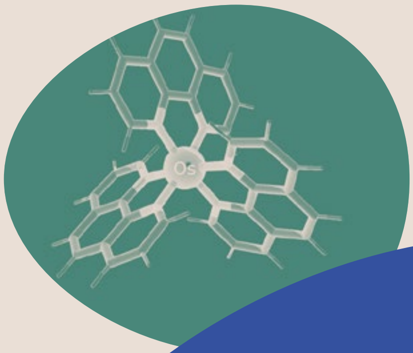
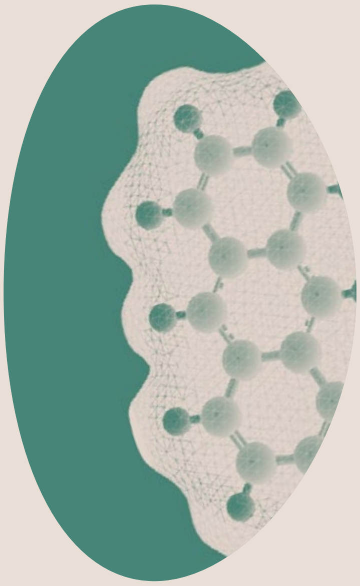
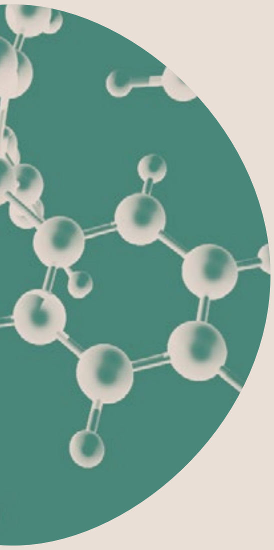
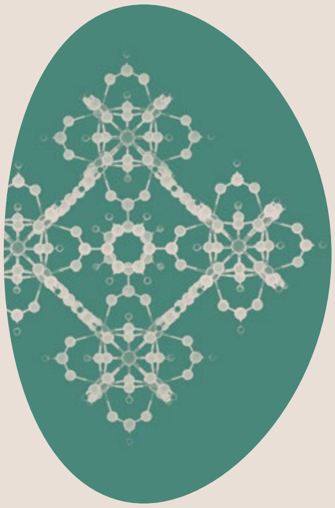




Hylleraas

Annual Report
2019





UiO : University of Oslo

UiT The Arctic
University of Norway

Norwegian
Centre of
Excellence

The Research Council of Norway

Hylleraas Centre for Quantum Molecular Sciences

The Hylleraas Centre 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. It receives an annual funding of 15 million NOK from the Research Council of Norway. In addition, it receives substantial financial support from UiO and UiT. The centre was established on October 1st 2017 for a period of five years with the possibility of an extension for a further five years following a mid-term evaluation.

The Hylleraas Centre is one of 23 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 students and postdocs from other research groups who wish to benefit from the expertise at the centre.

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From the Directors

The second full year of operation of the Hylleraas Centre was marked by several important events: the official opening of the Hylleraas Centre in September 2019, the establishment of the Young Researcher Parliament with participation of young researchers in the Management Team, the first visit of the Scientific Advisory Committee to the Hylleraas Centre, and the organization of the 10th Congress of the International Society of Theoretical Chemical Physics.

After nearly two years of full operation, the Oslo branch of the Hylleraas Centre moved into its refurbished premises at the Department of Chemistry, University of Oslo in June 2019. A few months later, on September 4 and 5, the Hylleraas Centre was officially opened in Oslo and Tromsø, respectively, with participation of Rector of the University of Oslo, Svein Stølen, and Prorector of the University of Tromsø – The Arctic University of Norway, Wenche Jakobsen as well as representatives of the Research Council of Norway, Liv Furuberg and Trude Dypvik. Our offices, seminar rooms, and other facilities in both Oslo and Tromsø are now in excellent shape and we are grateful to all who made this happen.

With the publication of 56 articles in international journals, 2019 was an active year for the Hylleraas Centre. Equally impressive is the broadness of our work, including studies of the fundamentals of density-functional theory, development of four-component relativistic methods for periodic systems, studies of electronic systems subject to lasers and ultrastrong magnetic fields, studies of CH activation, and studies of enzymatic systems. Indeed, the outstanding quality and broadness of our science were key elements of the report written by the Scientific Advisory Committee (SAC) of the Hylleraas Centre in November 2019. At the same time, the SAC pointed out that the potential of the centre for research across the different Research Themes (RTs) had not yet been fully realized. Several measures are now being introduced to strengthen the links between the six RTs at the centre – in particular, between the computational and methodological RTs. We would like to thank the SAC for their work in 2019 and, in particular, for their insightful and useful feedback on the research and other activities at the Hylleraas Centre.

Career development support was high on the agenda of the Hylleraas Centre throughout 2019. Indeed, as a result of the *Career Development Pilot Programme (KUPP)* initiated by the Hylleraas Centre in 2018, career development has become a priority at all Centres of Excellence at the University of Oslo and a report written on the KUPP initiative became an important input to career development work at the University in Oslo in 2019. At the KUPP workshop organized by the Hylleraas Centre in November 2019, experiences in career development were shared among the nine Centres of Excellence at the University of Oslo, aiming to improve career support at all centres. KUPP would not have been possible without the participation and leadership of Senior Advisor Olaug Kristine Bringager at the Research Support Office of the University of Oslo, for which we are very grateful.

As part of our efforts to improve career support at the Hylleraas Centre, a Young Researcher Parliament (YRP) was set up in 2019, whose representatives now participate in all decision making at the centre. More generally, the YRP takes an active part in all activities at the centre, including the organization of the Hylleraas Spring Meetings. It has its own budget, which may be used for workshops and other activities organized by the young researchers. We would like to thank all YRP members – in particular, its representatives Abril Castro, Karolina Eikås, Julie Héron, and Lukas Konecny – for their enthusiastic work and contributions to the centre.

In 2019, the Hylleraas Spring Meeting was held at Bardufoss May 13–15. We would like to thank Bin Gao for excellent organization of the meeting and, in particular, for the new format of the Spring Meetings he introduced for a more direct engagement of the participants in scientific and non-scientific activities at the meeting.

In July 2019, the Tromsø branch of the Hylleraas Centre with Kenneth Ruud as chair organized the *10th Congress of the International Society of Theoretical Chemical Physics (ISTCP)* in Tromsø. With more than 500 participants, it was not only the largest congress in theoretical chemistry worldwide in 2019 but also a resounding success – with a large number of excellent presentations and glorious weather. We would like to thank everyone who made ISTCP such a successful event and a wonderful inspiration for the Oslo branch of the Hylleraas Centre, who later in 2019 won the bid to organize the *13th Congress of the World Association of Theoretical and Computational Chemists* in Oslo 2023. In the course of the lifetime of the Hylleraas Centre, our members are thus on target to organize congresses in the three largest congress series in theoretical chemistry, recalling that Odile Eisenstein organized the *16th International Congress of Quantum Chemistry* in Menton in 2018, testifying to the high visibility of the Hylleraas Centre.

In his capacity as the Head of the Department of Chemistry at the University of Oslo, Jo Døhl has been the Chair of the Board of Directors of the Hylleraas Centre since 2017, helping to establish the centre. Having taken up the position as Director of the Faculty of Mathematics and Natural Sciences at the University of Oslo in November 2019, he stepped down from our board at the end of 2019. We would like to thank Jo Døhl for his valuable contributions and enthusiastic support of the centre. At the same time, we welcome Prof. Unni Olsbye, Deputy Head of the Department of Chemistry in Oslo, as our new chair and look forward to working with her.

We would also like to thank Stephanie Ramona Hansen for the excellent work she did as Administrative Assistant at the Hylleraas Centre in Tromsø from April 1 to October 31 2019. We wish her all the best in her new position as Adviser at the Faculty of Science and Technology in Tromsø.

Finally, we would like to thank all members and affiliates of the Hylleraas Centre for their great work in 2019, as documented by this Annual Report.

Trygve Helgaker

Prof. Trygve Helgaker

Director Hylleraas Centre
University of Oslo

Kenneth Ruud

Prof. Kenneth Ruud

Deputy Director Hylleraas Centre
UiT The Arctic University of Norway

(Photo: Ansgar Valbø/NORA)

From the Board of Directors

Another successful year for the Hylleraas Centre, but with more challenging times ahead.

2019 was another good year for the Hylleraas Centre. The scientific activity was high, with many novel and exciting results that have received well-deserved recognition as highlighted articles by journal editors. We also see increased collaboration across research themes and between the two centre nodes, in line with the centre's vision.

We congratulate centre director Trygve Helgaker with the 2019 Nansen Medal for Outstanding Research by the Norwegian Academy of Science and Letters, a well-deserved recognition of the high standards of his scientific work.

We are also happy to see that the first report of the Scientific Advisory Committee (SAC) confirms the high standards of the scientific activity of the centre. Although the SAC has identified areas where the full potential of the centre has not yet been realized, we are happy to see that the centre is actively following up on the recommendations of the SAC.

2019 saw the establishment of the Young Researcher Parliament at the centre. This is an innovative approach to build ownership to the centre among the young researchers. At the same time, it will also be a way of providing the young researchers with training and experience on the complexity of running a large research centre at the international research frontier. The board will follow the work of the Young Researcher Parliament with great interest.

The board commends members of the Hylleraas Centre, and Trygve Helgaker in particular, for the work done on the KUPP program. Through this program, aimed at improving awareness on career development for young researchers, the centre has had an impact far beyond its own scientific discipline, making a positive difference for young researchers.

Despite having been established only two and a half years ago, the Hylleraas Centre has already become an internationally recognized centre for quantum molecular sciences. The strong involvement of the centre in the *International Congress of Quantum Chemistry* chaired by Odile Eisenstein in 2018 and the *Congress of the International Society of Theoretical Chemical Physics* chaired by Kenneth Ruud in 2019 have contributed strongly to this centre visibility. Having won the bid to host the 2023 *Congress of the World Association of Theoretical and Computational Chemists*, the centre will continue to contribute to great meeting places for experts in quantum molecular sciences from all over the world.

On a closing note, we must address the ongoing corona pandemic. It is clear that this will have a huge societal impact. Universities are also affected in these challenging times and it is likely that the pandemic will have consequences both for research and training at the Hylleraas Centre.

The current crisis may impact PhD students and postdocs on temporary contracts, the recruitment of new staff, and the international visitors' program. We hope that the funders and the host institutions show as much flexibility as possible in this difficult situation, thereby helping to reduce the impact of the crisis on the scientific activities at the centre.

Since the research at the Hylleraas Centre is theoretical and computational in nature, it may continue from home offices and by means of web conferencing. Furthermore, the long experience the centre has with online group seminars and meetings will help ensure that its research to a large extent can continue uninterrupted.

The Board is confident that the leadership and members of the Hylleraas Centre will meet these challenges in the best possible way.

Jo Døhl (chair)
Head of Department
Dept. Chemistry
UiO

Camilla Brekke
Professor
Dept. Phys. Tech.
UiT

Atle Jensen
Professor
Dept. Mathematics
UiO

Nathalie Reuter
Professor
Dept. Bio. Sciences
UiB

Kajsa Ryttberg–Wallgren
Vice President
Vacuum Conveying Division
Piab Group, Sweden

From the Young Researchers

The Hylleraas Centre is committed to realize an inclusive work environment, where the young researchers (YRs) can actively shape their career development, define their own research lines, and at the same time contribute to the long-term scientific goals of the centre.

Part of the ambition was to create a platform for the YRs to voice our opinions and take part in the decision-making processes at the Hylleraas Centre. This vision was achieved by the establishment of the Young Researcher Parliament (YRP) during an open discussion session at the Hylleraas Spring Meeting in May 2019.

The YRP is run by young people for young people: undergraduate PhD students, postdoctoral fellows, and other young researchers that do not hold a permanent position at the Hylleraas Centre. The YRP is managed by two elected representatives and two substitutes with equal representation of each of the two Hylleraas Centre nodes. Everyone has the opportunity to bring matters to the YRP, and the representatives work actively with the Hylleraas Management Team to follow up decisions.

In 2019, we adopted a first plan of action and defined a political platform. Our vision, role, and scope are defined by a mandate with several key areas focused on monitoring and improving the well-being of the YRs during their stay at the Hylleraas Centre, promoting inclusion and fairness, motivating and aiding the YRs in the formulation of their career development plans, facilitating communication between senior and junior members of the centre, furthering the participation of YRs in the centre's dissemination and outreach, and encouraging ideas for new activities that fit both the mandate of the YRP and the objectives of the Hylleraas Centre.

As representatives of the YRP, our role is to inspire and empower the YRs to share ideas, suggestions, and opinions in an open and welcoming environment, gather these viewpoints, and to facilitate cultural and professional communication among all members of the centre. So far, we have seen a group of enthusiastic young researchers with many ideas on how to improve the day-to-day well-being at the centre and eager to establish creative arenas to formulate new, interesting research questions. Suggestions have been to teach one another newly developed or discovered tools, invite high-profile speakers from our field, as well as centre alumni to show their path in academia, industry, or other professions. The Young Researcher Parliament now has the mandate and budget in place, so more exciting work can begin.

Welcome to the Young Researcher Parliament!

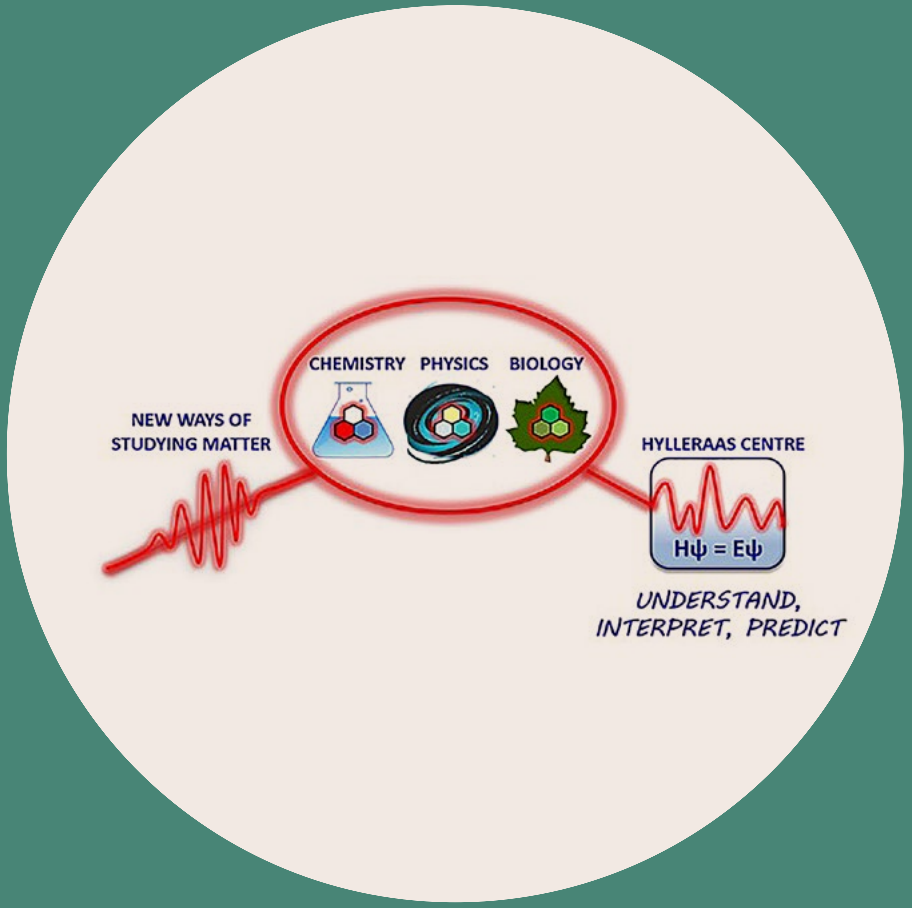
Abril Castro
Representative
UiO

Karolina Solheimslid Eikås
Representative
UiT

Julie Héron
Deputy representative
UiO

Lukas Konecny
Deputy representative
UiT

Elected YRP representatives 2019–2020



The Hylleraas Centre develops and applies computational methods to understand, interpret, and predict new chemistry, physics, and biology of molecules in complex and extreme environments.

2019 in Brief

Picture 1: *Back cover page of Dalton Transactions highlighting the article "Four-component relativistic ^{31}P-NMR calculations for trans-platinum(II) complexes: importance of the solvent and dynamics in spectral simulations" by Abril Castro et al.*

Picture 2: *ISTCP congress banner.*
© Michal Repisky

Picture 3: *Liv Furuberg presenting the SFF plaque to Trygve Helgaker at the opening of the Hylleraas Centre in Oslo.*
Photo: Bjarne Røsjø

WATOC
OSLO 2023

Picture 4: *Logo of WATOC 2023*
© Ferskvann Reklamebyrå AS

Publications

Members of the Hylleraas Centre published in total 56 articles in 2019, adding to the 82 articles published in late 2017 and in 2018. Most articles were published in *Journal of Chemical Theory and Computation* and *Journal of Chemical Physics* with eleven and five Hylleraas articles, respectively. However, members of the Hylleraas Centre also published work in several journals with broader readerships such as *Chemical Science, Journal of the American Chemical Society, Accounts of Chemical Research, ACS Catalysis,* and *Angewandte Chemie International Edition.*

In May 2019, the article *All-electron fully relativistic Kohn–Sham theory for solids based on the Dirac–Coulomb Hamiltonian and Gaussian-type functions*, published by Marius Kadek, Michal Repisky, and Kenneth Ruud in *Physical Review B*, was included in the *Editors' Suggestion list*, chosen by the editors and referees of that journal as being of particular interest, importance, or clarity. Likewise, the article *Isolation and study of ruthenium–cobalt oxo cubanes bearing a high-valent, terminal $\mathrm{Ru^V}$–oxo with significant oxyl radical character* published in the *Journal of the American Chemical Society* by David Balcells with researchers from UC Berkeley and UC Davis in November 2019 was highlighted in the *JACS Spotlights.*

In June 2019, the artwork of the back cover of *Dalton Transactions* represented a molecular dynamics simulation of a *trans*-platinum(II) complex in water solution, based on the publication *Four-component relativistic ^{31}P-NMR calculations for trans-platinum(II) complexes: importance of the solvent and dynamics in spectral simulations*, a collaboration of Abril Castro, Heike Fliegl, Michele Cascella, Trygve Helgaker, and Michal Repisky at the Hylleraas Centre, with Stanislav Komorovsky of the Slovak Academy of Sciences, Marcel Swart from the University of Girona, and María Ángeles Medrano and Adoración Quiroga from the Autonomous University of Madrid (*picture 1* ⇧).

Meetings and Conferences

The 2019 Hylleraas Spring Meeting was held May 13–15 at Haraldvollen Red Cross Centre in Bardufoss. The meeting was organized by Bin Gao and attended by forty members of the centre for three days of joint activities. Unlike earlier meetings, where traditional scientific presentations dominated, the program focused on joint activities within and across the research themes and between the two nodes of the centre.

The 2019 Almlöf–Gropen lecturer, Prof. Sharon Hammes-Schiffer of Yale University, delivered her lecture *Proton-coupled electron transfer in catalysis and energy conversion* on June 13 in Oslo and on July 11 in Tromsø, the latter as the opening lecture of the ISTCP congress (vide infra).

The Hylleraas Centre sponsored the *23rd European Conference on Organometallic Chemistry (EUCOMC)* at the University of Helsinki June 16–20 2019. Ainara Nova and Kathrin Hopmann, who co-organized one track at the conference, selected two computational chemists as speakers, Amalia Poblador from Université de Genève and Max Garcia from Trinity College Dublin, whose participation at the conference was sponsored by the Hylleraas Centre.

During July 11–17 2019, the Hylleraas Centre organized *the 10th Congress of the International Society of Theoretical Chemical Physics (ISTCP)* in Tromsø. With 545 registered participants, 202 lectures, and 280 poster presentations, it was the largest congress of theoretical chemistry world-wide in 2019. Blessed not only with excellent science but also with wonderful weather, the congress was an enormous success. The organizing committee was chaired by Kenneth Ruud, with the Hylleraas members at UiT The Arctic University of Norway in the local organizing committee (*picture 2* ⇧).

On August 22, the workshop *Combination of Theoretical/Computational Studies and Experiments toward Porous Coordination Polymers/Metal Organic Frameworks* was held in Oslo, organized by Hylleraas associate Dr. Michiko Atsumi as part of a collaboration between the Hylleraas Centre and Japanese research groups lead by Prof. Ehara (Institute of Molecular Science, Okazaki), Prof. Sakaki (Kyoto University), and Prof. Kitagawa (Kyoto University).

Following the refurbishment of the centre premises in Oslo during the first half of 2019, the Hylleraas Centre opened officially on September 4 in Oslo and on September 5 in Tromsø, after nearly two years of operation. In Oslo, the opening was attended by Rector Svein Stølen and Liv Furuberg from the Research Council of Norway; in Tromsø, by Prorector Wenche Jakobsen and Trude Dypvik from the Research Council of Norway. Members of the Hylleraas family were present in Oslo (*picture 3* ⇧).

The 2019 National Meeting of the Division of Quantum Chemistry and Modelling of the Norwegian Chemical Society was held at Radisson Blu Royal Garden Hotel in Trondheim October 8–9, organized by Prof. Ida-Marie Høyvik at the Norwegian University of Science and Technology. The meeting was supported by the Hylleraas Centre and attended by many of its members.

In December 2019, the Hylleraas Centre won the bid to organize *the 13th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC)* in 2023. The congress, which is expected to draw more than 1000 participants, will be held at Oslo Congress Centre July 19–25 2023. The organization committee consists of Hylleraas members at the University of Oslo and is chaired by Trygve Helgaker (*picture 4* ⇧).

Picture 5: *Banner for the meeting "Chemistry 2019 – On Odd Hassel's Shoulders". © Elina Melteig*

Picture 6: *Science writer Eivind Torgersen lecturing about the history of the periodic table to school children at Forskningsdagene in Tromsø on September 19. Photo: Stephanie Hansen*

Picture 7: *Senior Advisor Olaug Kristine Bringager prepared the KUPP programme together with Trygve Helgaker and chaired the KUPP workshops in 2018 and 2019. Photo: Oskar Mikael Bringager*

Ten fellows of the project *Molecules in Extreme Environments* at the Centre for Advanced Study (CAS) of the Norwegian Academy of Science and Letters visited the Hylleraas Centre in Oslo November 17–22 2019, completing work initiated during the academic year 2017–2018 at CAS.

In celebration of the 50th anniversary of Odd Hassel's Nobel Prize in Chemistry 1969, a two-day international meeting *Chemistry 2019 – on Odd Hassel's Shoulders* was held at the University of Oslo on October 31 and at the Norwegian Academy of Science and Letters on November 1. Hylleraas affiliates Prof. Ute Krengel and Prof. Einar Uggerud as well as Hylleraas Director Trygve Helgaker were among the five members of the organization committee, which was chaired by Senior Executive Officer Kari Kveseth at the Department of Chemistry. Odile Eisenstein was both a speaker at the meeting and a panellist in the discussion on whether increased focus on innovation suppresses the needs of long-term basic research (*picture 5* ↑).

Outreach and Dissemination

On February 19, March 5, and March 19 2019, high-school students from Oslo and Drammen visited the University of Oslo for an outreach activity focused on quantum chemistry. Trygve Helgaker gave a popular science talk on quantum mechanics and its application to chemistry, while David Balcells led an interactive session in which the students used their smartphones to perform quantum-chemical calculations on organic molecules.

The Hylleraas Day 2019 was held at Tromsø Museum on September 21, with four popular science presentations and a lecture on the life and work of Egil Hylleraas. The Hylleraas Day was organized as part of *Forskningsdagene 2019*, during which the Hylleraas Centre also celebrated 150 years of the periodic table in a collaboration with the Department of Chemistry at UiT The Arctic University of Norway (*picture 6* ↑).

As part of Forskningsdagene, the Tromsø Virtual Reality (VR) Lab was officially opened and visited by about 300 people over the next few days. The VR Lab was set up by Bjørn Olav Brandsdal, financed by the Research Council of Norway and the Faculty of Science and Technology in Tromsø. The visitors to the VR Lab explored chemical systems using real-time interactive molecular dynamics.

In the course of 2019, members of the Hylleraas Centre featured three times in the online journal Titan for science and technology at the University of Oslo. In January 2019, Trygve Helgaker and Prof. Stian Svelle at the Department of Chemistry, University of Oslo, were interviewed by Titan about the increasing importance of computations and simulations in chemistry. Shortly after, PhD student Audun Skau Hansen was also interviewed by Titan, about his project on coupled-cluster methods for periodic systems, supervised by Thomas Bondo Pedersen. Finally, in November 2019, Trygve Helgaker and Kenneth Ruud were interviewed about the research at the Hylleraas Centre and the long-term research goals of the centre.

Members of the Hylleraas Centre have appeared also in the online news journal forskning.no in 2019. In March, Simen Kvaal contributed the article *Hva tenker du på når du hører ordet "molekyl"?* to the Young Academy of Norway's blog in forskning.no.

