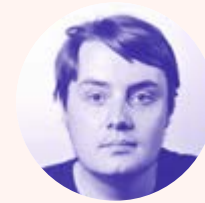
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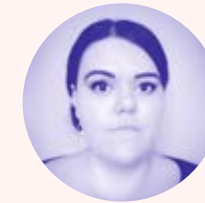
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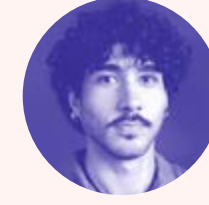
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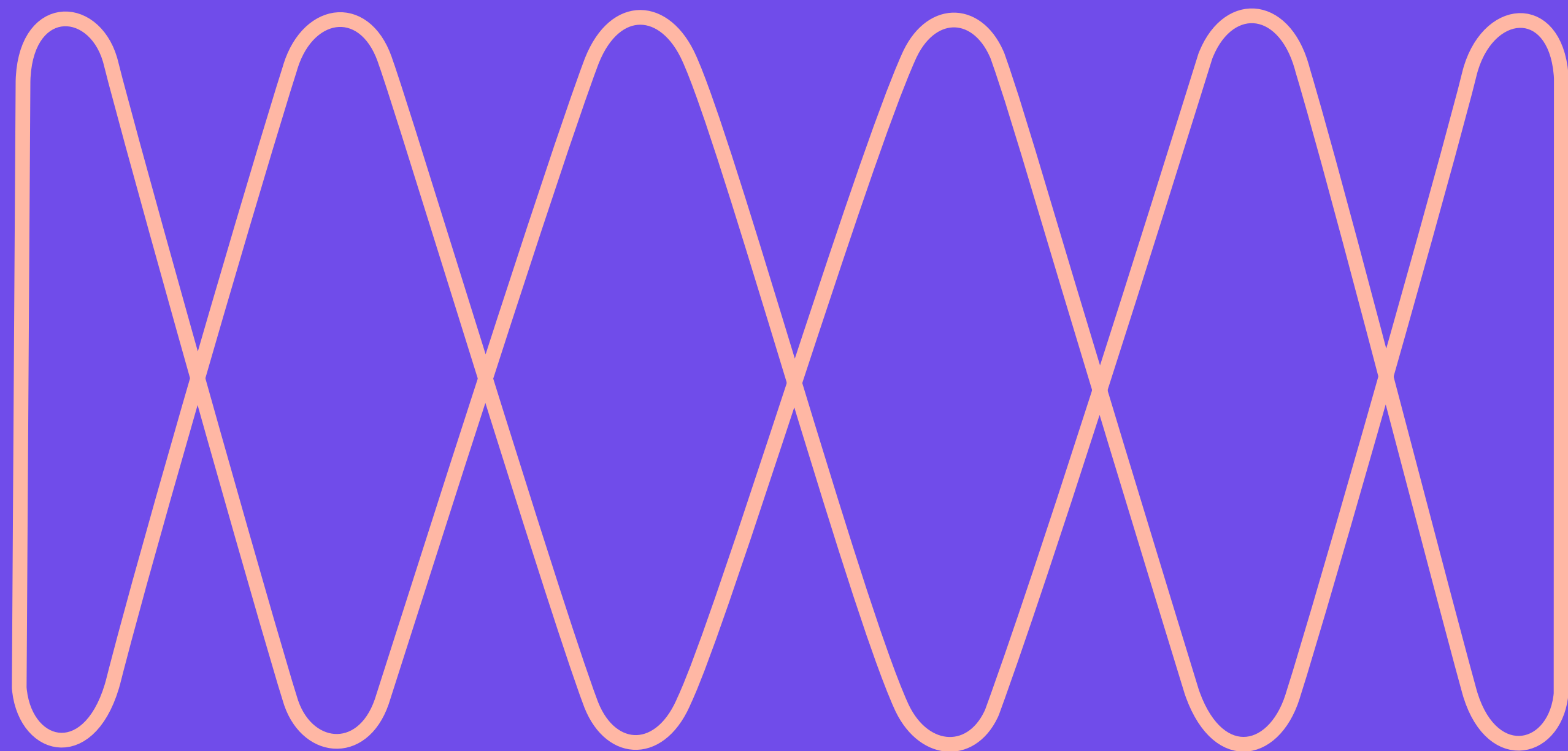