In 2019, Durek Verret, a self-proclaimed shaman and the boyfriend Norway's Princess Märtha Louise, claimed on a TV show that "In shamanism, we actually have the ability to access the atoms. We can rotate the nucleus as well as the electrons inside the atoms and that literally depletes the age from us". In an interview in forskning.no, Trygve Helgaker explained how scientists routinely rotate nuclei inside atoms but refuted as nonsense the claim that this reduces age.

Training and Career Support

Together with Patrick Norman (KTH Sweden) and Trond Saue (Toulouse, France), Kenneth Ruud organized the third *Molecular Response Properties Winter School* January 14–18 2019 at Haraldvollen in Bardufoss. The school was attended by 57 participants from eight European countries. Subsequently, the Hylleraas Centre held the annual "hackathon" workshop at Haraldvollen from January 21 to January 25.

Kathrin H. Hopmann wrote an editorial for *Organometallics* in her capacity as Associate Editor. The editorial, entitled *How to make your computational paper interesting and have it published* [*Organometallics* 2019, **38**, 603-605], gives useful advice to authors. The more than 4000 views in just over a year since its publication illustrates its impact on the organometallic and computational chemistry communities.

The Young Researcher Parliament became operational in September 2019, having received a mandate from the Hylleraas Management Team. Abril Castro and Karolina Eikås became its first elected representatives to the Management Team, with Julie Héron and Lukas Konecny as their substitute representatives.

On November 14 2019, a workshop on career development was organized by the Hylleraas Centre at the Norwegian Academy of Science and Letters. It was the third workshop in the KUPP programme for improved career development support at Centres of Excellence, launched by the Hylleraas Centre and Senior Advisor Olaug Kristine Bringager at the Research Support Office at the University of Oslo in 2018 (*picture 7* ↑). The workshop attracted participants from all Centres of Excellence in the Oslo region.

Within the framework of the career development program, David Balcells collected the contact details of the alumni associated with the Oslo node. They were invited to the Christmas dinner, with the aim of connecting them to the current members of the centre. Eight alumni, from both the private and public sectors, attended the event.

Visits

There were in total 39 visitors to the Hylleraas Centre in 2019. In Oslo, Prof. Jonathan Smith of Temple University, USA, stayed for the whole year. Both Oslo and Tromsø had three PhD students visiting from two to four months, doing research. Meetings, workshops, and conferences organized by the Hylleraas Centre attracted a large number of scientists to Norway, with more than 500 attending the ISTCP congress in Tromsø.

External Projects and Funding

In June 2019, a prestigious H2020–MSCA-ITN grant was funded by the Horizon 2020 Framework Program. The network *Cooperation towards a sustainable chemical industry (CO2PERATE)* involves seven universities and three industries in six European countries and is coordinated by Kathrin Hopmann with the support of Ainara Nova. The project funds a total of 15 PhD students, three of which will be hosted by the Hylleraas Centre with Hopmann and Nova as the main supervisors, while Luca Frediani, David Balcells, and Michele Cascella will act as co-supervisors.

In September 2019, Simen Kvaal and Thomas Bondo Pedersen were awarded the project *Attosecond quantum dynamics beyond the Born–Oppenheimer approximation* at the Centre for Advanced Study (CAS) at the Norwegian Academy of Science and Letters for the academic year 2021–2022.

David Balcells contributed as partner to the ERC Synergy Grant CUBE *Unravelling the secrets of Cu-based catalysts for C-H activation* led by Prof. Unni Olsbye (University of Oslo), awarded in October 2019.

In December 2019, the outcome of the 2019 FRIPRO call of the Research Council was announced. Kathrin Hopmann received a FRIPRO Research Grant for the project *CATCH ME IF YOU CAN: selective CO$_2$ conversion via chiral CO$_2$ trapping*, while Marius Kadek received a FRIPRO Mobility Grant, *First-principles modelling of magnetic topological materials from relativistic hybrid density functional theory*, allowing him to visit Prof. Arun Bansil at the Northeastern University in Boston, Massachusetts, for two years, before returning to the Hylleraas Centre for one year.

Picture 8: Trygve Helgaker with Prof. Øyvind Østerud, Chair of the Board of the Nansen Fund, at the award ceremony in Grand Hotel, Oslo, on May 3 2019. Photo: Thomas B. Eckhoff

Picture 9: Chandan Kumar with opponent Privatdozent Florian Weigend, Karlsruhe Institute of Technology, at the PhD defence on November 29, Department of Chemistry, University of Oslo. Photo: Trygve Helgaker

Personnel

At an award ceremony at the Annual Meeting of the Norwegian Academy of Science and Letters on May 3, Trygve Helgaker received the 2019 Fridtjof Nansen Award for Outstanding Research. The Nansen award is awarded annually to a Norwegian scientist or a scientist residing in Norway who has produced research of exceptional quality and international significance, alternating between humanities and social sciences and medicine and natural sciences (picture 8 ↑).

Kathrin Hopmann was appointed member of the Norwegian National Resource Allocation Committee (RFK) for e-infrastructure from January 2019. The RFK allocates national e-infrastructure resources such as computing time on the national supercomputers among researchers at Norwegian institutions.

Kenneth Ruud was in 2019 appointed vice chairman of the Board of the Research Council of Norway for a period of four years. The Research Council of Norway is the largest research funding organization in Norway, with an annual budget of one billion Euros. In May, he was appointed member of the Research and Innovation Advisory Group of EuroHPC, a billion-euro joint initiative to develop a world-class supercomputing ecosystem in Europe.

Kenneth Ruud was elected Vice President of the Norwegian Academy of Science and Letters and Chair of the Natural Sciences Division in September; in November, he was elected Fellow of the American Association for the Advancement of Science (AAAS) for invaluable contributions to science and technology. He is the ninth Norwegian to receive this distinction. In October 2019, Kenneth Ruud was elected to the Board of Directors of International Society of Theoretical Chemical Physics (ISTCP), joining Trygve Helgaker on this board. At the same time, Thomas Bondo Pedersen became the National Representative of Norway in the ISTCP.

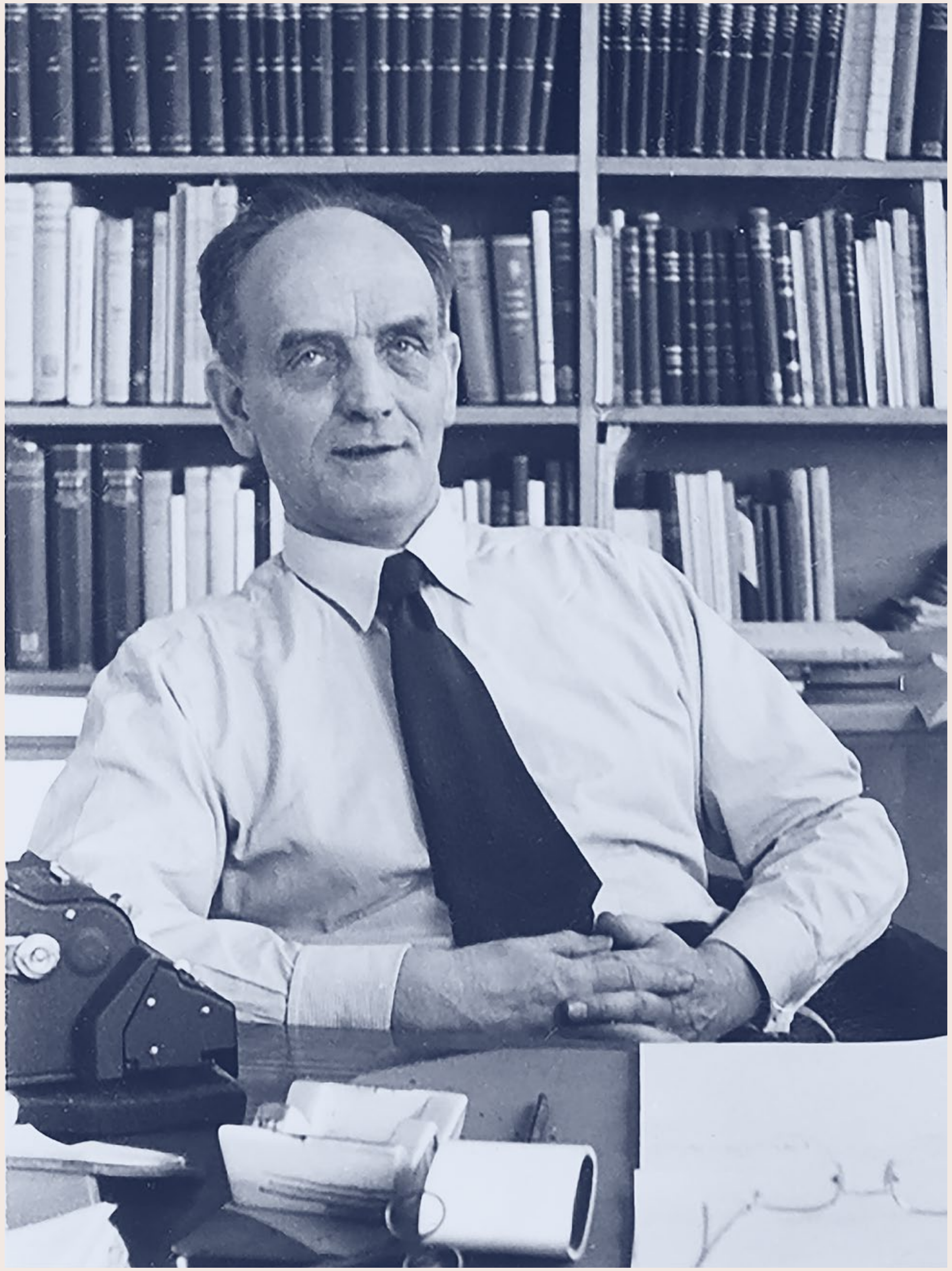
On November 29, Chandan Kumar defended his PhD thesis *Efficient calculations of magnetic and electric response properties for ground and excited states* at the Department of Chemistry, University of Oslo (picture 9 ↑).

Management

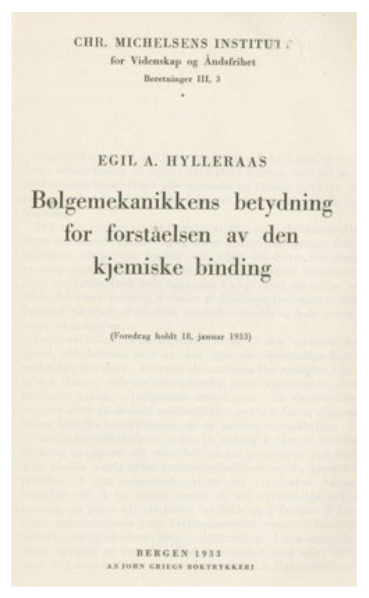
Stig Eide has been on leave of absence for all of 2019, acting as Head of the Administration at the Department of Chemistry at UiT The Arctic University of Norway. In his absence, Stephanie Ramona Hansen worked as Administrative Assistant at the Hylleraas Centre in Tromsø April 1–October 31, when she left to take up a position at the Faculty Administration in Tromsø.

On December 31, Jo Døhl stepped down as Chair of the Board of Directors of the Hylleraas Centre, having recently left the Department of Chemistry to become Director of the Faculty of Mathematics and Natural Sciences at the University of Oslo. He is replaced as chair by Prof. Unni Olsbye, Department of Chemistry, University of Oslo.

The Scientific Advisory Committee visited the Hylleraas Centre October 28–31, performing an evaluation of the science and organization of the centre for the Management Team. Their report gives important advice to the Management Team in the ongoing work to improve and develop the centre.



Egil A. Hylleraas (1898–1965)



CHR. MICHELSENS INSTITUT
for Videnskap og Åndsfrihet
Beretninger III, 3

EGIL A. HYLLERAAS

Bølgemekanikkens betydning
for forståelsen av den
kjemiske binding

(Foredrag holdt 18. januar 1933)

BERGEN 1933
A.S JOHN GRIEGS BOKTRYKKERI

Egil A. Hylleraas, "Bølgemekanikkens betydning for forståelsen av den kjemiske binding", Chr. Michelsens Institutt for Videnskap og Åndsfrihet, Beretninger III, 3. Bergen 1933

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 a popular science talk *Bølgemekanikkens betydning for forståelsen av den kjemiske binding* (*The importance of wave mechanics for understanding the chemical bond*) given at Chr. Michelsen Institute in Bergen in 1933, Hylleraas 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."

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. Four such research topics are here highlighted, showcasing recent and ongoing work at the centre, including work in fundamental theoretical chemistry, the development of new computational methods and techniques, and the use of computational chemistry to address challenging questions in modern science, often in collaboration with experimentalists.

Modeling and Tracing the Behavior of a *trans*-Platinum Complex, an Anticancer Drug, in Aqueous Solution

Abril C. Castro

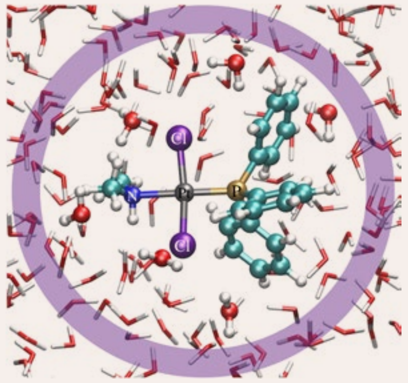


Figure 1: Structure of the *trans*-[PtCl$_2$(dma)PPh$_3$] complex surrounded by water molecules. *Illustration: Abril C. Castro*

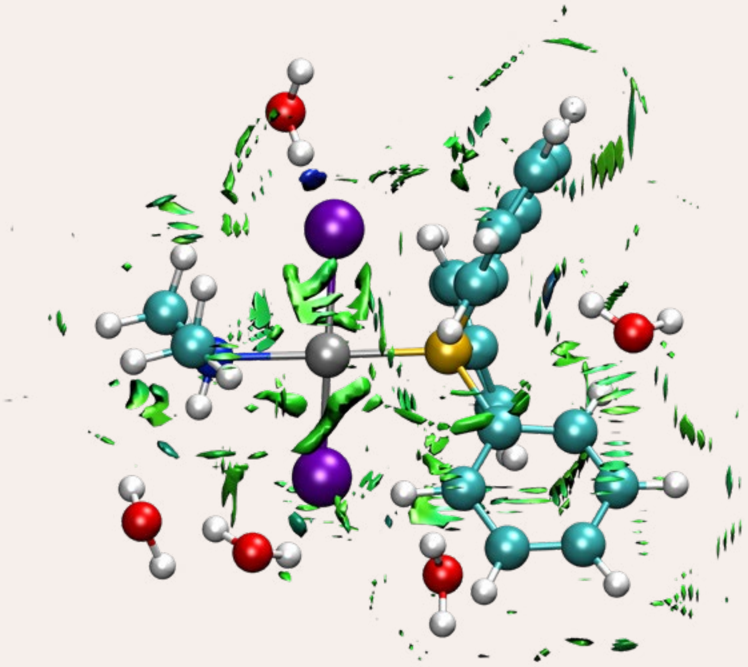


Figure 2: Molecular-dynamics snapshot of the *trans*-[PtCl$_2$(dma)PPh$_3$] complex with five explicit water molecules, identified based on the non-covalent interaction regions (in blue/green). *Illustration: Abril C. Castro*

How can we achieve high accuracy in the calculation of NMR shielding constants? Using theory to understand the ^{31}P NMR spectroscopy of platinum compounds is a challenging task, where relativity, solvation, and dynamics all play an important role.

In the last decade, a large number of studies have focused on the development of platinum-based anticancer drugs and non-classical *trans*-platinum complexes have emerged and demonstrated significant anticancer activity. Crucial for establishing their mechanism of action is the identification of the species formed in water solution, which has been studied in detail by several experimental techniques. In this regard, nuclear magnetic resonance (NMR) spectroscopy is a valuable tool for the characterization of complexes under physiological conditions; also, it allows theory and experiment to be connected.

A showcase study on this topic was made possible in an international collaboration between Spain (Girona and Madrid), Slovakia (Bratislava), and the two sites of the Hylleraas Centre (Oslo and Tromsø) in Norway. This combined experimental–theoretical study was devoted to the accurate calculation of ^{31}P NMR chemical shifts for the *trans*-[PtCl$_2$(dma)PPh$_3$] (dma = dimethylamine) complex and the speciation products in solution [1]. Validity and reliability of the computed values were assessed by comparing with experimental data – a challenging task, requiring robust computational models because of the strong influence of relativity, solvation, and dynamics. In other words, reproducing the experimental data required both an accurate representation of the system in solution and a high-level electronic-structure method for the property calculation itself (*figure 1*).

As the reliability of the computed values was found to be critically dependent on the proper inclusion of relativistic effects and on dynamical averaging, our computational strategy involved a combination of a full four-component relativistic electronic-structure method with *ab-initio* molecular dynamics (MD) simulations. As shown by NCI (non-covalent interaction) plot analyses, several water molecules are engaged in various types of weak interactions with the chemical groups of the platinum complex. These molecules were included explicitly in the simulations (*figure 2*).

With the inclusion of all these effects at a high level of electronic-structure theory, the ^{31}P chemical shifts were obtained in good agreement with experiment – in fact, for the *trans*-[PtCl$_2$(dma)PPh$_3$] complex, the calculated shielding constant was only 1 ppm away from the experimental signal. Our study set the stage for future studies in which calculations of ^{31}P NMR shielding constants are used in combination with experiment to elucidate how *trans*-platinum(II) complexes interact with their environment.

This work was made possible through the collaboration of several members of the Hylleraas Centre with complementary competences (MD simulations with Michele Cascella, electronic structure and spectroscopic processes with Trygve Helgaker, Michal Repisky, and Heike Fliegl) and scientists from other countries. The first author, Abril C. Castro, is presently on a Marie Sklodowska-Curie Individual Fellowship at the Oslo node of the Hylleraas Centre.

Reference:

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Highlight: Laser-Driven Many-Electron Quantum Dynamics

Thomas Bondo Pedersen and
Simen Kvaal

A fundamental understanding of the interaction between light and matter is crucial to modern science and technology and at the heart of the science at the Hylleraas Centre. To simulate such interactions, we must be able to model molecular electronic structure subject to intense laser pulses. At the Hylleraas Centre, we are developing quantum-chemistry methods to study such processes at high accuracy, using coupled-cluster theory.

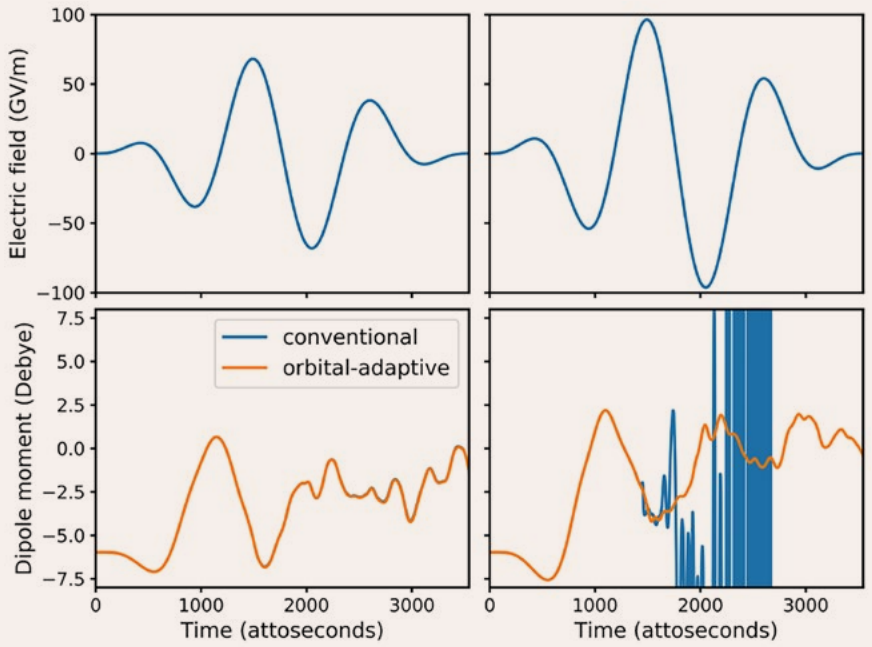

Figure 1: Comparison of conventional and orbital-adaptive coupled-cluster theories with two laser pulses of different intensities.

Top panels: electric field of the laser pulse as a function of time.

Bottom panels: simulated electric dipole moment of the LiH molecule as a function of time. The aug-cc-pVDZ Gaussian-type basis set was used in all simulations.

Illustration: Håkon Emil Kristiansen and Thomas Bondo Pedersen

Spectroscopy is undoubtedly the most important experimental tool to investigate the microscopic structure of matter and its atomic and molecular building blocks. Noting that the only thing we actually observe in spectroscopic experiments are photons (the quantum particles of light discovered by Planck and Einstein in the early 20th century) before and after their interaction with a molecular system, quantum theory is needed to connect the dots from photon detection to the concepts of molecular structure. In this context, molecular structure refers both to the geometric arrangement of the atoms of the molecule under study and to its electronic structure – that is, the detailed description of the many-electron quantum states. In other words, light is our primary source of information about atoms and molecules.

Under most experimental conditions, we may safely assume that photons act as slight disturbances of the electrons inside the molecule and, furthermore, that the light is turned on very slowly compared with the time scale of the electronic motion. These justified assumptions simplify the quantum mechanical treatment of the problem and leads to selection rules for spectroscopic transitions between the molecular energy levels and, in turn, to an interpretation of observed spectral lines in terms of molecular structure.

The characteristic time scale of electronic motion is roughly the time it takes for an electron to orbit the atomic nucleus and is on the order of attoseconds, 10^{-18} s. To appreciate the smallness of this number, note that an attosecond is to a second what a second is to the age of the universe. With the rapid development of ever more powerful light sources, it has become possible to generate laser pulses with a duration approaching the attosecond time scale and with a field strength comparable to the strength of repulsions and attractions between the negatively charged electrons and the positively charged nuclei of the molecule. To correctly interpret experimental data obtained with such lasers, we must first acknowledge that the basic assumptions underpinning the classic quantum-mechanical modelling of spectroscopic processes are no longer valid: the disturbance of the electrons by the photons is not small and the duration of the laser pulse is not long!

To interpret such experimental data, we must turn to explicitly time-dependent quantum mechanics, where the electronic state is computed in real time to account for the many-electron dynamics in the presence of an ultrashort, high-intensity laser pulse. This is a rather under-developed field of quantum chemistry and we have chosen to base our work on coupled-cluster theory, which has proven immensely successful for the accurate prediction of molecular electronic ground-state energies and properties such as electric dipole moments. Importantly, coupled-cluster theory also performs exceedingly well for excited electronic states, making it an attractive candidate for studies of laser-driven many-electron dynamics. In fact, single–doubles–perturbative-triples coupled-cluster theory is often referred to as the *Gold Standard* of quantum chemistry, since it defines the highest level of accuracy that we can at present routinely achieve in theoretical modelling of molecules.

Our investigations [1], however, have revealed that the conventional formulation of coupled-cluster theory, based on the Hartree-Fock mean-field approximation of the molecular electronic ground-state, fails miserably when the intensity of the laser pulse exceeds a certain value. The problem, it turns out, is that high-intensity laser pulses deplete the population of the electronic ground state [1]. Conventional coupled-cluster theory is explicitly designed to describe the ground state accurately and consequently, it tends to fail whenever the quantum-mechanical superposition of states generated by the laser pulse does not entail a significant contribution from the ground state.

The solution, therefore, is to remove the reliance on Hartree-Fock mean-field theory, while maintaining the high accuracy of coupled-cluster theory for both ground and excited states. Reviving older ideas by Pedersen *et al.* [2] and Kvaal [3], we have demonstrated that an orbital-adapted reformulation of coupled-cluster theory provides significantly improved stability [4]. An example is shown in figure 1, where conventional and orbital-adapted coupled-cluster models are compared for the LiH molecule in the presence of laser pulses of different intensities: 702 and 1404 $\mathrm{TW/cm^2}$ in the left and right panels, respectively. The left panels show that the conventional and orbital-adapted coupled-cluster theories yield the same time-dependent electric dipole moment with the less intense laser pulse. The right panels show that, whereas conventional coupled-cluster theory fails after about 1500 attoseconds, orbital-adaptive coupled-cluster theory remains correct when the intensity is doubled.

With these theoretical advances, our next step is to address one of the *Grand Challenges for Science in the 21st Century* [5]: controlling matter at the level of the electrons. We will study ionization processes and high harmonic generation, and investigate through simulations to what extent these processes can be controlled by varying the shape of the laser pulse and/or by the application of magnetic fields, thus establishing a collaborative link between RT1, RT3, and RT4. The CAS project *Attosecond quantum dynamics beyond the Born–Oppenheimer approximation* led by Kvaal and Pedersen (described elsewhere in the Annual Report) adds the quantum-mechanical description of nuclear motion to these efforts. This is a truly novel initiative made possible by the establishment of the Hylleraas Centre for Quantum Molecular Sciences.

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New Tools for Relativistic Molecular Property Calculations

Lukas Konecny,
Michal Repisky and
Kenneth Ruud

The solution of the time-dependent relativistic Dirac equation enables the study of light-matter interactions in the visible, ultraviolet, and X-ray spectral regions for a wide range of molecular systems – in particular, compounds containing heavy elements that can be used in molecular electronics and for white light-emitting diodes (LEDs).

Molecular properties and relativity

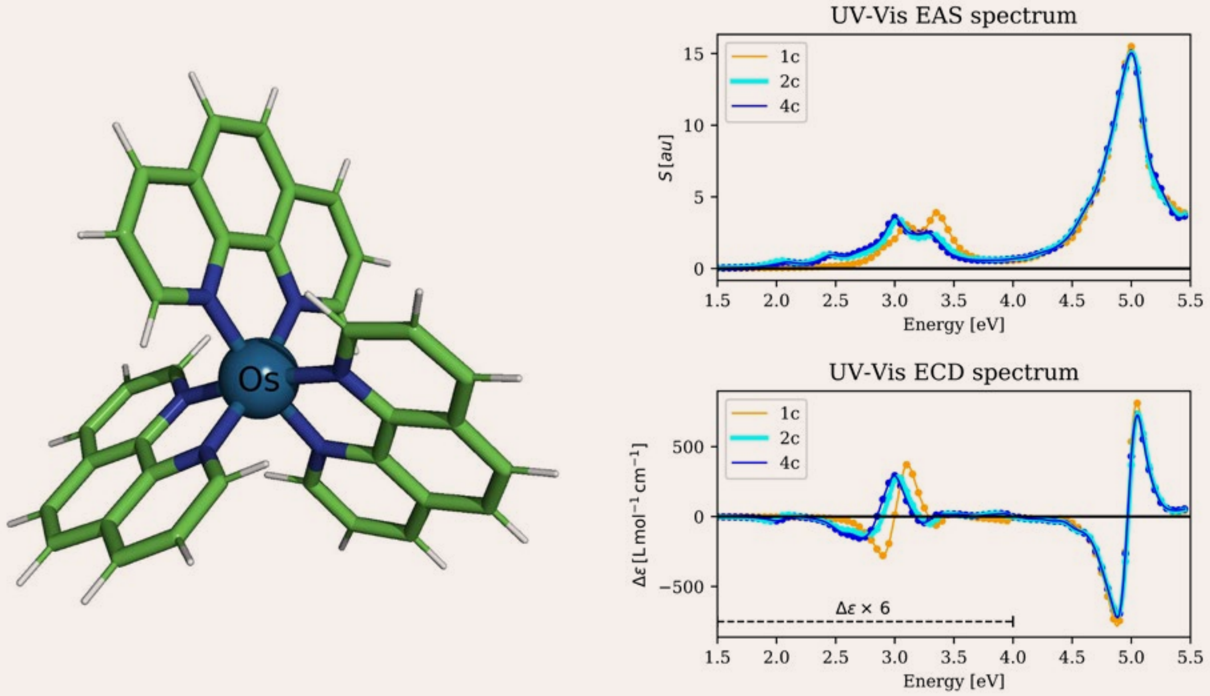
The description of matter and its interaction with light can often be reduced to the determination of the properties of the molecules it is made of. At the microscopic level, matter is described by the laws of quantum mechanics. For systems containing heavy-element atoms and for the electrons closest to the nuclei, the latter which is probed in X-ray spectroscopy, the special theory of relativity must be taken into account. The Dirac equation, rather than Schrödinger equation, must therefore be solved.

A successful framework for the application of (relativistic) quantum mechanics to many-particle molecular systems is time-dependent density functional theory (TDDFT). In TDDFT, a molecule subject to an external electromagnetic field is described by an equation for the evolution of the electron density in time as influenced by the applied field. This equation can be solved directly by propagating the electron density in time. This is the real-time TDDFT (RT-TDDFT) method, pioneered in the relativistic context by our group at the Hylleraas Centre and implemented in the quantum chemistry computer program ReSpect (www.respectprogram.org) [1]. This work complements the non-relativistic real-time development at the coupled-cluster level of theory described in the highlight by Pedersen and Kvaal.

Alternatively, the TDDFT equation can be formulated in the frequency domain and solved by one of two main approaches. In the first of these, the response of a molecule to an external field of a particular frequency is determined. In the second approach, the resonant frequencies that correspond to the molecule's excitation energies are calculated. Both these frequency-domain approaches are developed using perturbation theory, as the electromagnetic field is a small perturbation compared with the interactions within the molecule. Perturbation theory also allows us to separate first-, second-, and higher-order corrections to the molecular energy. In their linear response form, these two TDDFT approaches were in 2019 added to the ReSpect program [2, 3].

Perturbation and response

When a molecule is subjected to a weak external field, the molecule's response is dominated by the term linear in the external field and higher terms can in general be neglected. Moreover, the equation can be extended to account for the finite lifetimes of the molecular excited states by including a damping term. The resulting linear damped response TDDFT (DR-TDDFT) equation then still describes the response of the electron density to the external field, but unlike in RT-TDDFT, it is an algebraic matrix equation whose solution does not require time propagation. However, the sizes of the matrices in the equation prevent the use of direct matrix inversion or elimination techniques, and a tailored iterative method must instead be employed.



A heavy-metal (osmium) complex and its electronic absorption (EAS) and electronic circular dichroism (ECD) spectra calculated by means of linear damped response theory at the non-relativistic one-component (1c), quasi-relativistic two-component X2C (2c) and fully-relativistic four-component (4c) levels of theory. Relativistic effects are noticeable for low-energy metal-to-ligand excitations and less important for the ligand-to-ligand excitations around 5 eV. The ECD spectrum below 4 eV was enhanced six-fold to ease the visualisation of the less intense transitions present in that region. *Illustration: Lukas Konecny, adapted from M. Repisky, S. Komorovsky, M. Kadek, L. Konecny, U. Ekstrom, E. Malkin, M. Kaupp, K. Ruud, O. L. Malkina, and V. G. Malkin,* ***ReSpect: Relativistic Spectroscopy DFT program package****, J. Chem. Phys., 2020,* ***152****, 184101.*

Even with this caveat, DR-TDDFT is well suited for production calculations of linear response properties such as frequency-dependent polarizabilities, electronic absorption spectra, or natural chiroptical properties like optical rotation or electronic circular dichroism. This is because DR-TDDFT determines the response of a molecular system directly in the frequency domain for the spectral range of interest, yielding both the absorption and dispersion spectra simultaneously. In addition, this workflow makes DR-TDDFT advantageous for the treatment of high-frequency or high-density-of-states spectral regions that may prove challenging for alternative approaches. Therefore, the current research in the group aims at investigating X-ray spectra of heavy-metal complexes where core orbitals are strongly affected by relativistic effects.

Parallel to the work on DR-TDDFT, Michal Repisky co-authored an article on TDDFT for excitation energies, known as linear response TDDFT (LR-TDDFT) because of its origin in first-order perturbation theory [3]. This method is unique in that it can be applied to open-shell molecules, known to be challenging for relativistic methods that include spin–orbit coupling. An interesting feature of the relativistic open-shell method for excitation energies is that it can be used to determine excited-state spin–orbit splittings and phosphorescence radiative lifetimes.

A perturbation-theoretical Swiss army knife

The recent research by our group at the Hylleraas Centre and our co-workers has thus endowed the ReSpect program with three distinct methods for the calculation of dynamical molecular properties: RT-TDDFT [1], DR-TDDFT [2], and LR-TDDFT [3]. These three methods are complementary and the choice of the most appropriate method depends on the particular chemical problem at hand. Therefore, users may choose the most suitable approach within a single program.

References

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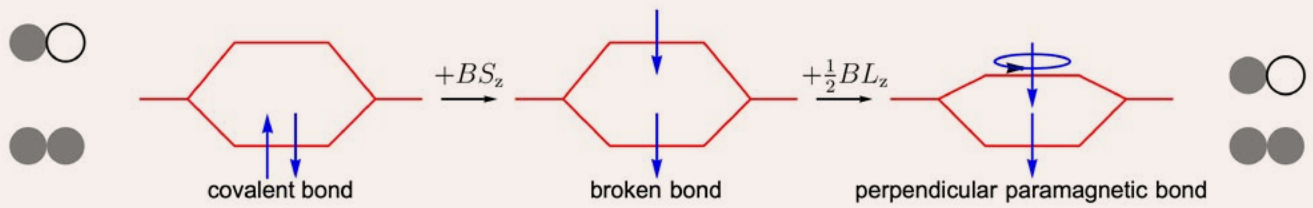
Magnetic Bond Breakers and Bond Makers

Erik Tellgren and
Trygve Helgaker



↑ **Figure 1:** A covalent bond is broken by the spin Zeeman interaction, which promotes an electron into the antibonding orbital. At the same time, the magnetic field induces a paramagnetic current in the antibonding orbital, which lowers the energy of the antibonding orbital by the orbital Zeeman interaction. This paramagnetic energy lowering is stronger the closer the two atoms are to each other, binding the atoms. *Illustration: Trygve Helgaker*

In ultrastrong magnetic fields, currents that are induced among the electrons in a molecule bind atoms in manners that are unknown on Earth but should occur under conditions such as those encountered in the atmospheres of magnetic white dwarf stars. Such bonding was first studied for the lowest triplet state of H_2 and the lowest singlet state of He_2. Recently, we have studied paramagnetic bonding in more general situations, in highly excited states and larger molecules, revealing a more detailed picture of paramagnetic bonding.

Traditionally, our terrestrial chemistry recognizes two main types of chemical bonding – namely, covalent bonds due to sharing of electrons and ionic bonds due to electrostatic interactions. In addition, there are weaker bonds such as van der Waals and hydrogen bonds that are the result of more subtle interactions between electron clouds.

Magnetic fields can fundamentally change this picture. While the magnetic fields that can be produced in a laboratory are weak and have only subtle effects on the electrons in a small molecule, much stronger fields exist around magnetic white dwarf stars and stronger fields still around spinning neutron stars. These fields are so strong that the magnetic interactions of the electrons in the molecule are able to compete with electrostatic interactions, generating a complicated, exotic new chemistry. Most surprisingly, the magnetic field changes in a fundamental manner how atoms bind and form molecules.

Consider the simple, covalently bound H_2 molecule. In the standard molecular-orbital (MO) picture of the electronic system, the MO of lowest energy is the bonding $1\sigma = 1s_A + 1s_B$ orbital, followed by the antibonding $1\sigma^* = 1s_A - 1s_B$ orbital. In the electronic ground state, both electrons occupy the bonding 1σ orbital, with opposite spins according to the Pauli principle. Since each electron has a lower energy than it would have in the 1s orbital of an isolated hydrogen atom, the molecule is bound. The bond is said to be covalent since the electrons are shared between the two atoms (*figure 1* ↗).

By contrast, if we promote one of the electrons to the antibonding 1σ* orbital, then the molecule falls apart since the energy of the two electrons is now higher than their energies in two isolated atoms. The covalent bond is broken. On Earth, this can be accomplished by ultraviolet radiation, whose photons have sufficient energy to excite electrons from the bonding to the antibonding orbital.

This is precisely what a strong magnetic field accomplishes but without the help of photons. In a magnetic field, the energy of the beta electron is lowered by the spin Zeeman operator BS_z, while the energy of the alpha electron is raised. If the field is sufficiently strong, then the alpha electron may lower its energy by jumping from the bonding to the antibonding orbital since the energy required for this quantum leap may be recovered if the electron at the same time switches its spin from alpha to beta. In this manner, the energy of the molecule is lowered, but the covalent bond is broken. *The spin Zeeman interaction is therefore a bond breaker* (*figure 1* ↑). We would then expect the molecule to fall apart.

However, this is not the end of the story. The antibonding 1σ* orbital has the shape of a distorted 2p orbital positioned at the centre of the molecule and oriented along the bond axis. The electron in the antibonding orbital therefore has an angular momentum, which is quenched in the absence of a magnetic field. A magnetic field perpendicular to the bond axis unquenches this angular momentum, setting up a paramagnetic current that lowers the energy of the electron by the orbital Zeeman interaction (*figure 2 next page* →). Moreover, this energy lowering is stronger the closer the two atoms are to each other as the antibonding orbital then more closely resembles the 2p orbital, effectively binding the atoms together. The *orbital Zeeman operator ½ BL_z is therefore a bond maker* and the chemical bond generated in this way is called a perpendicular paramagnetic bond (*figure 1* ↑).

Previous work on paramagnetic bonding focused on the lowest singlet state of He_2 and the lowest triplet state of H_2, which develop weak perpendicular paramagnetic bonds from 1s orbitals in field strengths comparable to those around magnetic white dwarfs [1]. Studies of higher electronic states in He_2 have revealed that paramagnetic bonding occurs in all antibonding orbitals – for example, in the antibonding 2σ* and 2π* orbitals in a diatomic molecule [2]. As the atoms move together, these orbitals acquire more and more 3p and 3d character, whose angular momentum is unquenched by a perpendicular magnetic field, leading to paramagnetic bonding. Our calculations on He_2 have also shown that the paramagnetic bonding in excited electronic states can be an order of magnitude stronger than the paramagnetic bonding previously observed in H_2 and He_2. This effect can be rationalized from the observation that excited states tend to have more diffuse electron clouds that enable larger current loops.

Paramagnetic bonding is directional in the sense that the strength of the bonding depends on the orientation of the orbital relative to the magnetic field. For the antibonding $1\sigma^*$ and $2\sigma^*$ orbitals, the situation is simple: these bonds prefer a perpendicular field orientation since the unquenched angular momentum and induced current is then perpendicular to the molecular bond axis [1]. By contrast, antibonding orbitals generated by atomic orbitals of nonzero angular momentum such as $2\pi^*$ have a preferred skew orientation to the magnetic field vectors [2]. The reason for this behaviour is that the total current in such orbitals is the sum of the permanent and induced currents, which may have different preferred directions. The total current in the $2\pi^*$ orbital, for example, is the sum of a permanent current about the molecular axis and an induced current perpendicular to the axis. As a result, this orbital prefers a near parallel orientation in weak magnetic fields and near perpendicular orientation in strong magnetic fields.

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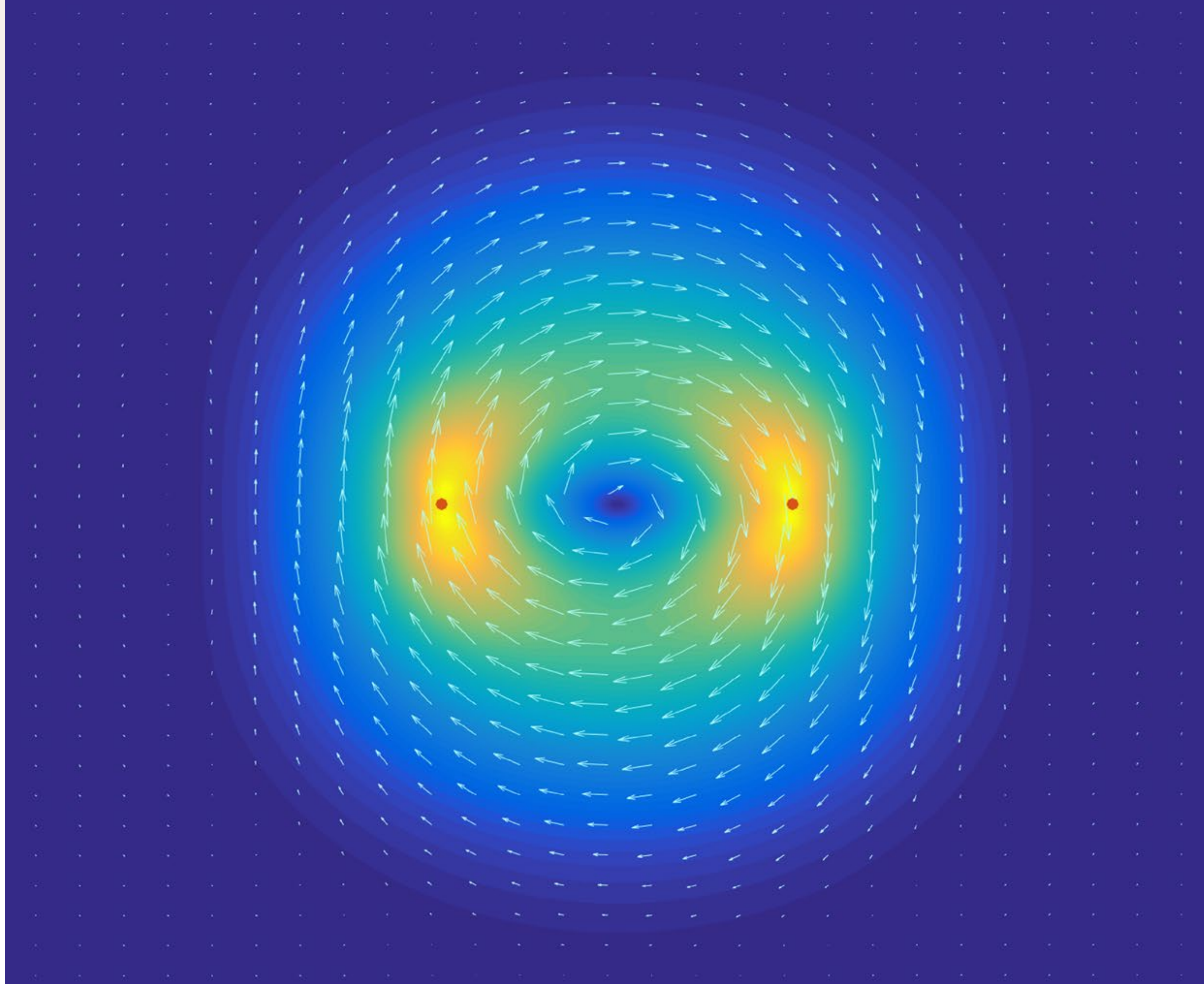

Figure 2: Clockwise paramagnetic current in the H_2 molecule generated by the magnetic field.
Illustration: Erik Tellgren

Almlöf–Gropen Lecture

The 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.

Previous Almlöf–Gropen lecturers

2008	**Prof. Bjørn 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. Arieh 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, Mühlheim, Germany:*	*Chemistry with the computer*

Prof. Hammes-Schiffer delivering the Almlöf–Gropen lecture at the Department of Chemistry, University of Oslo on June13 2019. *Photo: Trygve Helgaker*

Almlöf–Gropen Lecturer 2019: Professor Sharon Hammes-Schiffer

Proton-Coupled Electron Transfer in Catalysis and Energy Conversion

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June 13 2019, University of Oslo

July 11 2019, Clarion Hotel
The Edge, Tromsø

The research of Professor Hammes-Schiffer, John Gamble Kirkwood Professor of Chemistry, Yale University, USA, focuses on the development and application of theoretical and computational methods for describing chemical reactions in condensed phases and at interfaces. Her research is pursued in three areas: proton-coupled electron-transfer reactions, enzymatic processes, and non-Born–Oppenheimer electronic structure methods, aiming to elucidate the fundamental physical principles underlying charge-transfer processes and catalysis.

Professor Hammes-Schiffer has published over 340 papers and has received numerous awards for her work, including the Medal of the International Academy of Quantum Molecular Sciences. She is a fellow of the American Academy of Arts and Sciences, National Academy of Sciences, and American Association for the Advancement of Science, as well as the American Physical Society and the American Chemical Society.

In her lecture, Hammes-Schiffer discussed the role of proton-coupled electron-transfer (PCET) reactions in chemical and biological processes and described the key elements of a general theory developed to describe such reactions. The theory, which includes the quantum-mechanical effects of the active electrons and transferring protons as well as the motions of the proton donor–acceptor mode and solvent or protein environment, has assisted in the interpretation of experimental data and provided experimentally testable predictions. Hammes-Schiffer described applications to PCET in enzymes, molecular electrocatalysts for hydrogen production and water splitting, artificial photosynthesis, metal–oxide nanocrystals, proton discharge on a metal electrode, and photoreceptor proteins. Her studies have identified thermodynamically and kinetically favourable mechanisms and clarified the roles of proton relays, excited vibronic states, hydrogen tunnelling, reorganization, and conformational motions. The resulting insights are guiding the design of more effective catalysts and energy conversion devices.

Meetings and Events

Group picture of the participants and teachers at the winter school. *Photo: Hylleraas Centre*

Molecular Response Properties Winter School 2019

Haraldvollen Red Cross Centre, Bardufoss
January 14–18 2019

A record number of students participated in the third edition of the Molecular Response Properties Winter School.

The third edition of the *Molecular Response Properties Winter School* was held January 14–18 2019 at Haraldvollen Red Cross Centre, located at Bardufoss in Northern Norway. A total of 56 participants from seven European countries including Russia participated in this year's school – the largest number of participants in the history of the school. The school was organized by Patrick Norman (KTH, Sweden), Trond Saue (Toulouse, France), and Kenneth Ruud, who was also the local organizer.

This is the first time the winter school was held in Norway, the previous editions having been held in Chamonix and Luchon, both in France. In a slightly different form, the school has also been held twice as summer schools in Blacksburg (VA) in the US, in collaboration with Prof. Daniel Crawford.

The participants had an intense week of lectures and exercises at the end of the polar night period in Northern Norway. The curriculum of the school is based on the textbook by the three winter-school organizers, *Principles and Practices of Molecular Properties: Theory, Modeling, and Simulations*, which was published in 2018.

The participation of 18 Russian students and teachers was made possible by generous support of the Centre for Internationalisation of Education (DIKU), in a joint project between the Hylleraas Centre in Norway, and Tomsk State University and St. Petersburg State University in Russia.

Participants of the Haraldvollen Hackathon 2019. *Photo: Hylleraas Centre.*

Haraldvollen Hackathon 2019

Haraldvollen Red Cross Centre, Bardufoss
January 21–25 2019

The annual gathering of the Hylleraas Centre at Haraldvollen Red Cross Centre took place January 21–25 2019.

The meeting gathered many of the Hylleraas Centre members from Tromsø, as well as some participants from the UiO branch of the Hylleraas Centre. In addition, there were external participants from the Royal School of Technology (Stockholm, Sweden), Aarhus University (Denmark), University of Warsaw (Poland), and Cambridge University (UK).

With temperatures down to −27 degrees Celsius, the participants had no choice but to work, socialize and eat – in other words, an excellent setting for listening to nice talks, having constructive meetings, and working on the many interesting research projects at the Hylleraas Centre.

In line with previous gatherings, this year's gathering focused on group work in ongoing projects at the Hylleraas Centre, in combination with topical lectures of broad interest. These talks typically focus on generic tools that can be useful in method development, administration of research data, or best practices. This year, the group was introduced to Docker images as a way of distributing codes and testing programs across different machine architectures, to modular tools for program development, and to machine learning. In addition, a discussion session was held on open-access publishing and the requirements that have been put forth in PlanS for publication of research financed by the Research Council of Norway.

Hylleraas group photo at the Bardufoss meeting, with organizer Bin Gao in a red sweater in the first row. *Photo: Hylleraas Centre.*

Hylleraas Spring Meeting

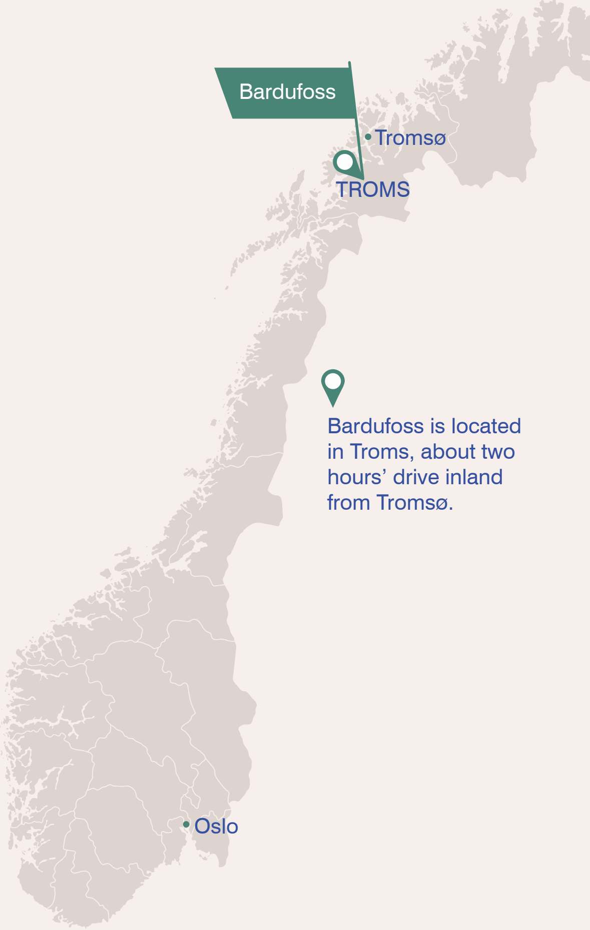
Haraldvollen Red Cross Centre, Bardufoss
May 13–15 2019

Every year all members of the Hylleraas Centre join for a three-day spring meeting of science and centre matters, combined with social activities. These meetings are chaired by young researchers and the organization alternates between the Oslo and Tromsø nodes. The 2019 Spring Meeting was held at Bardufoss, chaired by Bin Gao.