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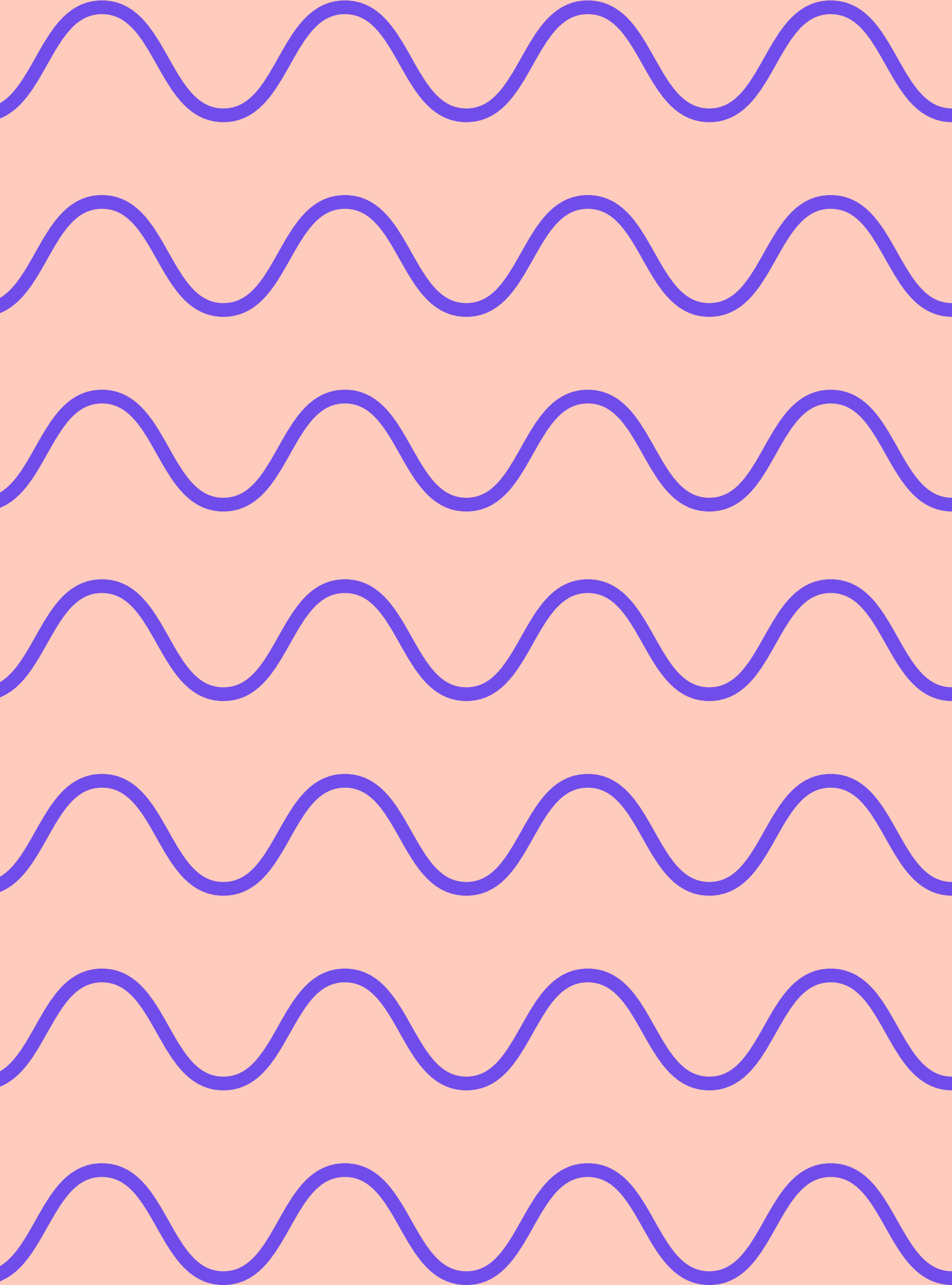
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Funding and Staff Report

“The [Hylleraas] Centre has been highly successful in its nationwide goals to train young people and to become a beacon of excellence in chemistry. It is internationally recognized as a world-leading centre for theoretical chemistry in its broadest sense. This accomplishment of the Centre is truly remarkable and cannot be rated high enough. As a result, it puts a burden onto the universities, as it is now their duty to make sure that the investment can be sustained after the end of the Centre in 2027.”

– excerpt from the 2022 Report of the Scientific Advisory Committee of the Hylleraas Centre.

Funding 2024

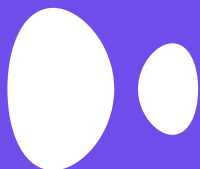
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Basic funding as agreed in the Centre contract	
Funding from Research Council (CoE grant)	17 283
Funding from home institutions	14 063
Total basic funding	31 346
Additional funding from external projects	
Research Council funding	22 683
International funding	4 538
Public funding	0
Private funding	0
Total additional funding	27 221
Total funding	58 567

Staff Report 2024

(in man-years)

Professors and researchers	18.8
PhD Candidates	21.7
Postdoctoral Fellows	11.5
Visiting Researchers	4.7
Administrative and technical staff	3.7
All staff	60.3



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