In May 13–15 2019, 41 members of the Hylleraas Centre gathered for three days at Haraldvollen in Bardufoss, about two hours' drive inland from Tromsø. The program focused on joint activities within the centre's Research Themes (RTs) and across the two nodes of the centre.

After a presentation of the vision for the Hylleraas Centre by Trygve Helgaker, the principal investigators gave a status update for each RT and their views on the road ahead. This overview was followed by group work by the PhD students and postdocs in each RT on how the RT should be developed, building on the joint expertise of all Hylleraas members.

In addition to the scientific program, there were social activities, including a hike to Øverli overlooking Bardufoss and a "Puzzled Pint Quiz" organized by Karen Dundas, Marius Kadek and Lukas Konecny.



Bardufoss is located in Troms, about two hours' drive inland from Tromsø.

↑ **Picture 1:** The official ISTCP-X conference photo. *Photo: Luca Frediani*

ISTCP 2019 Congress

Clarion Hotel The Edge, Tromsø
July 11–17 2019

July 11–17 2019, the Hylleraas Centre organized the 10th Congress of the International Society of Theoretical Chemical Physics in Tromsø. With 545 registered participants, it was the largest congress held in this congress series and the largest conference in theoretical chemistry in 2019.

During seven sunny and fairly warm days in July 2019, almost 550 researchers from around the world gathered in Tromsø for *the 10th Congress of the International Society of Theoretical Chemical Physics (ISTCP-X)*. With 202 lectures given in plenary sessions and 14 topical parallel sessions and 280 poster presentations, the participants were able to enjoy the latest scientific advances in the field of theoretical and computational physics (*picture 1* ↑).

The conference was opened in the afternoon of July 11 with two plenary talks – first by Prof. Sharon Hammes-Schiffer from Yale University, who delivered her 2019 Almlöf–Gropen lecture as part of the conference opening. In her lecture, she presented her work on describing the coupled motion of electrons and nuclei in molecules with applications to a wide range of problems in chemical physics.

This lecture was followed by a talk by Trygve Helgaker, who presented the life and science of the Norwegian physicist Egil Hylleraas, from whom the Hylleraas Centre has taken its name. Helgaker showed that Hylleraas was ahead of his time and that the methods he developed around 1930 are still extensively used today. Indeed, one of the topical sessions at the conference was named *90 years of r12: Hylleraas Symposium*, with a focus on current research that builds on the seminal work of Egil Hylleraas (*picture 2* ↗).

Picture 2: Trygve Helgaker presenting his plenary lecture. *Photo: Luca Frediani* →

↑ **Picture 3:** Kersti Hermansson presenting her plenary lecture. *Photo: Luca Frediani*

↑ **Picture 4:** Kathrin Hopmann presenting her lecture on how to ensure that your reaction mechanism is correct. *Photo: Luca Frediani*

The conference program was busy, starting at 08:30 in the morning and lasting until 21:00 on the days with poster sessions. Most days began with two plenary lectures followed by three groups of four talks in three to four parallel sessions, ending at 18:30.

The plenary speakers had been selected by an international scientific committee that also identified 14 scientific topics that should be the focus of the conference. The scientific committee invited internationally leading scholars to chair symposia on the selected topics and in turn invite whom they thought to be the leading international scholars within these different topics.

At the end of a busy week, the conference was closed on July 17 by two excellent plenary lectures given by Prof. Monica Olvera de la Cruz, Northwestern University, who spoke about the properties and modelling of molecular electrolytes, and by Prof. Kersti Hermansson, Uppsala University, who spoke about the challenges one faces when modelling complex materials, especially if water is involved (*picture 3* ↑).

Highlighting research at the Hylleraas Centre

The ISTCP-X conference was a great venue to promote the research carried out at the Hylleraas Centre. In addition to Helgaker giving a plenary lecture, Michele Cascella, Luca Frediani, Kathrin Hopmann, and Michal Repisky had been invited by session chairs to present their research. Bjørn Olav Brandsdal stepped in on short notice when one of the scheduled speakers missed his flight and thus could not attend the conference (*picture 4* ↑).

In addition, ten younger members of the Hylleraas Centre presented their research at the poster sessions and several Hylleraas members were co-authors on posters and lectures. The conference thus showcased research at the Hylleraas Centre to a broad international audience.

Photo: Luca Frediani

Picture 5: 13 of the 17 staff members that were hard at work during the conference.

Back row from left:
Diego Garcia-Lopez,
Karen O.H.Dundas,
Nikolaj S. W. Ravn,
Marc Obst,
Marc Joosten,
Peter Wind

Front row from left:
Marius Kadek,
Anders M. Brakestad,
Stig R. Jensen,
Katarzyna Jakubowska,
Karoline S. Eikås,
Magnar Bjørgve,
Lukas Konecny

Staff members not present:
Sigbjørn L. Bore,
Geir V. Isaksen,
Jogvan M. H. Olsen,
Matej Veis

Promoting equal opportunities

The ISTCP-X conference was praised by the participants for the high quality of the scientific program. The program featured 66 females among the 202 invited speakers and 5 females among the 12 plenary speakers, making it the most gender-balanced large conference in the field of theoretical chemical physics in recent years.

Conference attendance is often complicated for primary caregivers, in part because necessary facilities may not be available at the conference and in part because additional costs are incurred when someone else may have to take care of the children while their parents attend a conference. The collaboration with the conference venue, Clarion Hotel The Edge, allowed the conference to offer a nursing room for participants with children. Through a generous sponsorship, the conference also offered bursaries to primary caregivers to cover their additional expenses. In total, six such bursaries were provided to participants.

Innovative conference measures

In addition to its focus on promoting gender balance, the ISTCP-X conference implemented a number of measures to reduce waste (and in this way also keep costs, and conference fee, low). The conference did not offer any printed book of abstracts – instead, the program and abstracts were available online, in a format well suited to portable devices such as mobile phones and tablets. This online program, which was developed in-house by Michal Repisky, was very well received by the conference participants.

The welcome package was kept to a minimum, containing only a certificate of attendance, a name badge, and food and drink vouchers. At the end of the conference, participants were encouraged to hand in their lanyards; about a third of these were returned to the conference organizers.

Poster prizes

The conference had received support from several scientific journals for awarding 14 poster prizes to students and postdocs who had elected to participate in the poster prize competition. This support was much appreciated, bearing in mind that poster awards are important for the future career of young scientists.

Organization

The local organization was handled by the Tromsø node of the Hylleraas Centre, the members of the local organization committee being Maarten Beerepoot, Bjørn Olav Brandsdal, Stig Eide, Luca Frediani, Bin Gao, Stephanie R. Hansen, Kathrin Hopmann, Michal Repisky and Kenneth Ruud (chair) (*picture 5* ↑).

In addition to this local organizing committee, the smooth operation of the conference relied heavily on the active participation of many of the younger members of the Hylleraas Centre, mainly from Tromsø but also with participation from Oslo and a few visiting students. They were outfitted with a characteristic yellow T-shirt when on duty. In total, 17 young people participated as such assistants during the conference, ensuring that everything ran smoothly. At the end of the conference, the yellow T-shirts were recognised as a symbol for high quality of service.

Sponsors

The ISTCP-X conference received generous support from the Research Council of Norway and from UiT The Arctic University of Norway: Department of Chemistry, Faculty of Science and Technology, and the rector of UiT. Their support is gratefully acknowledged.

Rector Svein Stølen addressing the audience at the opening ceremony in Oslo. *Photo: Yngve Vogt*

Official Opening of the Hylleraas Centre

University of Oslo & UiT The Arctic University of Norway
September 4–5 2019

Following the refurbishment of the Hylleraas premises, the official opening of the Hylleraas Centre took place in September 2019 at the two host universities, with participation of representatives of the two universities and the Research Council.

After nearly two years of operation, the Hylleraas Centre was officially opened in 2019, on September 4 in Oslo and on September 5 in Tromsø. In Oslo, a large number of invited guests attended the event in Auditorium 2 at the Department of Chemistry, which was chaired by Hylleraas affiliate Einar Uggerud. As befits a centre shared by two institutions, the first addresses were by Rector of the University of Oslo, Svein Stølen, and Prorector of UiT The Arctic University of Norway, Wenche Jakobsen. After a presentation of the Centre of Excellence programme of the Research Council of Norway, Special Advisor Liv Furuberg presented Trygve Helgaker with the official SFF plaque.

Trygve Helgaker's presentation of the Hylleraas Centre was bookended by musical performances of the violinist Mari Okshovd, who played traditional music from Engerdal, where Egil Hylleraas grew up. The opening ceremony was concluded by addresses by the Vice Dean for Research at Faculty of Mathematics and Natural Sciences, Solveig Kristensen, and by the Head of the Department of Chemistry and Chairman of the Hylleraas Board, Jo Døhl.

After the official opening, refreshments were served at a well-attended reception in the refurbished premises of the Hylleraas Centre. Among the many guests were four generations of the Hylleraas family, including Egil Hylleraas' daughter Inger Hylleraas Bø.

The opening of the Hylleraas Centre in Tromsø on September 5 was chaired by Kathrin Hopmann. After a welcome address from UiT The Arctic University of Norway by Prorector Wenche Jakobsen and a presentation of the centre by Trygve Helgaker, the audience was addressed by Trude Dypvik from the Research Council of Norway, Dean of the Faculty of Science and Technology, Arne Smalås, and Head of the Department of Chemistry, Annette Bayer. There was musical entertainment by the group *Norwegian Moods*. After the opening ceremony, all guests were invited to reception at the Hylleraas Centre.

At the opening of the Hylleraas Centre, the representatives of both universities emphasized the shared value of the centre for both institutions and the importance of the long-term collaboration set up by the Centre for Theoretical and Computational Chemistry (CTCC) during its ten years of operation 2007–2017 and now continued with the Hylleraas Centre.

Four generations of descendants of Egil Hylleraas at the reception in Oslo.

From left to right:
granddaughter Ingvild Hylleraas Bø,
granddaughter Siri Margrete Hylleraas Bø,
great-great-granddaughter Edda Hylleraas Myklebust,
great-grandson Erlend Eide Bø, and
daughter Inger Mathilde Hylleraas Bø.
Photo: Elina Melteig

Prorector Wenche Jakobsen at the opening of the Hylleraas Centre in Tromsø. *Photo: Jan Ingar Johnsen*

Refreshments, including hot dogs and home brew beer, were served in the new kitchen "Onsager" at the Hylleraas Centre in Oslo. *Photo: Elina Melteig*

Opening of the Hassel meeting by Rector at the University of Oslo, Svein Stølen.
Photo: Merethe Alm

Chemistry 2019: on Hassel's Shoulders

University of Oslo and the Norwegian Academy of Science and Letters

October 31 – November 1 2019

In celebration of the 50th anniversary of Odd Hassel's Nobel Prize in Chemistry in 1969, a two-day seminar was held in Oslo with members of the Hylleraas Centre in the organizing committee.

In 1969, Prof. Odd Hassel (1897–1981) together with Prof. D. H. R. Barton, UK, was awarded the Nobel Prize in Chemistry "for their contributions to the development of the concept of conformation and its application in chemistry." The pioneering work of Odd Hassel on the conformations of cyclohexane had been published in the late 1940s.

In celebration of the 50th anniversary of Hassel's Nobel Prize, a two-day meeting *Chemistry 2019: on Hassel's Shoulders*, was held in Oslo October 31–November 1 2019. The meeting highlighted the importance of Hassel´s establishment of the structure of cyclohexane and the field of conformation analysis and its relevance for our understanding of chemistry, biology, medicine, material sciences and catalysis.

The meeting consisted of three separate events. On Thursday October 31, there were opening addresses by Rector Svein Stølen and Dean Morten Dæhlen in Vilhelm Bjerknes's House followed by a panel debate *Innovation at the cost of long-term basic research or room for both?* with participation of Odile Eisenstein. Later the same day, an exhibition on Hassel and his work was opened at the Department of Chemistry, followed by a dinner at the Academy of Science and Letters.

On Friday, there was a workshop at the Academy of Science and Letters, with presentations by Prof. Gerard Meijer, Fritz Haber Institute of the Max Planck Society, Prof. Thomas Ebbesen, University of Strasbourg, Prof. Pekka Pyykkö, University of Helsinki, Prof. Omar Yaghi, UC Berkeley, Prof. Laura Hartmann, University of Düsseldorf, Prof. Donald Hilvert, ETH, Prof. Tanja Kortemme, UC San Francisco, Prof. Richard Henderson, Cambridge, and Odile Eisenstein, Hylleraas Centre.

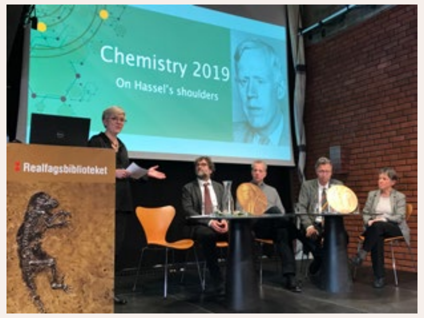
The organizing committee consisted of Kari Kveseth (chair), Hylleraas affiliate Einar Uggerud, Trygve Helgaker, Hylleraas affiliate Ute Krengel, and Mohamed Amedjkouh. Kari Kveseth and Trygve Helgaker are both previous members of the Gas-Phase Electron-Diffraction Group at the Department of Chemistry, University of Oslo, established by Odd Hassel.

Speakers and organizers of the Hassel meeting at the Norwegian Academy of Science and Letters.

Standing left to right:
Mohamed Amedjkouh,
Gerard Meijer, Ute Krengel, Jo Døhl,
Tanja Kortemme, Laura Hartmann,
Einar Uggerud, Donald Hilvert,
Richard Henderson, Trygve Helgaker.

Sitting left to right:
Pekka Pyykkö, Kari Kveseth,
Omar Yaghi, Thomas Ebbesen,
Odile Eisenstein.
Photo: Merethe Alm

Opening of the Hassel exhibition at the Department of Chemistry.
Photo: Merethe Alm



Panel debate at Vilhelm Bjerknes House.
From left to right:
Moderator Marina Tofting,
Norwegian Academy of Science and Letters,
Kay Gastinger, *Kavli Institute*,
Carl Henrik Gørbitz, *University of Oslo*,
Thomas Ebbesen,
University of Strasbourg,
and Odile Eisenstein,
Hylleraas Centre.
Photo: Merethe Alm

Molecules in Extreme Environments – post-CAS week

Hylleraas Centre, University of Oslo
November 18–22 2019

CAS fellows visiting Oslo.
From left to right:
Peter Schwerdtfeger,
Dage Sundholm,
Wim Klopper,
Stella Stopkowicz,
Lukas Pasteka,
Trygve Helgaker,
Andy Teale,
Maria Dimitrova,
Hans Joachim Werner,
Trond Saue, and
Jürgen Gauss.
Photo: Elina Melteig

In November 2019, ten of the fellows of the project *Molecules in Extreme Environments* at the Centre for Advanced Study (CAS) at the Norwegian Academy of Science and Letters returned to Oslo, for one week of concentrated work.

During the academic year 2017–2018, thirteen quantum chemists worked at the Centre for Advanced Study (CAS) at the Norwegian Academy of Science and Letters in Oslo, participating in the project *Molecules in Extreme Environments*, led by Trygve Helgaker. Their work at CAS concerned a variety of themes related to extreme environments such as the stability of atoms and molecules in strong magnetic fields, excitations and ionizations in strong magnetic fields, closed-shell paramagnetism, density-functional theory in a magnetic field, confined electronic systems, melting in strong magnetic fields, magnetically induced currents, and quantum electromagnetism.

Ten of the CAS fellows came to the Hylleraas Centre in Oslo for a workshop November 18–22 2019, continuing the collaboration started during the CAS project: Dr. Maria Dimitrova (University of Helsinki, Finland), Prof. Jürgen Gauss (University of Mainz, Germany), Prof. Wim Klopper (Karlsruhe Institute of Technology, Germany), Dr. Lukas Pasteka (Comenius University, Slovakia), Trond Saue (University of Toulouse, France), Peter Schwerdtfeger (Massey University, New Zealand), Dr. Stella Stopkowicz (University of Mainz, Germany), Dage Sundholm (University of Helsinki, Finland), Asst. Prof. Andy Teale (University of Nottingham, UK), and Prof. Hans Joachim Werner (University of Stuttgart, Germany). The workshop was enjoyable and productive, leading to the submission of two manuscript and progress on other projects.

Career Development

Morning session at the KUPP workshop November 14 2019.
Photo: Trygve Helgaker

Career Development Pilot Programme (KUPP) Workshop 2019

Norwegian Academy of Science and Letters
November 14 2019

Following up on the Career Development Pilot Programme (KUPP) initiated by the Hylleraas Centre in 2018, a one-day KUPP workshop was held at the Norwegian Academy of Science and Letters on November 14 2019 with participants from all Centres of Excellence in Oslo, who shared their experiences over the last year and discussed the path forward.

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In 2018, the Hylleraas Centre initiated a Career Development Pilot Programme (KUPP) to improve the career support of the young researchers at the nine Centres of Excellence at the University of Oslo. The KUPP programme was developed in collaboration with Senior Advisor Olaug Kristine Bringager in the Research Support Office at the University of Oslo. At two one-day KUPP workshops in 2018, the participants discussed aspects of career support and, in particular, how to improve the career support at centres of excellence. The report from these two workshops, *Videreutvikling av karrierestøtten til forskere i tidlige karrierefaser*, written by Bringager and Helgaker, was used as input for further development of career support at the university.

On November 14 2019, a third KUPP workshop was held at the Norwegian Academy of Science and Letters, attended by 50 participants – centre directors, heads of office, senior researchers, and young researchers representing all Centres of Excellence in the Oslo region. The purpose of this workshop was to learn from the experiences of others, to receive feedback on implemented activities, to generate ideas for the next steps, and discuss the way forward.

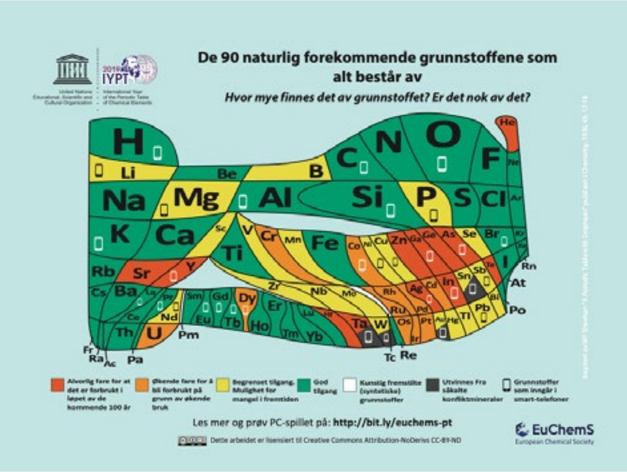
After an overview and recapitulation by Bringager, who also informed participants about ongoing work on career support at the University of Oslo, each participating Centre of Excellence reported on their own career-development work, discussing the successful and less successful measures that had been taken since 2018. After lunch, group work was carried out on three topics: career planning, mentoring of young researchers, and arenas for young researches. After a general discussion on the way forward, a tapas dinner was served. All participants expressed enthusiasm about the ongoing KUPP work and commitment to improved career support in the years ahead.

Young Researcher Parliament

A primary concern of young scientists is their future career. Securing a permanent position in academia requires not only hard work but also a strategy to get there. Still, the majority of young researchers who begin their career in academia will eventually pursue a career outside academia. An important task of the Young Researcher Parliament (YRP) is therefore to motivate and aid the young researchers in the formulation of their career development plans. To this end, several young members of the YRP as well as senior members of the Hylleraas Centre attended the KUPP workshop at Norwegian Academy of Science and Letters in November 2019, exchanging ideas on career planning, mentoring, and arenas for young researcher such as the YRP.

As a result of the KUPP initiative that began in 2018, a framework has been formulated together with the PIs at the Hylleraas Centre to ensure that all the young researchers: 1) will become well integrated into the centre and its goals and values (onboarding), 2) will achieve a fulfilling and productive stay at the centre (ongoing), and 3) will leave well equipped for their future careers with a solid plan and proper tools (off-boarding).

Outreach



The EuChemS Periodic Table

Tromsø museum
Photo: Trygve Helgaker

Hylleraas Day 2019

Tromsø Museum
September 21 2019

The Hylleraas Day 2019 consisted of a biographical talk on the life and work of the Norwegian physicist Egil Hylleraas and four popular science talks on current work at the Hylleraas Centre.

The Hylleraas Day took place on Saturday September 21 at Tromsø Museum, in connection with Forskningsdagene (Science Days) September 19–29 2019. Trygve Helgaker first gave a presentation of the life and science of the Norwegian physicist Egil Hylleraas (1898–1965), the founding father of quantum chemistry in Norway. Hylleraas performed a number of pioneering computational studies in the early days of quantum mechanics, including the first accurate calculations on the helium atom (confirming the validity of quantum mechanics for more than one particle) and the calculation of the cohesive energy of the LiH crystal (the first quantum-mechanical study of a crystal). Many techniques introduced by Hylleraas are in use today.

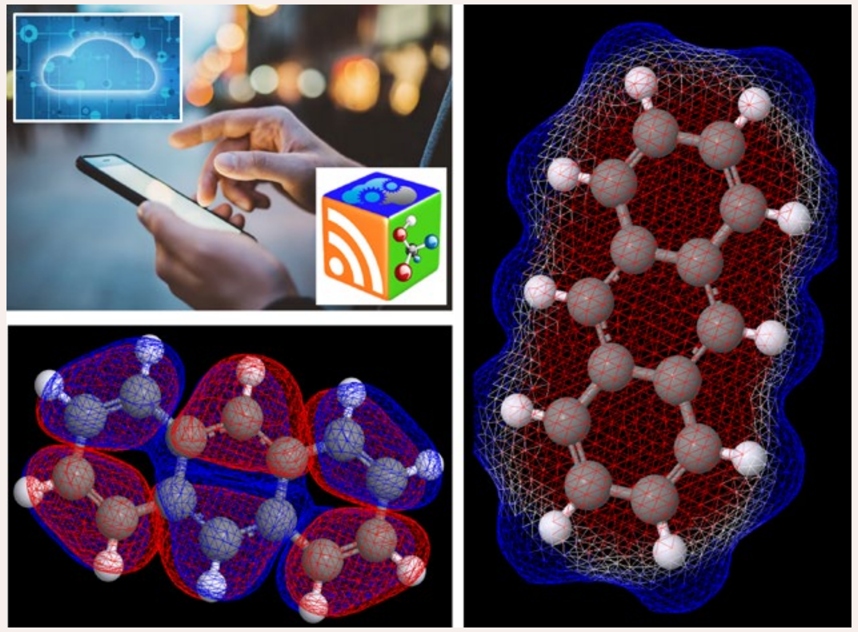
After a short coffee break, four short popular science talks were given by members of the Hylleraas Centre: *Utenomjordisk kjemi* (Trygve Helgaker), *Relativt god kjemi* (Kenneth Ruud), *Kuldetilpasninger* (Bjørn Olav Brandsdal), and *Can we transform carbon dioxide into something useful?* (Ainara Nova).

The Hylleraas Day was attended by only about 20 people. It had been announced by e-mail to everyone at the Faculty of Science and Technology (UiT) and by social media. However, Tromsø Museum is both off-campus and outside the city centre. Competition with several simultaneous activities held as part of Forskningsdagene in the city centre may also explain the disappointing turnout at the Hylleraas Day event at Tromsø Museum.

However, the Hylleraas Day also included, in collaboration with the Department of Chemistry at UiT The Arctic University of Norway, a celebration of 2019 as the International Year of the Periodic Table, highlighting the 150th anniversary of the first periodic table by Dmitri Ivanovich Mendeleev and the 100th anniversary of the International Union of Pure and Applied Chemistry (IUPAC).

In Tromsø, we targeted school children and a total of six lectures for groups of 30 school children were given by Eivind Torgersen on September 19. His lectures presented selected curious facts about chemistry and the periodic table, taken from his book: *Genier, sjarlataner og 50 bøtter med urin. Historien om det periodiske system.* As the principles of quantum mechanics are the foundation of the periodic table, his lectures gave almost 200 school children an entertaining introduction to the consequences of our quantum world.

Kenneth Ruud is a member of the Executive board of the European Chemical Society (EuChemS). As a memento, the school children were provided with the EuChemS Periodic Table highlighting the abundance of the different elements.



Quantum chemistry on a smartphone – doing quantum-mechanical calculations with the Mo3 app. *Illustration: David Balcells*

School Outreach

Reaching out to young people is important for the recruitment to science in general and chemistry in particular. During 2019, members of the Hylleraas Centre engaged in several outreach activities to students from upper secondary school.

In Oslo, members of the Hylleraas Centre gave popular science talks to school classes from Drammen, Nesbru and Asker upper secondary schools on February 19, March 5 and March 19 2019, respectively. After welcoming the students, Trygve Helgaker gave a popular science talk *Kvantemekanikk og kjemi* on quantum mechanics and its application to chemistry. David Balcells then led an interactive activity in which the students engaged by using their smartphones to perform quantum-mechanical calculations on organic molecules. The feedback from the students was positive and we are looking forward to similar events in the future.

In Tromsø, Bjørn Olav Brandsdal and PhD student Tor Arne Heim Andberg contributed to *Kjemikonferansen* March 14–15 2019, which gathered about 200 students and teachers from upper secondary schools in Nordland, Troms and Finmark, with a four-hour session devoted to antimicrobial resistance. The students were given hands-on practical exercises where the proteolytic stability of antimicrobial compounds was examined using computational docking and scoring methods.

School visit from Nesbru upper secondary school on March 5 2019. *Photo: David Balcells*

Bente Sirin Barge and Magnus Burkow playing with a DNA binding protein in a VR environment. *Photo: Bjørn Olav Brandsdal*

Families visiting the VR lab during the Science Days were allowed to interact with two different chemical systems in VR using real-time molecular dynamics simulations. *Photo: Bjørn Olav Brandsdal*

Tromsø Virtual Reality Lab

Virtual reality (VR) offers a new way to teach, communicate, and engage with concepts that have traditionally been considered difficult to understand. It can be particularly useful for explaining complex molecular concepts in chemistry and biology, when three-dimensional molecular structures are involved and combined with atomic motions.

The Tromsø VR Lab was established in the autumn of 2019 with the installation of one server (48 cores and a powerful GPU card) along with six clients. This multiuser simulation environment allows for six people to be in the lab at the same time. The VR lab, which was built as a replica of Dr. David Glowacki's lab at the University of Bristol in UK, is part of Bjørn Olav Brandsdal's Toppforsk grant and will be used for visualization and data analysis. Additional funding has been received from the Faculty of Science and Technology at UiT for teaching and outreach activities.

The Tromsø VR Lab was opened in connection with the Science Days 2019, during which students from upper secondary school visited the lab on September 19. The VR lab was also open to the general public on September 22.

The opening was a great success, with close to 300 persons visiting the lab, where they played and interacted with two different chemical systems using real time interactive molecular dynamics (MD) simulations [1]. The first chemical system was the relatively simple C_{60} molecule, where they could grab individual atoms and manipulate the real-time molecular-dynamics simulation using two wireless controllers. Users were also able to pass the molecule to one another. The second simulation system involved threading of a methane molecule through a nanotube, which most visitors were able to achieve with some practice. All visitors gave positive feedback and thought this was an intuitive way of learning about chemistry.

In addition to the Science Days, we hosted school visits during the last months of 2019. Apart from interacting with the C_{60} molecule and threading methane through a nanotube, the visiting students explored the binding and unbinding of a drug from its protein receptor by means of real-time interactive molecular dynamics.

In 2020, we will continue to host school visits for chemistry and biology students and participate in the International Day of Women and Girls in Science as well as the Science Days. The VR activities will be expanded to include modelling of chemical reactions using real-time density-functional theory [2] and of antimicrobial resistance using real-time interactive molecular dynamics.

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1 M. O'Connor, H.M. Deeks, E. Dawn *et al.*, *Sci. Adv.* 2018, **4**, eaat2731.

2 S. Amabilino, L. A. Bratholm, S. J. Bennie, A. C. Vaucher, M. Reiher, D. R. Glowacki, *J. Phys. Chem.* A 2019, **123**, 4486–4499.

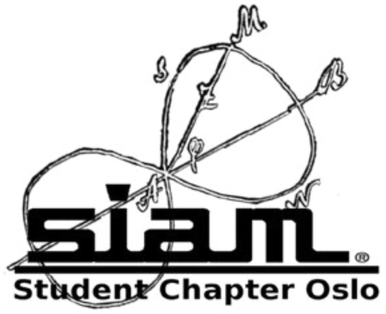
PhD student Fabian Faulstich
(Photo: George Bergman)

SIAM Student Chapter Oslo

To foster applied and computational mathematics, PhD student Fabian Faulstich at the Hylleraas Centre has set up the first SIAM student chapter in Norway.

The Society for Industrial and Applied Mathematics (SIAM) encourages the formation of student chapters at universities all around the world to foster applied and computational mathematics. The Hylleraas Centre, together with the University of Oslo, is official sponsor of the very first SIAM student chapter in Norway (the second SIAM student chapter in all of Scandinavia). The aspiration of the SIAM student chapter at the University of Oslo is the interdisciplinary participation of students and faculty from a variety of departments in providing valuable opportunities to develop networks with faculty members outside the classroom, share ideas and research with people with similar interests, learn about career options, and develop leadership skills. Important objectives of the SIAM student chapter at the University of Oslo are

- to promote mathematics in research and industry,
- to foster relations between chapter members and the local scientific community,
- to work with SIAM chapters across the globe to further applied and computational mathematics,
- to establish an environment where academic and industrial participants interact on a regular basis.



Fabian's logo of the SIAM student chapter in Oslo

PhD Defences 2019

Chandan Kumar

University:	University of Oslo
Date:	November 29 2019
Thesis:	*Efficient calculations of magnetic and electric response properties for ground and excited states*
Trial Lecture:	*Quantum chemical calculation of molecular properties*
Supervisors:	Dr. Heike Fliegl, Karlsruhe Institute of Technology, Germany Trygve Helgaker, University of Oslo
Committee:	Privatdozent Florian Weigend, *Karlsruhe Institute of Technology, Germany* Assoc. Prof. Perttu Lantto, *University of Oulu, Finland* Prof. Ute Krengel, *University of Oslo*

Visits and Mobility

Interview with Visiting Researcher

Maria del Sagrario Rossano Tapia

Maria del Sagrario Rossano Tapia is a PhD student in the group of Prof. Alex Brown at the University of Alberta in Edmonton (Canada). She visited the Hylleraas Centre from September to December 2019.

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

As part of my PhD research, my supervisor, Prof. Alex Brown at the University of Alberta (Edmonton, Canada), and I were exploring the effects that the environment has on two-photon absorption processes in fluorescent proteins, where the chromophores contain non-canonical amino acids. A perfect tool for this research is the quantum mechanical/molecular mechanical (QM/MM) polarized embedding model as implemented in the Dalton electronic structure package. As the Hylleraas Centre hosts many of the Dalton developers and some of the most high-profile researchers in this area, we contacted Prof. Kenneth Ruud and Dr. J. Magnus H. Olsen to ask about their interest in collaboration. They drew our attention to the visitors' program, and I decided to apply for Fall 2019.

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

My stay at the Hylleraas Centre gave us the opportunity to complete four entire projects around emissive properties and environment effects on multi-absorption processes in fluorescent proteins and fluorescent protein chromophores containing non-canonical amino acids. The results of these projects will help me shape significant parts of my doctoral thesis to be submitted in early to mid 2021. Importantly, the stay and my interactions with Hylleraas Centre members provided me with excellent practical and theoretical experience, especially with the models and tools implemented in the Dalton software package. During my stay, I got the chance to hold fruitful discussions with expert researchers in the field of multi-photon absorption processes and QM/MM models, including the polarized embedding model. Also, I consider this visit the beginning of what might be a longer-standing scientific relationship between the Hylleraas Centre and Prof. Alex Brown's research group, especially in the area of multi-photon absorption processes.

How did you find the working conditions and social and scientific environment at the Hylleraas Centre?

Visiting PhD student María del Sagrario Rossano Tapia at the top of Storsteinen with the island of Tromsø in the background. *Photo: Evellin Battistela*

The working conditions at the Hylleraas Centre allow you to thrive in your projects because of its tolerant, respectful, enthusiastic, diverse, and supportive scientific environment. Through their weekly meetings held with Oslo via video conference, the Hylleraas Centre gave me the opportunity to become familiar with the research undertaken by many of their well-trained members including graduate students, post-doctoral fellows, and faculty. Also, through the Hylleraas Centre, I got the chance to attend the 2019 Annual Meeting in Quantum and Computational Chemistry in Trondheim, which was a wonderful opportunity to get a better understanding of the research that is being carried out in Norway in the realm of quantum and computational chemistry. In many different ways, the Hylleraas Centre gave me the opportunity to interact with its members – for example, at lunchtime, when everyone gathered to eat and talk about a wide range of topics, including Tromsø lifestyle. In the coffee room, I got to know people outside Kenneth Ruud's research group, talk about their research, and even get feedback about my own research while I was enjoying a nice cup of coffee.

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

I found Tromsø to be a very suitable place to live while carrying out research, keeping in mind I visited from September to December – that is, the start of winter. Tromsø is full of unique natural landscapes and, at the same time, urban spots where I got the chance to spend my leisure time. For example, I visited the Storsteinen mountain three times and there I had beautiful views of the whole island and even the stunning Northern lights. From my visit, I found the people in Tromsø and Norway to be kind and always willing to help you. I look forward to visiting again – maybe in the summer next time!

Outgoing Visits

Abril Castro visited Masaryk University in Brno, the Czech Republic, for three months in 2019, working in the group of Prof. Radek Marek. Masaryk University is the second largest university in the Czech Republic.

Fabian Faulstich visited the University of Helsinki for two weeks in 2019, working with Dr. Sushi Lehtola.

Michele Cascella spent two weeks at Ca'Foscari University in Venice in 2019, working with Prof. Achille Giacometti. The photo is of the main hall of Ca'Bottacin, a historic building in Venice and the location of "European Centre for Living Technology", an interdisciplinary centre led by Giacometti.

During 2019, members of the Hylleraas Centre attended schools, specialist workshops, meetings, and conferences, presenting their own work in talks or in posters. In addition, many members visited research groups abroad, establishing new collaborations or continuing old ones. In the following, we include only visits that lasted for a week or longer.

PhD student Fabian Faulstich worked with Prof. Lin Lin at the Department of Mathematics, UC Berkeley for five months in the first half of 2019, financed by a Peder Sather Grant. Together with Dr. Andre Laestadius, he also visited Jiri Pittner at J. Heyrovsky Institute of Physical Chemistry in Prague for one week in July, working on coupled-cluster theory. On internationalization support from UiO:LifeScience, Faulstich then spent six weeks at the Technical University of Berlin. Finally, he worked with Dr. Susi Lehtola at the University of Helsinki for two weeks in December 2019.

Apart from his visit to Prague, Andre Laestadius visited the Max Planck Institute for the Structure and Dynamics of Matter in Hamburg for ten days in August 2019, working with Dr. Markus Penz and Dr. Michael Ruggenthaler on the fundamentals of density-functional theory, supported by the Sønneland Foundation.

Michele Cascella visited Universidade Federale do ABC, São Bernardo do Campo in Brazil for a week in October 2019, establishing a scientific collaboration with Prof. Mauricio Coutinho-Neto. Within the framework of a COST Action, Cascella visited Prof. Achille Giacometti at Ca' Foscari University Venice for one week in December. Furthermore, as part of an ongoing collaboration with Prof. Jürgen Gauss, Cascella visited the University of Mainz several times in 2019. Likewise, Trygve Helgaker travelled a number of times to Aarhus, for collaboration with Prof. Poul Jørgensen and Prof. Jeppe Olsen at Aarhus University on a monograph, *Principles of Density-Functional Theory*.

PhD student Sigbjørn Løland Bore visited Prof. Giuseppe Milano at Yamagata University for one month in January and February 2019. Drs. Michiko Atsumi and Erik Tellgren also travelled to Japan in 2019, visiting Prof. Masahiro Ehara at Institute of Molecular Science in Okazaki and Prof. Shigeyoshi Sakaki at Kyoto University for one week during the summer.

Dr. Jógvan Magnus Haugaard Olsen visited the Hebrew University of Jerusalem in May and KTH, Stockholm for one week in October and one week in December. Dr. Magnus Ringholm spent all of 2019 at KTH, on a mobility grant from the Research Council of Norway.

From October 2019, Dr. Abril Castro made a research stay of three months at CEITEC (The Central European Institute of Technology), Masaryk University in the Czech Republic, starting a collaboration with Prof. Radek Marek to work on her MSCA-IF project *Relativistic and Dynamic effects in Computational NMR Spectroscopy of transition-metal complexes* (ReaDy-NMR). She also made a visit of one week to the Institut Charles Gerhardt, University of Montpellier in France, as part of an ongoing collaboration with Dr. Christophe Raynaud and Odile Eisenstein.

In July 2019, Drs. Ainara Nova and David Balcells made a research stay of four weeks at CIQSO (Research Centre for Sustainable Chemistry), in the University of Huelva (Spain), reinforcing collaborations with Profs. Antonio Martínez and Pedro Pérez in the fields of catalytic CO_2 reduction and methane oxidation. Members of the Hylleraas Centre have extensive collaboration with Prof. Don Tilley at UC Berkeley. During 2019, Odile Eisenstein and PhD student Julie Héron visited Tilley for three weeks and one week, respectively. Dr. Torstein Fjermestad visited the University of Iceland for two months in 2019, hosted by Prof. Egill Skúlason.

Regarding internal Hylleraas visits, PhD Lluis Artus Suarez and Dr. Ainara Nova from the Hylleaas Centre in Oslo visited Tromsø for one and two weeks, respectively. Dr. Diego Garcia Lopez from Tromsø visited Michele Cascella and Ainara Nova in Oslo for two months in 2019, to learn ab initio molecular dynamics and to establish whether there is solvent assistance at the early stages of C–C forming reactions using CO_2. Dr. Roberto Di Remigio from Tromsø visited the Oslo node of the Hylleraas Centre for one week in November, working with Thomas Bondo Pedersen and Simen Reine on coupled-cluster theory.

Incoming Visits

There were in total 39 visitors to the Hylleraas Centre in 2019. In addition, meetings and workshops organized by the Hylleraas Centre attracted a large number of scientists to Norway, with more than 500 attending the ISTCP congress in Tromsø.

Visitors to Oslo

Prof Jonathan Smith	Temple University, USA	January 1–December 31
PhD Markus Penz	Max Planck Institute, Hamburg, Germany	January 10–25
MSc Till Kirsch	Johannes Gutenberg University of Mainz, Germany	March 8–9
Prof Jürgen Gauss	Johannes Gutenberg University of Mainz, Germany	April 3–6
Prof Taku Onishi	Mie University, Japan	April 22–28
MSc Till Kirsch	Johannes Gutenberg University of Mainz, Germany	May 24–June 14
Prof Sharon Hammes-Schiffer	Yale University, USA	June 12–14
PhD Alexandre Patrick Bazante	University of Florida, USA	June 14–28
Prof Takeshi Satō	University of Tokyo, Japan	June 19–July 2
Prof Ludwik Adamowicz	University of Arizona, USA	June 28–July 12
PhD Jiri Pittner	J. Heyrovsky Institute of Physical Chemistry, Czech Republic	July 8–10
PhD Örs Legeza	Wigner Research Centre for Physics, Hungary	July 8–10
MSc Sebastián Franco-Ulloa	Italian Institute of Technology, Italy	September 1–November 30
MSc Zsuzsanna Iker	Budapest University of Technology and Economics, Hungary	September 16–15
MSc Sri Harsha Pulumati	University of Iceland, Iceland	September 13–20
MSc Juan A. de Gracia Triviño	KTH Royal Institute of Technology, Sweden	October 1–December 31
MSc Irene Casademont Reig	University of the Basque Country, Spain	October 16–December 31
Prof Giuseppe Milano	Yamagata University, Japan	November 11–13
Prof Trond Saue	Toulouse University, France	November 16–22
PhD Maria Dimitrova	University of Helsinki, Finland	November 17–22
Prof Wim Klopper	Karlsruhe Institute of Technology, Germany	November 17–22
PhD Lukas Felix Pasteka	Comenius University, Slovakia	November 17–22
Prof Peter Schwerdtfeger	Massey University, New Zealand	November 17–22
PhD Stella Stopkowicz	Johannes Gutenberg University of Mainz, Germany	November 17–26
Prof Dage Sundholm	University of Helsinki, Finland	November 17–22
Prof Jürgen Gauss	Johannes Gutenberg University of Mainz, Germany	November 19–23
PhD Aleix Comas-Vives	Autonomous University of Barcelona, Spain	November 20–22
MSc Chandan Kumar	VU Amsterdam, the Netherlands	November 22–29
Prof Ida Marie Høyvik	Norwegian University of Science and Technology, Norway	December 18–19

39 visitors in 2019

545 congress participants

Visitors to Tromsø

MSc Charles J. C. Scott	University of Cambridge, UK	January 19–February 2
Prof Olav Vahtras	KTH Royal Institute of Technology, Sweden	January 22–25
MSc Peter Reinholdt	University of Southern Denmark, Denmark	January 28–February 1
MSc Till Kirsch	Johannes Gutenberg University of Mainz, Germany	March 4–7
MSc Nikolaj S. W. Ravn	Aarhus University, Denmark	March 11–July 19
Asst Prof Mehboob Alam	Indian Institute of Technology Bhilal, India	May 15–30
MSc Katarzyna Jakubowska	University of Warsaw, Poland	July 11–19
MSc Evelin Battistella	Federal University of Rio de Janeiro, Brazil	August 1–October 31
MSc Maria Rossano-Tapia	University of Alberta, Canada	September 28–December 20
MSc Daniel Gryko	Polish Academy of Science, Poland	December 11–12

Externally Funded Projects

The financial support that 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 new external research grant proposals that have been approved for funding during the report period. Progress in these projects will in the future be reported as part of the activities of the research themes.

CO_2PERATE Innovative Training Network

Kathrin Hopmann (UiT)
Ainara Nova (UiO)
–
Marie Skłodowska-Curie Innovative Training Network
2020–2024

Beneficiaries and partners of the CO_2PERATE ITN.

Kathrin Hopmann has successfully initiated the CO_2PERATE Innovative Training Network, consisting of 10 nodes across 6 European countries. Ainara Nova leads of one of the work packages in CO_2PERATE.

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The CO_2PERATE Innovative Training Network (ITN) has a simple but essential vision: Training of young European researchers in the synthesis of indispensable molecules from sustainable carbon sources with sustainable catalysts. This will involve development of novel and industrially relevant methods for employing CO_2 as a carbon synthon, alongside renewable biomass, catalysed by non-precious metals. The main focus is on C-C bond formation with CO_2, which is an important but insufficiently developed area. CO2PERATE has 15 PhD research projects (P1-P15), divided into four work packages (WP1–WP4) using both computational and experimental approaches to achieve their goals. The ITN is funded by the European Union's Horizon 2020 research and innovation programme with financing from 2020 to 2024.

Carboxylic acids and esters from CO_2

The goal of WP1 is to find efficient non-precious metal catalysts for the formation of carboxyl and ester motifs from CO_2 and sustainable starting materials. Six projects are part of this work package, including one PhD project concerned with the computational analysis of CO_2-based carboxylation of hydrocarbons, under the supervision of Kathrin Hopmann.

Carbamates from CO_2

WP2 focuses on finding homogeneous and immobilized catalysts for the efficient and enantioselective formation of carbamate motifs from CO_2. The work is carried out within three projects, two using experimental and one using computational approaches. The latter will deal with the computational analysis of symmetric and asymmetric oxazolidinone formation from CO_2, also under the supervision of Kathrin Hopmann.

Amides and ketones from CO_2

WP3 aims to find efficient non-precious homogeneous and heterogeneous catalysts for the formation of amides and ketones via carbonylation and aminocarbonylation processes with CO_2. Three projects are part of this work package, one of them experimental. The two other projects are titled *Computational insights into the conversion of CO_2 to CO and carbonylation reactions* and *Theoretical studies on catalytic alkoxycarbonylation and carbonylation reactions with CO_2*, respectively.

Labelled compounds from CO_2

WP4 is concerned with the development of new versatile technologies for the isotopic labelling of chemicals, pharmaceuticals, and proteins with $^{11}CO_2$, $^{13}CO_2$, and $^{14}CO_2$. The three projects are all experimental.

Hylleraas members in CO2PERATE

Kathrin H. Hopmann is the consortium leader and Ainara Nova is the leader of WP4.

Attosecond Quantum Dynamics Beyond the Born–Oppenheimer Approximation

Simen Kvaal (UiO) and
Thomas Bondo Pedersen (UiO)
–
Centre for Advanced Study (CAS)
Norwegian Academy of Science and
Letters 2021–2022

Pedersen (left) and Kvaal (right) outside a book store and café in Telluride, Colorado. In this store, the idea that sparked the CAS application was born in 2017. *Photo: Simen Kvaal and Andreas Grüneis*

In the autumn of 2019, Simen Kvaal and Thomas Bondo Pedersen were awarded a Centre for Advanced Study (CAS) project for the academic year 2021–2022.

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A CAS project allows international researchers to have an up to one-year long sabbatical in the premises of CAS at the Norwegian Academy of Science and Letters in Oslo. Besides Kvaal and Pedersen, the core members of the project are Prof. Ludwik Adamowicz (University of Arizona, USA), Prof. Reinhold Schneider (TU Berlin, Germany), Assoc. Prof. Takeshi Satō (University of Tokyo, Japan), and Prof. Lars Bojer Madsen (Aarhus University, Denmark). Additionally, several internationally renowned researchers will spend time at CAS during the project. The project is highly interdisciplinary, with researchers from mathematics, physics, and chemistry, united towards the challenging problem of developing novel methods for *ab initio* quantum dynamics beyond the Born–Oppenheimer approximation.

Our understanding of the geometric structures of molecules and materials is based on the Born–Oppenheimer approximation, which, roughly speaking, treats the nuclei as classical particles while the electrons are quantum particles. In a secondary quantization procedure, quantal nuclear motion is then defined for each electronic state separately. The range of validity of the Born–Oppenheimer approximation is well established, both theoretically and experimentally. Indeed, it is hard to imagine most of our chemical knowledge without this approximation and its "world view".

With the advent of ever brighter and stronger light sources, we are now able to interrogate experimentally molecular systems with unprecedented resolution in time and space, all the way down to the characteristic time scale of the electron – the attosecond (10^{-18} s) time scale. As the electrons and nuclei interact with an ultrashort, high-intensity laser pulse, a superposition of states is generated, containing contributions from a large number of quantum states, including excited electronic states.

As the Born–Oppenheimer approximation assumes stationary conditions, its application becomes questionable and could lead to erroneous interpretations of experimental data and the risk of missing new important quantum-dynamical phenomena.

In the project *Attosecond Quantum Dynamics Beyond the Born–Oppenheimer Approximation*, we aim to formulate new computationally realizable models for the quantum dynamics of electrons and nuclei without invoking the Born–Oppenheimer approximation, thereby testing its limits of validity.

CATCH ME IF YOU CAN:

Selective CO_2 Conversion via Chiral CO_2 Trapping

Kathrin Hopmann (UiT)

FRIPRO Researcher Project
2020–2024

Most carbon employed in the synthesis of thousands of essential everyday chemicals comes from non-sustainable fossil resources such as oil, which society will run out of in the future. Other sources of carbon such as carbon dioxide (CO_2) are needed but, for CO_2 to become a valuable carbon source, novel chemistry must be developed. CATCH ME IF YOU CAN aims to develop C-CO_2 bond-forming reactions from CO_2, focusing on chiral trapping of CO_2 with the goal to make the reactions enantioselective and to provide chiral carboxylic acids – an important feature of many pharmaceuticals.

CO_2 is a natural resource that has the potential to be used in chemical synthesis as a carbon source. This requires the development of CO_2 conversion reactions – in particular, towards C-CO_2 bond formation, since C-C linkages constitute the core of all organic molecules. The project CATCHME will employ computational and experimental methods to investigate C-CO_2 bond formation towards formation of chiral carboxylic acids.

Three fundamental research questions will be addressed:

- How does CO_2 behave during C-CO_2 bond formation?
- Can CO_2 be trapped and activated towards C-CO_2 bond formation?
- Can chiral CO_2-trapping molecules promote asymmetric carboxylation?

C-C bond formation with CO_2 typically involves metal-bound carbon nucleophiles. Our recent research on C-CO_2 bond formation indicates that, in many reactions of this type, CO_2 does not interact with the metal in the C-C bond formation step and thus experiences no activation from the metal centre. The unbound state of CO_2 may be the reason why attempts towards enantioselective CO_2 conversion are often unsuccessful, because the free CO_2 is little affected by the chiral metal complexes that are employed. CATCHME proposes a novel strategy for enantioselective CO_2 conversion, involving trapping of CO_2 prior to C-C bond formation.

Although many molecules are known that can trap CO_2 (e.g., N-heterocyclic carbenes or frustrated Lewis pairs), they are typically employed in CO_2 hydrogenation or O-C bond formation, but not in C-C bond forming reactions. A critical aspect of CATCHME is to identify CO_2 adducts that are active in C-C bond formation. Furthermore, if these adducts are chiral, this could provide a new approach towards enantioselective C-C bond formation with CO_2.

CATCHME will employ high-level quantum-chemistry methods to obtain general insights and identify promising trapping molecules, followed by organic chemistry approaches to test chiral CO_2 trapping in enantioselective formation of carboxylic acids. The project will employ three postdoctoral researchers with a total budget of 12 MNOK and last for a period of four years 2020–2024.

> "Every attempt to employ mathematical methods in the study of chemical questions must be considered profoundly irrational. If mathematical analysis should ever hold a prominent place in chemistry – an aberration which is happily impossible – it would occasion a rapid and widespread degradation of that science."
>
> *Auguste Comte (1798–1857)*

> "The more progress sciences make, the more they tend to enter the domain of mathematics, which is a kind of center to which they all converge. We may even judge the degree of perfection to which a science has arrived by the facility with which it may be submitted to calculation."
>
> *Adolphe Quetelet (1796–1874)*

First-principles Modeling of Magnetic Topological Materials from Relativistic Hybrid Density Functional Theory

Marius Kadek (UiT)

RCN FRINATEK Mobility Grant
2020–2023

The RCN Mobility Grant allows Marius Kadek to establish an independent scientific profile and network by pursuing a personalized research project in collaboration with the group of Prof. Arun Bansil in Boston, USA. The project addresses major challenges that hinder DFT simulations of interacting topological materials exhibiting strong spin–orbit coupling and nontrivial magnetic structures.

Marius Kadek has received funding from The Research Council of Norway for the project *First-principles modeling of magnetic topological materials from relativistic hybrid density functional theory*. The research targets a class of materials that have attracted considerable attention in the theoretical and experimental condensed-matter community due to their exceptional properties with many technological applications in spintronics and quantum computing. In particular, the immunity of certain states to impurities present in realistic samples can be used to mitigate the decoherence problem of quantum computers, to control magnetic states with currents, or to store information with high density in memory devices. These properties often originate in the spin–orbit coupling, which requires a relativistic description based on the Dirac equation of the electronic motion and is significantly enhanced for materials containing heavy elements.

The identification of potential topological systems as well as the prediction of new materials require first-principles approaches that are (i) reliable (for correct characterization of states), (ii) systematic (to enable high-throughput screening of materials), and (iii) efficient (to bring the cost of simulations to an affordable level). The research project will advance the field of material simulations by providing a method that fulfils these criteria for magnetic systems.

The project combines expertise in mathematics, physics, and chemistry, and brings Kadek's previous work on modelling solids in the fully relativistic framework with Gaussian-type orbitals into a new area. The ReSpect code – a program package designed for large-scale relativistic calculations – will be extended to handle spin–orbit-coupled magnetic systems. The use of cutting-edge technology of local basis functions, quaternion algebra, and fast multipole methods will enable large magnetic unit cells to be used, a necessary condition for calculations on complex magnetic structures.

The research will be carried out in two phases: During the outgoing phase, Kadek will be hosted in the group of Prof. Arun Bansil in USA. Bansil has a long-standing record in first-principles simulations of topological materials as well as established collaborations with experimental groups. Kadek will return to the Hylleraas Centre in the second phase to back-transfer the knowledge acquired. The project starts in July 2020, has a budget of 3375 kNOK, and will fund Kadek's postdoc position for three years.

> "I hope by this means to give a proof of an idea advanced by several very distinguished chemists – that we are perhaps not far removed from the time when we shall be able to submit the bulk of chemical phenomena to calculation."
>
> Joseph Louis Gay-Lussac (1778–1850)

> "The underlying physical laws necessary for the mathematical treatment of a large part of physics and the whole of chemistry are thus completely known and the difficulty is only that the exact application of these laws leads to equations that are too complicated to be soluble. It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation."
>
> Paul Dirac (1902–1984)
> in "Quantum mechanics of many-electron systems",
> *Proc. R. Soc. Lond. A*, 1929, **123**, 714

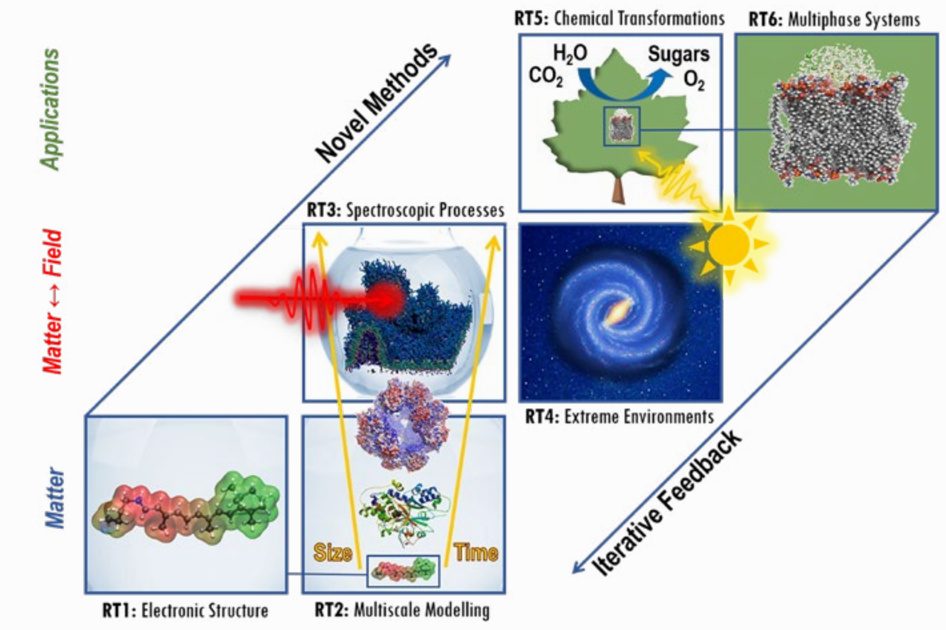
Research Theme Activity Reports

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):

- Electronic Structure (RT1)
- Multiscale Modelling (RT2)
- Spectroscopic Processes (RT3)
- Extreme Environments (RT4)
- Chemical Transformations (RT5)
- Multiphase Systems (RT6)

Each RT has its own deliverables, directed towards the common goal of the centre. The first two themes, RT1 on electronic structure and RT2 on multiscale modelling, describe matter in isolation, providing the backbone for our work. The next two themes, RT3 and RT4, introduce fields and photons. They are at the heart of the centre, dealing with spectroscopic processes and extreme environments. The tools developed in these four RTs will enable our application themes to address problems that are today beyond the reach of computation. We focus on chemical transformations in RT5 and on multiphase systems in RT6 – areas that, among many other things, aim to secure clean energy and to combat antimicrobial drug resistance.

In the following, the 2019 report is provided for each RT.



Hylleraas Research Themes

RT1

RT1: Electronic-Structure Theory

Principal investigators:
Thomas Bondo Pedersen and
Luca Frediani

Aiming at improved computational accuracy and efficiency, RT1 has made important progress in multiwavelet-based density-functional-theory for computational catalysis studies and in new developments in coupled-cluster theory ranging from fundamental mathematical analysis through solid-state studies to novel multireference and stochastic formulations. Finally, development of a modern Python-based platform has been initiated, making the Dalton and LSDalton software packages more accessible to computational chemists and method developers alike.

Multiwavelets

The activity in the group of Luca Frediani has focused on the development of the MRChem code and related applications. The code is now ready for production calculations of energies and linear response properties. We have started a collaboration with RT5 (Chemical Transformations) and the group of Kathrin Hopmann on several benchmark studies.

In particular, PhD student Anders Brakestad has performed an extensive benchmark of polarizabilities of small molecules to verify the precision of large Gaussian-type orbital basis sets and currently uses MRChem to obtain basis-set-error-free reaction energies of a set of metal complexes. Peter Wind and Stig Rune Jensen have improved the parallelization scheme of MRChem to address the issue of the large memory footprint of multiwavelet calculations on large systems with hundreds of electrons or more. Gabriel Gerez has successfully defended his master thesis on the implementation of continuum solvation for MRChem, with a variational and cavity-free approach. He is now enrolled as a PhD student and will continue developing this model in his PhD project. PhD student Magnar Bjørgve has worked on introducing periodic boundary conditions (PBCs) in MRChem. He has been working on improving the precision of the results (a non-trivial task for PBCs), with the aim of producing basis-set-error-free PBC benchmarks. During the autumn, Evelin Battistella (visiting student from Brasil sponsored by the IAESTE program) worked on the Python interface of our multiresolution library, VAMPyR (Very Accurate Multiresolution Python Routines), expanding its features considerably.

Frediani has supervised the work of the PhD students and worked on completing the linear response implementation (GGA functionals as well as exact exchange are now available). The group has met regularly every week to coordinate the various activities and plan the work ahead. Moreover, we have started organizing “hackathon days” where we meet off-campus to focus on code development (*picture 1* ↑).

Picture 1: The MRChem group at Eidkjosen, during the off-campus coding & sailing day in September 2019. From left to right: Stig Rune Jensen, Gabriel Gerez, Magnar Bjørgve, Evelin Battistella, Anders Brakestad. *Photo: Luca Frediani*

Stochastic coupled-cluster theory

The Hylleraas Centre and RT1 are involved in a collaboration with Cambridge University (UK) and Virginia Tech (USA) on the development of Monte-Carlo coupled-cluster methodologies for molecular properties. This project is spearheaded by Roberto Di Remigio and supported by the RCN Mobility grant *Stochastic Methods for Molecular Chiroptical Properties*. Recent results of the project have been presented at the Telluride Science Research Center workshop on *Stochastic Methods in Electronic Structure Theory* in 2019.

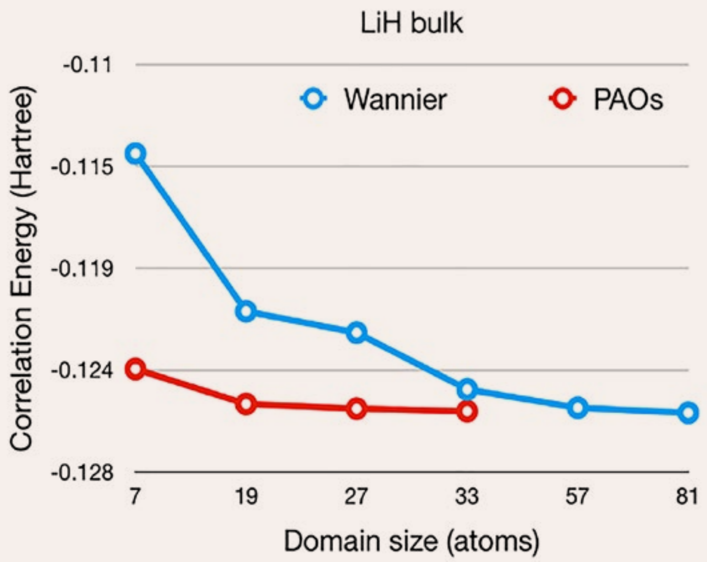
BIVAQUM

The ERC Starting Grant project *BIVAQUM (Bivariational Approximations in Quantum Mechanics and Applications to Quantum Chemistry)* entered its fifth year in 2019. In addition to the project leader Simen Kvaal, the group at this point consists of postdocs Tilmann Bodenstein and Andre Laestadius and PhD students Fabian Maximillian Faulstich and Benedicte Ofstad. The BIVAQUM project is centred around the *bivariational principle*, an unconventional formulation of quantum mechanics that naturally leads to the coupled-cluster hierarchy of computational methods. We focus on a mathematical analysis of bivariational methods and the development of new computational methods. In particular, we are aiming for novel attacks on the multireference problem.

In 2019, an analysis of the coupled-cluster method tailored by tensor network states (TNS-TCC) was published, in a collaboration with Prof. Reinhold Schneider in Berlin and Dr. Örs Legeza in Budapest [1]. This is the first mathematical analysis of a multireference coupled-cluster scheme in the literature and was followed up by a numerical study on the nitrogen dimer [2].

The activity in the BIVAQUM group now focuses on the multireference problem. Bodenstein and Kvaal have developed and implemented a novel method, the first multireference coupled-cluster method based on the bivariational principle. The results are promising and a journal article is in preparation.

Several workshops and conferences were attended. In particular, Kvaal attended the workshop *New Developments in Coupled-Cluster Theory* in Telluride, USA in 2019. Faulstich and Laestadius attended the 2019 Sanibel Symposium.



↑ **Figure 2:** Second-order Møller–Plesset correlation energy per unit cell of bulk LiH as a function of local-excitation domain size (measured as number of nearest-neighbour atoms). *Illustration: Lorenzo Maschio*

Periodic coupled-cluster theory

The RCN FRIPRO research project *Coupled-Cluster Methods for Periodic Systems*, led by Thomas Bondo Pedersen, ended on November 30 2019, but PhD student Audun Skau Hansen and master student Einar Aurbakken continue to work on the project in collaboration with Pedersen.

In 2019, the X-DEC code for periodic linear-scaling coupled-cluster calculations has been substantially rewritten in response to our findings reported in a manuscript submitted in late 2019 [3] in collaboration with Prof. Lorenzo Maschio in Turin (now accepted for publication). In this paper, we demonstrate that, despite being more local according to commonly used measures, localized orthonormal virtual Wannier orbitals (LVOs) are far inferior to simple projected atomic orbitals (PAOs) with respect to capturing electron-correlation effects with as few virtual functions as possible (*figure 2* ↑). The PAOs, however, are linearly dependent and non-orthonormal, forcing us to redesign the X-DEC code. In this process, the code has been refactorized to better exploit translational symmetry, including significant acceleration through a fully periodic implementation of the Coulomb-attenuated resolution-of-the-identity approximation to the electron-repulsion integrals. This work was mainly done by Hansen, while Aurbakken has developed an automatic spline-based determination of cut-off distances for long-range interactions, as required for a reliable calculation of correlation energies at minimal computational cost. These developments are currently being optimized for computational efficiency and the methodology is being tested through theoretical determination of equilibrium lattice parameters of ionic and covalent crystals and van der Waals-dominated surface adsorption distances. A manuscript is under preparation and will be submitted for publication in 2020.

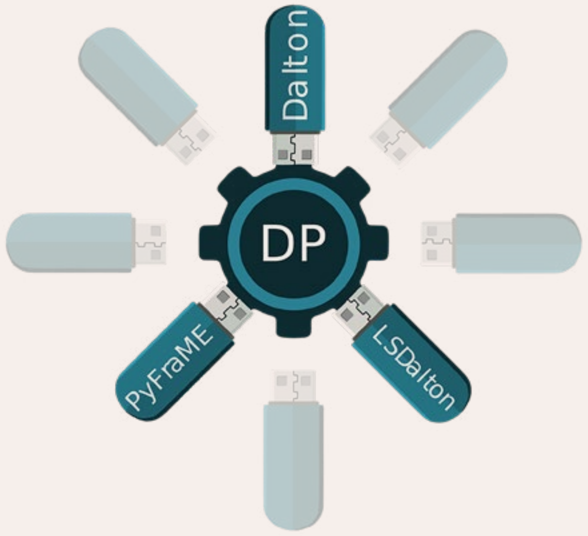
The Dalton Project

The use of quantum-molecular modelling is growing due to its increasing predictive power, the complexity of chemical systems that can be studied, and the emergence of more complex novel predictions and insights. To address these challenges, we need a paradigm change in the software engineering practices in the field of quantum chemistry to more easily develop, sustain and maintain large and complex general-purpose software ecosystems.

In 2019, the Dalton community took the important first step in this direction by initiating the *Dalton Project*.

The Dalton Project provides a uniform platform for accessing the full-fledged quantum-chemistry codes Dalton and LSDalton along with the PyFraME library for automatic fragmentation and parameterization of complex molecular environments. The Dalton platform is written in Python and provides the software infrastructure for library communication and interaction. Intermediate data such as molecular integrals are exposed through the platform and made accessible to the user in the form of NumPy arrays. Complex computational protocols, such as environment fragmentation and configuration-space sampling of biochemical systems, are facilitated by the Dalton platform, which also provides support for extraction, analysis, and visualisation of computational results. An article describing and illustrating the Dalton Project platform has been published [4].

The development of the Dalton platform lays an important foundation for the design of a sustainable software ecosystem for the core activities of the Hylleraas Centre. The platform is designed both to interface existing, often monolithic, codes in a unified framework and to host modular software libraries (*figure 3* ↑). Although the Dalton community today covers part of the activities of the centre, the experience of Simen Reine with the design and implementation of the Dalton Project will benefit the ambitions of the Hylleraas Centre to develop a collaborative software platform to accelerate inter-RT collaborations.



↑ **Figure 3:** Logo of the Dalton Project. *Illustration: Iulia-Emilia Brumboiu.*

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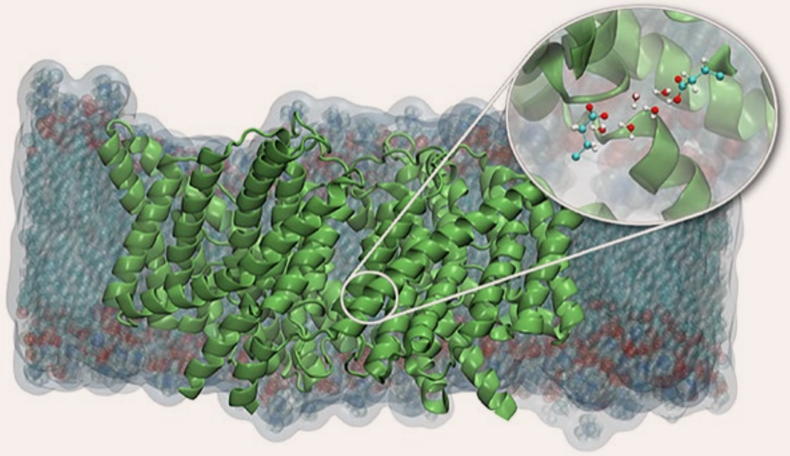
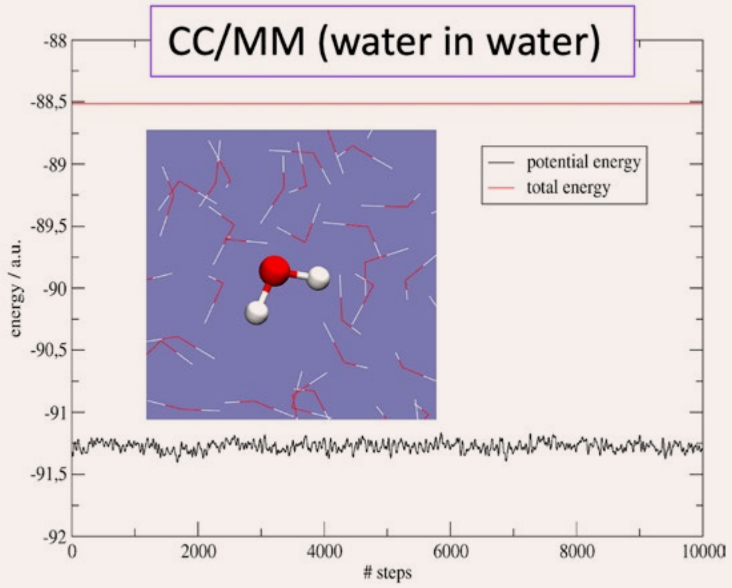
RT2

Multiscale Modelling

Principal investigators:
Michele Cascella and
Bjørn Olav Brandsdal



↑ **Figure 1:** ClC-ec1 ion channel embedded in a lipid membrane with the QM region in the inset; solvent not shown. The remaining more than 150,000 atoms are treated at the MM level. *Reprinted with permission from Ref. [1]. Copyright 2019 American Chemical Society.*



↑ **Figure 2:** Water-in-water hybrid coupled-cluster QM/MM molecular dynamics simulation using the MiMiC-based CFOUR/CPMD interface. Under NVE conditions, the total energy is conserved over 105 simulation steps.

RT2 is devoted to the development of computational methods from quantum mechanics to the mesoscale and to build algorithmic bridges across multiple resolutions. 2019 has been a year of investment, with a relatively small number of publications, but with important intermediary work that will pay off in the coming years.

The MiMiC project

Jógvan Magnus Haugaard Olsen from UiT heads a collaborative effort to develop a highly flexible and efficient multiscale modelling framework for computational chemistry (MiMiC). The MiMiC framework, whose design principles were published in early 2019 [1], promises high flexibility and performance through a design that allows coupling of separate programs, where each program can use their own optimal parallelization strategy and communicate through network-based solutions employing high-performance interconnects.

QM/MM molecular dynamics

The MiMiC framework has been used to implement a multiscale quantum-mechanics/molecular-mechanics (QM/MM) model based on density-functional theory (DFT) for the QM part. Here the CPMD program was used to run a molecular dynamics (MD) simulation using CPMD and GROMACS for the QM and MM contributions, respectively, while MiMiC computed the contributions due to QM/MM interactions using a highly efficient and scalable algorithm. The performance of the implementation was demonstrated in a publication [2]. On a system consisting of a ClC-ec1 ion-channel protein embedded in a lipid membrane (*figure 1* ↑), we reached a peak performance of 14 seconds per simulation time step for Born–Oppenheimer MD with a hybrid exchange–correlation functional. To obtain this level of performance, we used 13,440 CPU cores with more than 70% strong scaling parallel efficiency.

In a collaboration with Prof. Jürgen Gauss (Johannes Gutenberg University, Mainz), we have established a protocol to run both ab-initio MD (AIMD) and hybrid QM/MM simulations with coupled-cluster theory. Using the MiMiC framework, we have coupled AIMD and QM/MM routines in the CPMD package to the CFOUR quantum chemistry software (*figure 2* ↗). The implementation, which was done by PhD student Till Kirsch in Mainz, has been tested for the calculation of IR/Raman spectra of simple molecular systems both in vacuo and in solvent, reproducing both harmonic and anharmonic frequencies with excellent accuracy. A manuscript on the implementation and first application is in preparation [3].

Hybrid particle/field model

In 2019, the UiO group continued the development of the hybrid particle/field (hPF) methodology.

In early 2019, the generalized formalism for the treatment of electrostatic interactions in hPF calculations in non-homogeneous phases was published in the *Journal of Chemical Theory and Computation* [4]. By defining the total electrostatic energy as a function of the displacement field **D** and the dielectric function ε (*figure 3 next page* →), we can deduce that a particle of type K is subject to the potential

$$V_{\mathrm{ext},K} = q_K\psi(\mathbf{r}) - \frac{1}{2}\frac{\partial\epsilon(\{\phi(\mathbf{r})\})}{\partial\phi_K(\mathbf{r})}(\nabla\psi(\mathbf{r}))^2$$

where the first term is the electrostatic potential energy of the charge and the second arises from polarization. We have demonstrated that this scheme reproduces the partitioning of ideal ions in water/oil mixtures and that it can predict the correct low permeability of both zwitterionic and charged membranes to ideal ions [4].

A major challenge in density-based models is to properly determine the full internal pressure tensor. Since the density is a local quantity, functionals that depend on the density function alone cannot account for anisotropic effects. As a consequence, interfacial properties – in particular, surface tensions – cannot be properly described by density-based models. To correct this situation, PhD student Sigbjørn Bore has introduced a generalization of the interaction energy functional, adding a term that takes into account interface energy contributions dependent on the gradient of the densities of the various moieties composing the system:

$$H = H_0(\{\mathbf{r}_i\}) + W[\{\phi(\mathbf{r})\}] + W_1[\{\nabla\phi(\mathbf{r})\}]$$

The new term guarantees the appearance of anisotropic contributions to the pressure in the presence of ordered molecular organization in the system – in particular, at interfaces. The correct description of surface tension guarantees, for example, the formation of regular spherical shapes for small oil droplets in water (*figure 4* ↑) and the correct area per lipid in lipid bilayers during constant pressure simulations. A manuscript on these advances has been published in 2020 [5].

The project involves the crucial collaboration with Prof. G. Milano from Yamagata University, Japan.

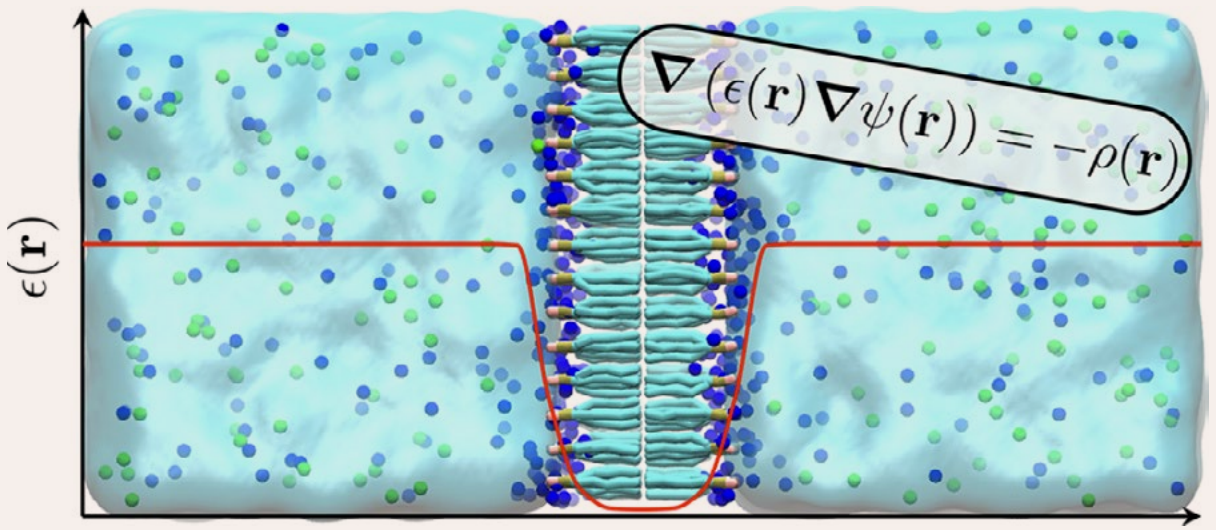


Figure 3: Schematic representation of a lipid bilayer and the corresponding drop in the dielectric function. *Reprinted with permission from Ref [4]. Copyright (2019) American Chemical Society.*

The original formulation of the hPF method relies on the definition of a simple interaction energy, which depends on a set of parameters χ_{ml} (were m,l are indexes running over all particle types) that have the precise physical meaning of mixing free energies. While such an interaction matrix can be easily set up for simple polymer melts – for example, using the Flory-Huggins model – its determination is much more difficult for complex moieties, especially in the presence of long-range interactions. Our most recent developments have introduced a significant number of free parameters into the model – specifically, one dielectric constant for every particle type and a second interaction matrix for interfaces, K_{ST}, which has in principle the same dimensionality as χ_{ml}.

With such a complicated representation of the interaction energy, any protocol based on simple modelling, and eventual ad-hoc manual optimization, becomes unpracticable. During the last year, PhD student Morten Ledum has devised a protocol based on Bayesian optimization, where all interaction parameters are globally derived. The optimization is obtained by machine learning, training the potential to reproduce as accurately as possible properties that are deemed to be relevant for the system of interest. The algorithm has been particularly successful in systematically refining potential energy terms previously obtained from the Flory–Huggins model, as demonstrated for phospholipid bilayers (*figure 5* ⊕).

A manuscript describing this protocol has been published in 2020 [6].

Funding / Personnel

Sigbjørn Bore submitted his PhD thesis in December 2019, with defence planned for spring 2020. Two new PhD students, Manuel Carrer and Samiran Sen, began their studies at UiO during fall 2019.

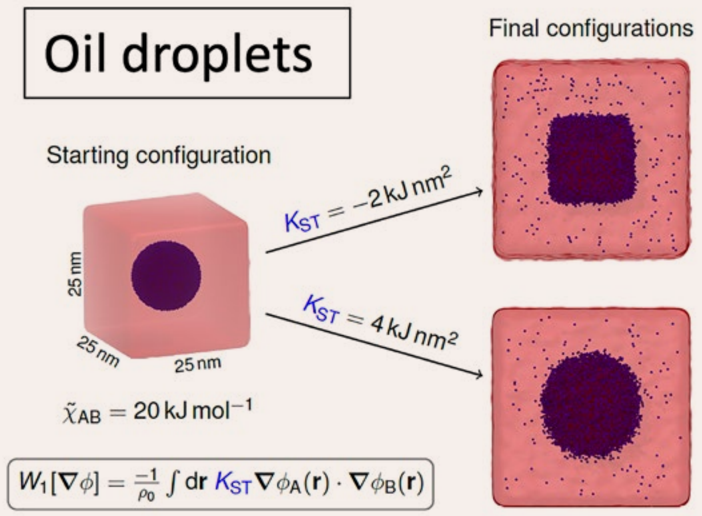


Figure 4: Shape of an oil droplet as a function of the surface tension constant K_{ST} in hPF simulations.

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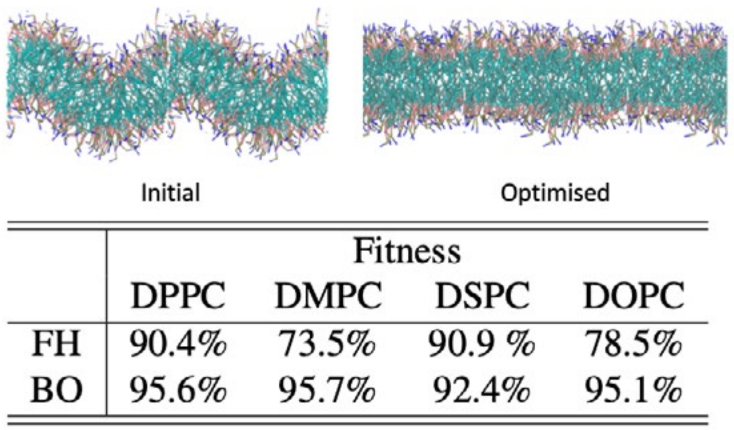


	Fitness			
	DPPC	DMPC	DSPC	DOPC
FH	90.4%	73.5%	90.9 %	78.5%
BO	95.6%	95.7%	92.4%	95.1%

Figure 5: Similarity of lateral density profiles for DPCC, DMPC, DSCP, and DOPC phospholipid bilayers to reference MARTINI CG simulations from Flory–Huggins (FH) and Bayesian optimization (BO)

RT3

Spectroscopic Processes

Principal investigators:
Kenneth Ruud and
Thomas Bondo Pedersen

In RT3, we develop computational tools for describing the experimental observations that will be realized at the new light sources. RT3 builds on the developments in RT1 and RT2 to describe spectroscopic processes of increasingly complex systems.

Consolidation and outreach

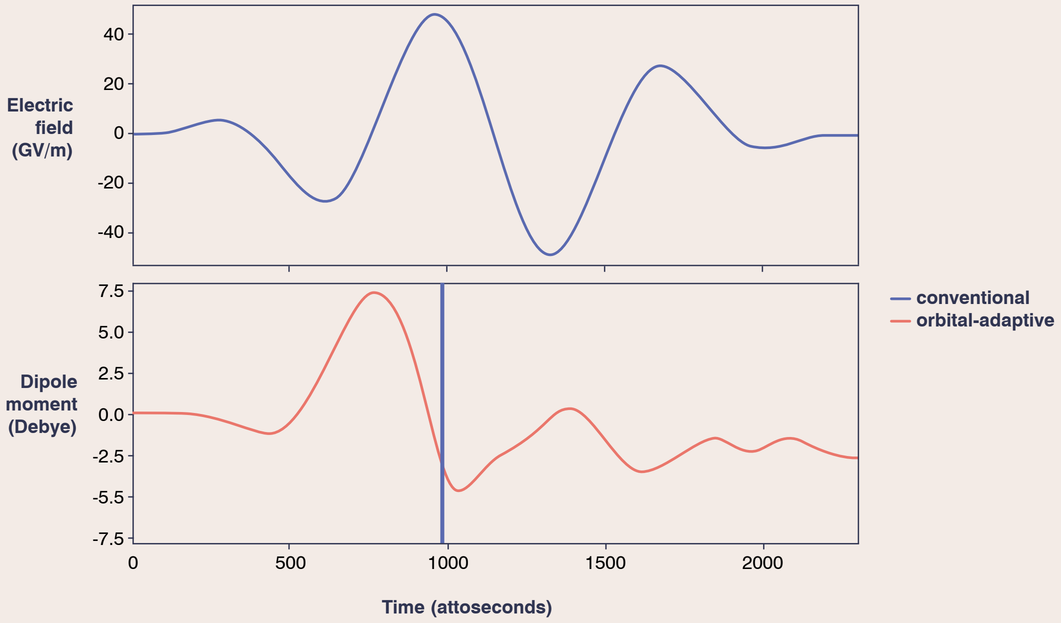
As described in the reports of RT1 and RT2, much effort has in 2019 been spent on preparing for code releases and documenting the functionality of code developed at the Hylleraas Centre. In addition to the Dalton Project and LSDalton developments, all relevant to the work in RT3, efforts have been devoted to finalizing a release of OpenRSP [1] in the framework of the Dalton Project and linked to the LSDalton linear-scaling program. This will open new opportunities in the size of systems that can be studied, for instance, for multiphoton absorption processes, as well as new functionalities through the open-ended integral-derivative schemes for geometric perturbations. A major effort has also been invested in preparing a manuscript describing the ReSpect program for two- and four-component relativistic density-functional theory (DFT) calculations for molecules and solids [2].

Laser-driven many-electron dynamics

The rapid development of laser sources capable of producing ultrashort, high-intensity pulses makes it possible to investigate transient phenomena of atomic and molecular electronic systems. This poses a challenge to quantum-chemical modelling, which relies on steady-state populations of energy levels to make transients subside. Focusing on energies and frequencies, the conventional quantum-chemical models become delocalized in time and not well suited for the description of laser-driven many-electron dynamics.

Facing this challenge, Thomas Bondo Pedersen and Simen Kvaal have put significant effort into the development of real-time time-dependent coupled-cluster theory. In a paper published in early 2019 [3], a new interpretation of coupled-cluster theory based on the time-dependent bivariational principle was proposed along with a numerically stable algorithm for integrating the equations of motion in the presence of an external laser pulse. A key finding of this work is that the conventional formulation of coupled-cluster theory – using the static Hartree–Fock ground state as the reference determinant – becomes numerically unstable in the presence of an intense laser pulse, as it pumps the many-electron system into a superposition of states that is essentially orthogonal to the reference determinant.

It thus becomes evident that a reformulation of time-dependent coupled-cluster theory is needed to make accurate computational studies of high-field phenomena possible. Based on earlier work by Pedersen *et al.* [4] and Kvaal [5], PhD students Håkon Emil Kristiansen at the Hylleraas Centre and Øyvind Sigmundson Schøyen at the Department



↑ **Figure 1:** The dipole moment (bottom) induced in the Be atom by an intense laser pulse (top). The orbital-adaptive coupled-cluster model provides an excellent agreement with the exact wave function, whereas conventional coupled-cluster theory fails after about 1000 attoseconds. *Illustration: Håkon Emil Kristiansen and Thomas Bondo Pedersen*

of Physics (co-supervised by Pedersen) have implemented the orbital-adaptive time-dependent coupled-cluster model and shown that it provides significantly improved stability in strong laser pulses [6] (*figure 1* ↑). The Hartree–Fock ground-state determinant is replaced by time-dependent biorthonormal determinants that capture the main effects of the laser pulse in concert with the correlation description provided by the cluster amplitudes. Supported by numerical evidence, it is conjectured in [6] that the time-dependent biorthonormal determinants are excellent approximations to the Brueckner determinant – the single determinant closest in Hilbert space to the exact (full configuration interaction) wave function – and that this is the key to numerical stability. This work is also described in a Highlight in this Annual Report.

Based on these results, the goals of the near future are to embark on computational studies of strong-field ionization processes and higher-harmonic generation, theoretical and computational interpretation of the coupled-cluster state with applications to transient phenomena such as Rabi oscillations, and control of the electron dynamics by means of magnetic fields (relating here to RT4).

Liouville-space response theory

Magnus Ringholm is hired on a mobility grant from the Research Council of Norway, spending all of 2019 in Stockholm with Prof. Patrick Norman at the Royal Institute of Technology (KTH). Ringholm has in 2019 been working on developing a Liouville-space formulation of approximate-state response theory along the lines of existing non-Liouville-space response-theory formulations developed in the Scandinavian research community [7]. The goal is to improve the treatment of various damping/dephasing effects in this approach. Connected to this work is also the implementation of functionality to describe the behavior of molecules in a response-theory framework subject to electromagnetic fields with time envelopes of a non-limiting form. A basic form of this pulse time-envelope functionality is being implemented in the program VeloxChem – a program being developed in the research group of Norman at KTH in Stockholm. Ringholm has also participated in the ongoing development of the OpenRSP program library and its interface to other modules/programs.

Relativistic response theory

Lukas Konecny and Michal Repisky have in 2019 been engaged in the development of different approaches for calculating molecular response properties. Whereas our relativistic DFT program ReSpect for a long time has had the ability to calculate linear and nonlinear response properties using real-time propagation of the electron density in the presence of a electromagnetic perturbation [8], Konecny and Repisky have together with Dr. Stanislav Komorovsky at the Slovak Academy of Sciences developed a damped linear-response theory approach [9]. This approach allows linear electric and mixed electric–magnetic response properties to be calculated analytically, describing simultaneously the scattering and absorption processes that occur when electromagnetic light interacts with the electron density of a molecule. This work is described in more detail in a Highlight in this Annual Report.

In parallel with this work, Repisky has together with Komorovsky developed an open-shell time-dependent DFT formalism at the four-component relativistic DFT level [10], in which transition moments to individual excited states can be addressed. A particular feature of this formalism is its applicability to open-shell molecules known to be challenging for relativistic methods that include spin–orbit coupling. An interesting consequence of relativistic open-shell calculations of excitation energies is the ability to determine excited-state spin–orbit splittings and phosphorescence radiative lifetimes. More information can be found in the Highlight elsewhere in this Annual Report.

Relativistic solid-state density-functional theory

A major highlight of 2019 was the publication of the implementation of a fully relativistic four-component, all-electron DFT approach to systems with periodic boundary conditions in one, two, and three dimensions using Gaussian-type atomic orbitals [11], described in a Highlight in the 2018 Annual Report of the Hylleraas Centre. In 2019, much effort was spent on reducing the memory footprint of the code and improving computational efficiency as well as the scalability on parallel computers. This work was led by Marius Kadek together with Repisky. In December 2019, Kadek was awarded a mobility grant from the Research Council of Norway for 2020–2023, to extend this work to the study of topological magnetic materials.

In parallel, PhD student Marc Joosten has implemented nuclear electric-field gradients in the solid-state relativistic code. Nuclear electric-field gradients probe the electron density close to the nucleus, where relativistic effects are particularly important. The approach commonly used in solid-state codes using plane waves – namely, to describe the core electrons by pseudopotentials – therefore cannot be applied. In addition to being important as a means of unraveling the electron density in solids, nuclear electric-field gradients are important for determining nuclear quadrupole moments, one of the fundamental properties of nuclei with spin greater than one half. In collaboration with Prof. Pekka Pyykkö at the University of Helsinki, we have targeted the nuclear quadrupole moment of the Bi nucleus, for which atomic and molecular determinations of the nuclear quadrupole moment disagree, hoping that our solid-state calculations on Bi-oxyhalides can be combined with previous experimental observations to help resolve this conundrum.

The calculations on the Bi-oxyhalides (*figure 2*). proved to be computationally demanding. Joosten has therefore spent significant time during 2019 to implement the resolution-of-the-identity approximation in the solid-state code, significantly speeding up the calculations, allowing us to provide basis-set limit results for the electric-field gradients at the nuclei at the density-functional level of theory for systems with periodic conditions in one, two, and three dimensions.

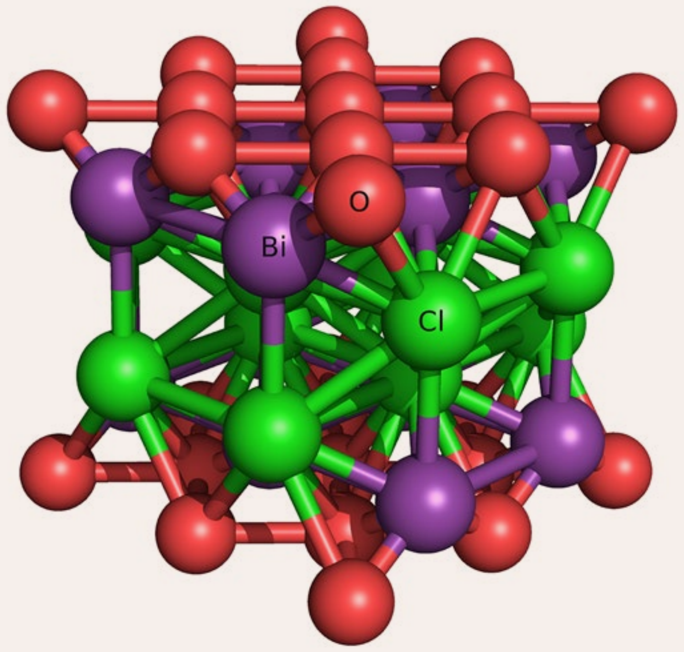


Figure 2: The properties of solid-state BiOCl are now being studied at the Hylleraas Centre using four-component relativistic DFT. *Illustration by Marius Kadek.*

Vibrational spectroscopy of embedded systems

PhD student Karen Dundas has continued her work on an open-ended response theory framework for the calculation of vibrational spectroscopies within the framework of the Dalton Project (see the RT1 Activity Report), extending the OpenRSP module, whose lead developer has been Ringholm, in combination with FraME and PyFraME developed by Magnus Olsen, and LS-Dalton, whose main developer at the Hylleraas Centre is Simen Reine. As part of her work, Dundas has included the development of a new Python framework for visualization and analysis of (anharmonic) infrared and Raman spectra, SpectroscPy, where the automatic averaging of multiple vibrational spectra calculated from snapshots taken from molecular dynamics simulations is a novel feature.

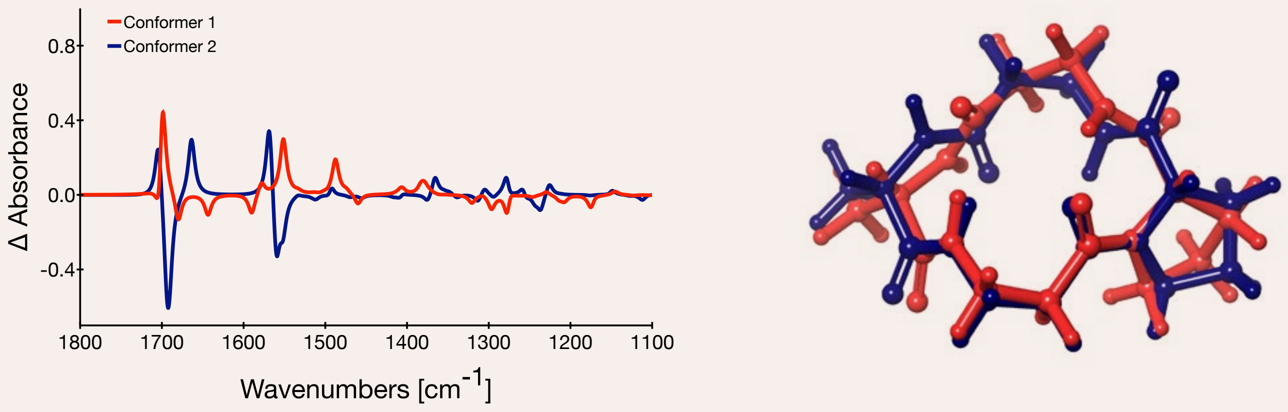
The work on integrating multiple program modules has proven to be more time consuming than expected due to a legacy of non-modular programming practices. At the same time, it has brought forward new developments in the evaluation and integration of exchange–correlation functionals for the analytic evaluation of higher-order geometric derivatives of exchange–correlation kernels, developed by Dr. Radovan Bast at the HPC group at the IT services department at UiT The Arctic University of Norway.

With all these elements being finalized and documented through the Dalton Project paper and two manuscripts in preparation, attention has in 2019 also been on the demonstration of the capabilities of the approach for multiscale modeling of solvent effects on harmonic infrared and Raman spectra as well as anharmonic hyper-Raman spectra of solvated molecules.

Vibrational chiroptical spectroscopy

PhD student Karolina Eikås has continued her work on establishing a computational protocol for the calculation of vibrational chiroptical spectra – in particular, vibrational circular dichroism (VCD) spectra of natural compounds based on cyclic polypeptides. This work is part of the larger Digibiotics project, a project funded by the Research Council of Norway involving researchers from three faculties at UiT The Arctic University of Norway, including Bjørn Olav Brandsdal and Kenneth Ruud from the Hylleraas Centre. The ambition is to bring novel marine natural products into drug design and development with the goal of identifying and optimizing new antibiotics, with a focus on polycyclic peptides beyond the Lipinski rule-of-five [12]. A milestone for 2019 was the installation of a vibrational circular dichroism (VCD) instrument at the premises of the Department of Chemistry at UiT The Arctic University of Norway.

Karolina Eikås' work has focused on how to reliably model vibrational chiroptical spectra of these complex molecules. Even small changes in the structure resulting from different conformational equilibria can have dramatic effects on the calculated spectra



↑ **Figure 3:** Calculated VCD spectra of two different conformers of cyclic (Ala-β-Ala-Pro-β-Ala). Conformer 1 (red) has rather small structural changes from Conformer 2 (blue), but the VCD spectrum of the two conformers differ dramatically, especially in the frequency range 1450–1750 cm^{1}. *Illustration by Karolina Eikås.*

(*figure 3* ↑). It is therefore important to design a computational protocol that can efficiently identify *all* relevant conformers and accurately calculate their relative stability and chiroptical spectra. This work has initially focused on compounds for which experimental data exist in the literature and which are complex enough to test the protocol but small enough to allow reference results to be obtained. In parallel with this, following the recommendations of the Digibiotics Scientific Advisory Committee, Eikås has contributed to a case study demonstrating a significant part of the planned pipeline for potential drug candidates by applying experimental and theoretical chiroptical spectroscopy to determine the molecular structure and chirality of a molecule synthesized in the laboratory of one the Digibiotic partners, Prof. John Sigurd Svendsen.

Computational studies

In addition to the method developments described thus far, there has been significant work on applying the new functionality to the study of molecular properties of chemical interest. Some of the work done in this respect concerns heavy-element NMR properties and has been performed by Odile Eisenstein and Abril Castro and is described in RT5.

Dr. Michiko Atsumi has studied NMR properties of small molecules in excited electronic states, giving new insight into the electron densities in electronically excited states and how these may affect NMR properties of molecules [13].

Kenneth Ruud has, together with Prof. Radek Marek of Masaryk University in the Czech Republic and his PhD student Pankaj Bora and other collaborators, studied the electronic spin structure and metal-ligand bonding in open-shell systems by means of relativistic DFT calculations of electron paramagnetic resonance and paramagnetic NMR spectra [14].

Ruud has been involved in several studies of photophysical properties of molecules, including fluorescence lifetimes of hybrid compounds of nitro-spiropyrans together with Dr. Vladimir Pomogaev of Tomsk State University [15]. Together with long-term collaborator Dr. Swapan Chakrabarti, he has studied the breakdown of the commonly assumed Kasha rule (stating that emissions occur primarily from the lowest singlet or triplet excited state) as a consequence of strong Duschinsky mixing on an organic phosphor [16].

Several applications have focused on core-electron excitations and X-ray spectroscopy. Bin Gao has together with colleagues at Nanjing University of Science and Technology and KTH in Stockholm studied the X-ray photoelectron and absorption spectra of the K edges of carbon and nitrogen atoms in g-C_3N_4 nanosheets, including vibronic effects [16]. Postdoc Rolf Myhre has, together with Prof. Sonia Coriani at the Danish University of Technology and Prof. Henrik Koch at the Norwegian University of Science and Technology, performed highly accurate studies of the X-ray and UV spectra of glycine using coupled-cluster linear response theory [18].

Finally, at the interface with RT2, Magnus Olsen has published a tutorial review on modeling response properties of embedded molecules [19], while Roberto Di Remigio and Luca Frediani have developed a fully polarizable QM/Fluctuating-Charge approach to two-photon absorption in aqueous solutions together with colleagues at the Scuola Normale Superiore in Pisa (Italy) [20].

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RT4

Extreme Environments

Principal investigators:
Trygve Helgaker and
Kenneth Ruud

In RT4, we explore the exotic, squeezed chemistry of ultra-strong magnetic fields and high pressure. In 2019, we studied ionization of atoms in magnetic fields, atoms and molecules in nonuniform magnetic fields, atomic and molecular confinement, and Kohn-Sham theory in magnetic fields.

We have published five papers within RT4 in 2019. These papers concern the Kohn–Sham energy decomposition for molecules in a magnetic field [1], the calculation of ionization energies in a magnetic field using *GW* and coupled-cluster theory [2], excited states of molecules in strong uniform and non-uniform magnetic fields [3], the foundations of current-density-functional theory (CDFT) [4], and convergence of the Kohn–Sham iterations [5]. In addition, two papers submitted in 2019 and accepted in early 2020 deal with molecules in soft confinement potentials [6] and magnetically induced currents in molecules obtained from CDFT [7]. Ongoing projects in RT4 concern the stability of larger molecules in strong magnetic fields and the electronic states of the helium molecule in strong magnetic fields – some results from these projects are described in a Highlight in this Annual Report.

Kohn–Sham theory in a magnetic field

In the paper *Kohn–Sham energy decomposition for molecules in a magnetic field* [1], we studied the total molecular electronic energy and its Kohn–Sham components within the framework of magnetic-field DFT (BDFT), an alternative to CDFT for molecules in the presence of magnetic fields. For a selection of closed-shell dia- and paramagnetic molecules, we investigated the dependence of the total electronic energy and its Kohn–Sham components on the magnetic field. Comparing with results obtained from Lieb optimizations based on field-dependent coupled-cluster singles-and-doubles (CCSD) and second-order Møller–Plesset (MP2) densities, we showed that popular approximate exchange–correlation functionals at the generalized-gradient-approximation (GGA), meta-GGA, and hybrid levels of theory provide a good qualitative description of the electronic energy and its Kohn–Sham components in a magnetic field – in particular, for diamagnetic molecules.

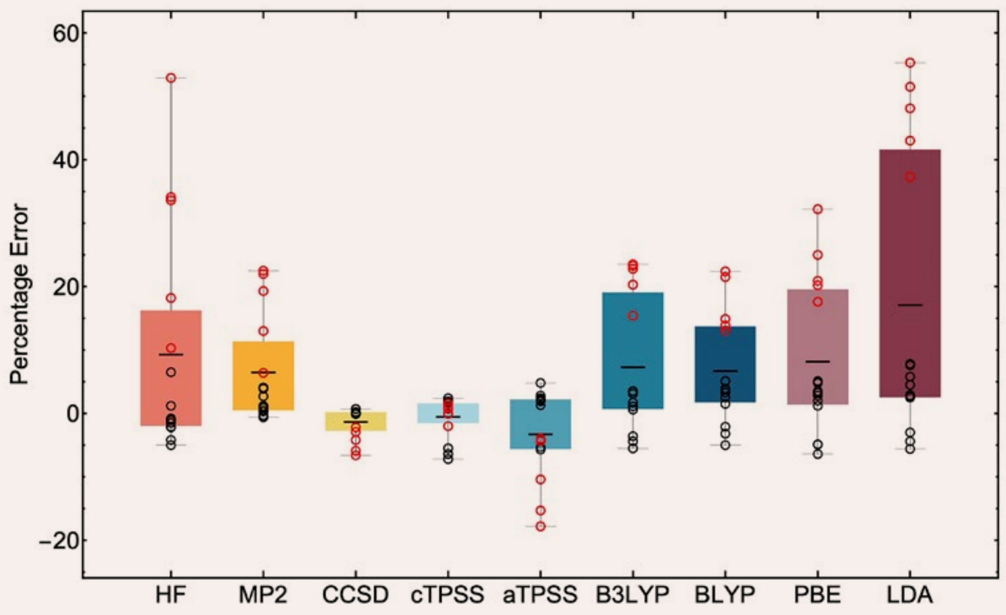


Figure 1: Mean percentage error for different models in the component of the magnetizability perpendicular to the magnetic field for the diamagnetic systems He, H_2, He_2, Be, H_2O, HF, Ne, N_2, CO, NH_3, C_6H_6, C_4H_5N (black circles) and the paramagnetic systems BH, CH, AlH, SiH, BeH (red circles). All errors are for magnetizabilities calculated in the uncontracted aug-cc-pVTZ basis relative to CCSD(T)/aug-cc-pCVQZ magnetizabilities. *Reproduced from Ref. [1] by permission of Taylor & Francis.*

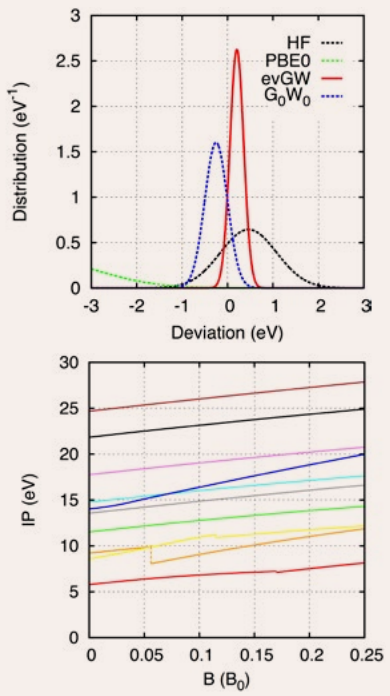
Furthermore, BDFT magnetizabilities calculated with different exchange–correlation functionals were compared with highly accurate magnetizabilities obtained using coupled-cluster singles–doubles–perturbative–triples (CCSD(T)) theory. These comparisons showed that the TPSS meta-GGA functional adapted to systems in a magnetic field performs well. The cTPSS functional, in particular, with a current-corrected kinetic-energy density, performs excellently, providing an accurate and balanced treatment of dia- and paramagnetic systems and outperforming MP2 theory (*figure 1* ↑).

Ionization energies in a magnetic field

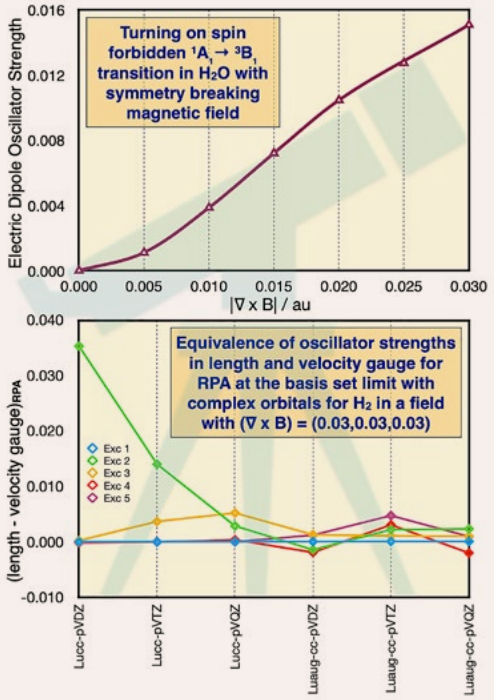
A central question regarding atoms and molecules in a strong magnetic field is their stability. In Ref. [2], we computed the ionization potentials of the first-row atoms H–Ne as the negative *GW* quasiparticle energies, comparing the results with ionization energies calculated using Hartree–Fock (HF) theory, DFT, and equation-of-motion coupled-cluster singles–and–doubles (EOM-CCSD) theory. This is the first systematic study of ground-state ionization potentials of the first-row atoms at field strengths up to $0.25B_0$ (with B_0 = 235kT), characteristic of magnetic white dwarfs. We found that the eigenvalue-only self-consistent *GW* model with the PBE0 functional (ev*GW*@PBE0 model) provides quasiparticle energies in good agreement with CCSD values and substantially more accurate than HF values and DFT values obtained with the PBE0 functional (*figure 2* →).

In the field range considered, the ionization potentials increase in a near-linear, concave manner. To understand this behaviour, we first note that the Zeeman interactions of an electron with the magnetic field are the same before and after ionization, while the diamagnetic energies are different. For an ionized electron, the diamagnetic energy increases linearly with the magnetic field; for an electron in an atom, it initially increases quadratically and then linearly as the atom enters the Landau regime, with $B > B_0$. For the field strengths considered here, therefore, the change in the ionization energy with increasing field strength is dominated by the linear increase in diamagnetic energy of the ionized electron, while the quadratic increase of the energy of the electron in the atom modifies the linear increase slightly, giving the ionization curves in figure 2 a slight concavity.

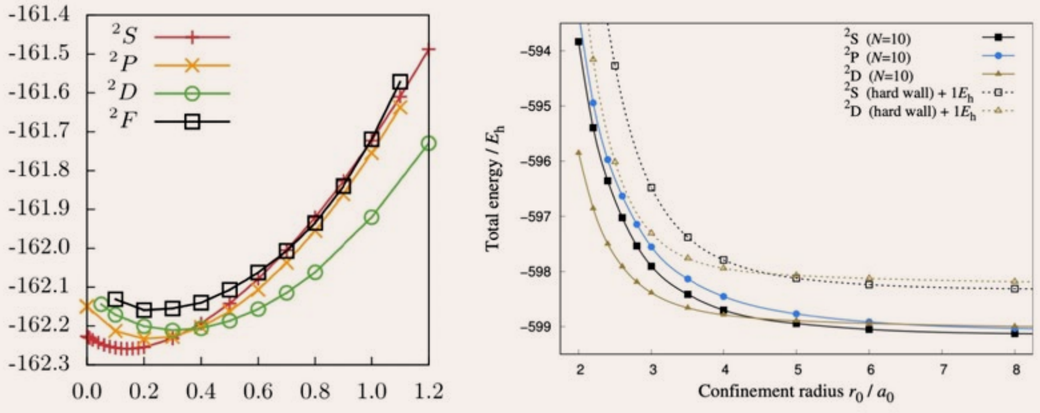
The erratum to Ref. [2] concerns an inconsistency in our definition of the charge fluctuation and does not affect our implementations of the *GW* method nor any numerical results in Ref. [2].



↑ **Figure 2:**
Above: Normalized Gaussian distributions of the Hartree–Fock, PBE0, evGW, and G_0W_0 deviations from the CCSD reference values.
Below: Ionization potentials of the first-row atoms as a function of the magnetic field strength. *Figures reproduced from Ref. [2] with the permission of AIP Publishing.*



↑ **Figure 3:** Spin breaking can be induced by nonuniform magnetic fields leading to spin-forbidden electronic transitions becoming possible (top panel). The equivalence of the length and velocity gauges for electric-dipole oscillator strengths has been established numerically (bottom panel). *Illustration: Sangita Sen*



↑ **Figure 4:** Left: The energy of the lowest states of the Na atom as a function of the magnetic field strength *B* (in units of B_0 = 235 kT)[8]. Right: The energy of the lowest states of the K atom as a function of confinement radius r_0 (in units of a_0 = 52.9 pm) for stiffness parameter *N* = 10 and the hard-wall limit *N* = ∞ [6]. *Figure to the left reproduced from Ref. [8] with the permission of AIP Publishing. Figure to the right reprinted from Ref. [6] by permission of Taylor & Francis.*

Excited states in strong uniform and nonuniform magnetic fields

In Ref. [3], Sangita Sen, Kai Lange, and Erik Tellgren reported an implementation of Hartree–Fock linear response theory for computing electronic spectra of molecules in strong external magnetic fields. Their implementation is general, allowing for spin-restricted, spin-unrestricted, and general two-component reference states. The implementation is applied to small molecules placed in strong uniform and nonuniform magnetic fields of astrochemical relevance. For uniform fields, where comparison is possible, the spectra are found to be qualitatively similar to those recently obtained with equation-of-motion coupled-cluster (EOM-CC) theory. The paper also contains a study of the behavior of spin-forbidden excitations with progressive loss of spin symmetry induced by nonuniform magnetic fields. The equivalence of length and velocity gauges for oscillator strengths when using complex orbitals is investigated and found to hold numerically (*figure 3* ↑).

Confined electronic systems

There are many similarities between confined electronic systems and electronic systems in a strong magnetic field – in particular, both systems are squeezed to occupy a smaller volume than they would otherwise do. In the paper *Atoms and molecules in soft confinement potentials* [6], we explored atomic and molecular electronic systems in confinement potentials of the form $V_N(r) = (r/r_0)^N$ of stiffness parameter *N* and confinement radius r_0. When *N* = 2, we recover the harmonic potential, similar to the diamagnetic part of the kinetic energy in a magnetic field except that the diamagnetic operator confines the system only in the directions perpendicular to the magnetic field. In the limit when *N* tends to infinity, we recover hard-wall confinement.

The similarities between magnetic fields and confinement are seen in figure 4, where we compare the energies of the lowest states of the sodium atom as a function of the magnetic field strength and the energies of the lowest states of potassium atom as a function of the confinement radius r_0 for different stiffness parameters *N* (*figure 4* ↗).

It is noteworthy that the magnetic field and the confinement potential both reverse the ordering from S < P < D to D < P < S. This behaviour can be rationalized by noting that the expectation value of the radius of the hydrogen orbital is $(3n^2 - l(l+1))/2$, where *n* is the principal quantum number and *l* the angular-momentum quantum number. Thus, for a fixed principal quantum number *n*, the hydrogen atom becomes more compact with increasing angular momentum, meaning that states of high angular momentum are less penalized by applied pressure and magnetic field.

The compression of the electronic density and the increasing importance of high-angular momentum states in a strong magnetic field and under high pressure means that it becomes more difficult to converge the basis set for systems under such conditions [6,8]. Standard basis sets lack the flexibility necessary to describe high-angular momentum states and their Gaussian exponents are not optimal for compressed systems. In our experience, however, this compression does not represent a problem for systems in magnetic fields of strength up to about one atomic unit B_0. Indeed, it may be preferable to use flexible traditional basis sets for field strengths up to B_0 since such sets sometimes provide a smoother field dependence than basis sets with field-dependent exponents [2].

We have also studied CH_4 both in magnetic fields and in confinement. In a spherical confinement potential, the one-electron density of CH4 becomes more spherical as the molecule becomes compressed (*figure 5* →).

It is interesting to note that the total electronic energy increases while the correlation energy decreases (increasing in magnitude) as pressure is applied, demonstrating the importance of electron correlation for the correct description of squeezed systems (*figure 6* →).

An ongoing related project is the structure of CH_4 in strong magnetic fields. While it is clear that covalent bonds are broken by the spin Zeeman effect and new bonds are formed by the orbital Zeeman effect, the precise nature

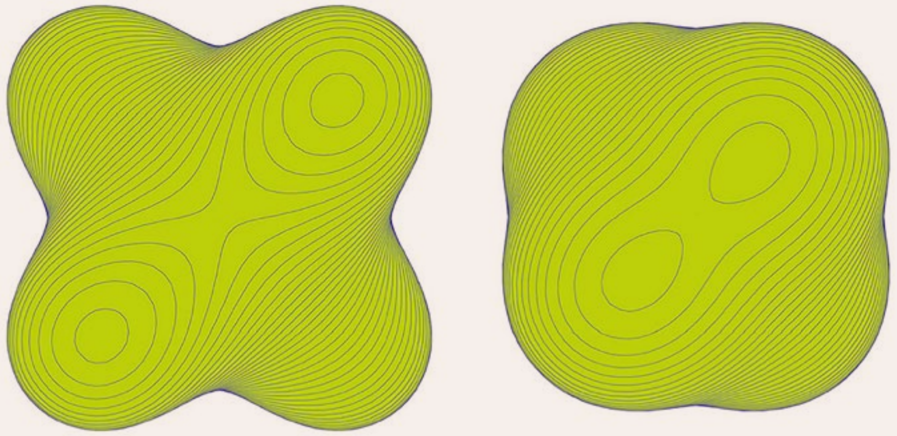


Figure 5: One-electron density of free (left) and confined (right) CH$_4$ (N = 10, r_0 = 2.4 a_0). Isodensity surfaces of $0.1a_0^{3}$ are shown on the same scale. *Reproduced from Ref. [6] by permission of Taylor & Francis.*

of these bonds in CH$_4$ is still unclear. We have established that the molecule remains bound at field strengths of one atomic unit, but the equilibrium structure is not yet known. A planar symmetrical arrangement with the four hydrogen atoms around the central carbon atom is a saddle point; the minimum is less symmetric, with the hydrogen atoms arranged in a half-circle rather than full circle around the carbon atom.

Fundamentals of DFT

In 2014, we established Moreau–Yosida regularization as a mathematical tool to achieve rigorous functional differentiability in DFT [9]. In the article *Kohn-Sham theory with paramagnetic currents: compatibility and functional differentiability* [4], we extended this tool to CDFT, the most common density-functional framework for magnetic field effects. The extension includes a well-defined Kohn–Sham iteration scheme with a partial convergence result, relying on a formulation of Moreau–Yosida regularization for reflexive and strictly convex function spaces. A crucial prerequisite for the convex formulation of paramagnetic CDFT, termed compatibility between function spaces for the particle density and the current density, is pointed out and analyzed. Several results about compatible function spaces are given, including their recursive construction. The regularized, exact functionals are calculated numerically for a Kohn–Sham iteration on a quantum ring, illustrating their performance for different regularization parameters. In Ref. [5], the exact Kohn–Sham iteration of generalized DFT in finite dimensions with a Moreau–Yosida regularized universal Lieb functional and an adaptive damping step is shown to converge to the correct ground-state density.

Personnel and funding

Apart from RT leader Trygve Helgaker and co-leader Kenneth Ruud, the personnel on RT4 are Erik Tellgren, Sangita Sen, PhD-student Jon Austad, and Asst. Prof. Andy Teale, University of Nottingham, who is hired in a 20% position at the Department of Chemistry, University of Oslo.

Sangita Sen was on maternity leave March–December 2019 and will leave in 2020 to take up a position at the Indian Institute of Science Education and Research (IISER) in Kolkata in May 2020. Jon Austad left in July 2019 for a position at the University Centre for Information Technology at the University of Oslo and will defend his thesis in 2020.

Two postdocs, Dr. Tanner Culpitt and Dr. Laurens Peters, have been hired for three years on the project *Magnetic Chemistry*, financed by the Research Council of Norway. They will begin work in July 2020.

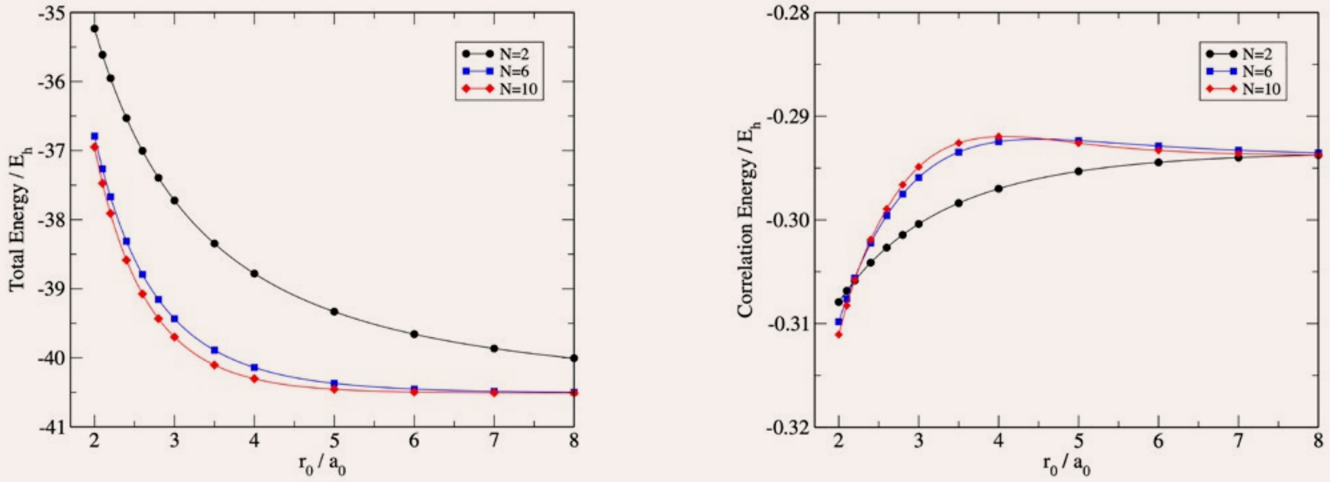


Figure 6: Total CCSD(T) energy (left) and total electron correlation energy (right) for the soft-wall confined CH$_4$ molecule plotted against the confinement radius r_0 for stiffness parameters N = 2, 6, 10. *Reproduced from Ref. [6] by permission of Taylor & Francis.*

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RT5

Chemical Transformations

Principal investigators:
Odile Eisenstein and
Kathrin Hopmann

RT5 applies state-of-the art computational methods to analyse and understand reactions in chemistry, often in collaboration with experimental groups. RT5 focuses on topics that can make chemistry more environmentally friendly. Research is carried out on the functionalization of CO_2 and water oxidation. Catalysis and chemical reactions based on main-group elements and earth-abundant metals, as well as on metal complexes with unusual oxidation states (Au(III)), are being considered. Relationships between reactivity patterns and spectroscopic properties are analysed and machine learning tools for homogeneous catalysis are being developed. RT5 increasingly benefits from the complementary competences present in the other RTs.

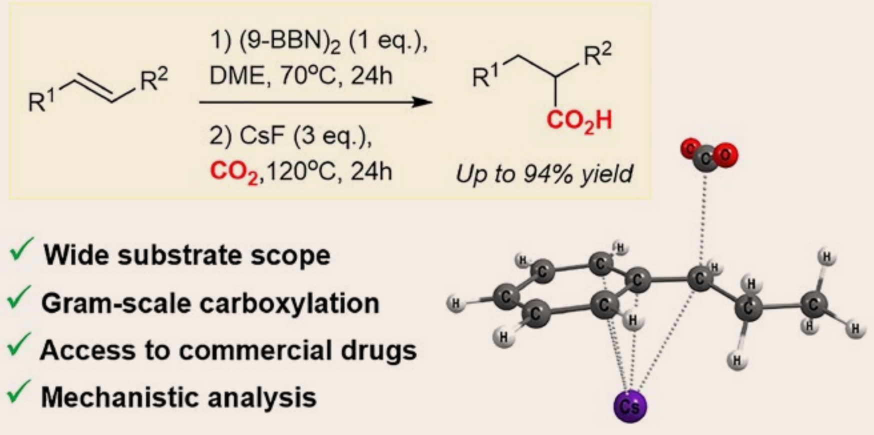
Water oxidation

Following the collaboration established through a visiting scholarship in 2017 [1], David Balcells investigated the electronic structure and reactivity of a cubic cobalt-oxide doped with ruthenium [2]. This species was oxidized and fully characterized in a Ru(V)-oxo state, analogous to that postulated as key intermediate in the catalytic oxidation of water. The oxo state mimics the structural and functional properties of metal-oxide materials and oxidase enzymes. The work involved a diverse team of researchers with expertise in synthesis (Prof. Tilley, UC Berkeley), spectroscopy (Prof. Britt, UC Davies) and modelling (Balcells, Hylleraas). The calculations made it possible to identify the orbital interactions between the support and dopant metal centres, which, at the core of the cube, stabilize the high oxidation state. Another key feature revealed by the calculations is the localization of the radical character into the Ru(V)-oxo, supported by experiments showing the high activity of this moiety in the C–H oxidation of organic substrates.

Under the supervision of Balcells and Trygve Helgaker, MSc student Bastian Skjelstad also contributed to the investigation of the cubic oxides. His work focused on the exploration of a large chemical space in which the cobalt core is doped with different transition metals at the limit of the oxo wall. The goal of this project is to understand which support-dopant metal combinations yield an optimal balance between stability (i.e., aqua-to-oxo redox potentials) and reactivity (i.e., energy barriers for C–H and water oxidations).

Carbon–carbon bonds with CO_2

Efforts were pursued to study CO_2 as a source of carbon in chemical reactions. PhD student Marc Obst from Kathrin H. Hopmann´s group studied the Cu-catalysed carboxylation of organoboranes. The study showed that non-benzylic C_{sp^3} substrates prefer a transition state where CO_2 is interacting with the metal centre (*inner*-sphere pathway), while for benzylic C_{sp^3} substrates both transition states with metal-interacting CO_2 and non-interacting (*outer*-sphere pathway) CO_2 are accessible [3]. Moreover, calculations performed by Obst indicated that the reaction for some substrates may not be Cu-catalysed but rather Cs-mediated. The Cs-mediated carboxylation of benzylic and allylic substrates was experimentally verified. Obst performed a computational study of the Cs-mediated reaction using artificial force-induced analysis of reaction pathways (AFIR), indicating that benzylic organoboranes are transformed to organocaesium intermediates, which then react with CO_2 via a nucleophilic attack [4] (*figure 1* ↑).



↑ **Figure 1:** Cs-assisted carboxylation of allylic and benzylic substrates. From Ref. [4] – *Published by the Royal Society of Chemistry.*

Inspired by the findings indicating different pathways for CO_2 incorporation, Diego Garcia Lopez, a postdoc in Hopmann´s group, worked on a systematic mechanistic evaluation of the CO_2-incorporating step of C–CO_2 forming reactions catalysed by different metal catalysts and using different substrates (submitted for publication). The work showed that Pd- and Rh-benzyl complexes as nucleophiles strongly favour *outer*-sphere CO_2 insertion, while the picture is not that clear for Cu-benzyl complexes, where the insertion mode seems to depend on ligand size. For metal-C_{sp^2} complexes, an *inner*-sphere pathway of CO_2 insertion was preferred for all tested metals (Cu, Rh and Pd), in line with previous computational results on Cu- and Rh-C_{sp^2} systems.

Under the supervision of Hopmann, PhD student Ljiljana Pavlovic followed up on the mechanistic study of the Rh-catalysed hydrocarboxylation [5] with a search for chiral ligands to improve the enantioselectivity of the reaction by automatized modelling of enantioselectivity with the program AARON (An Automated Reaction Optimizer for New catalyst) by Prof. Steven E. Wheeler (Texas A&M, USA). Promising candidates for highly selective chiral ligands were identified and will now be investigated experimentally in collaboration with the group of Assoc. Prof. Annette Bayer (UiT). PhD student Cuong Dat Do joined Hopmann´s group in late 2019. He has started to investigate the mechanism of a base metal-catalysed lactonization reaction using CO_2, developed by Prof. Timo Repo (Aalto University, Finland).

CO_2 reduction

In the last year of her FRIPRO Young Research Talent project, Ainara Nova has focused on the hydrogenation of CO_2 to methanol by two different approaches: 1) homogeneous bifunctional catalysis, and 2) MOF-supported catalysis (MOF = Metal Organic Framework).

The most efficient processes for the homogeneous hydrogenation of CO_2 to methanol involve amines as co-catalysts and amides as reaction intermediates (*figure 2* →). PhD student Lluís Artús Suárez has focused his research on studying the mechanism of the deaminative hydrogenation of amides by using base-metal catalysts [6,7,8]. His work revealed that the reaction mechanism depends on both the nature of the metal (Fe or Mo) and the amide substituents. Furthermore, it was found that the yield of the process can be significantly enhanced by co-catalysis. This work was carried out in collaboration with the groups of Profs. Wesley Bernskoetter at the University of Missouri (USA) and Matthias Beller at the LIKAT institute (Germany).

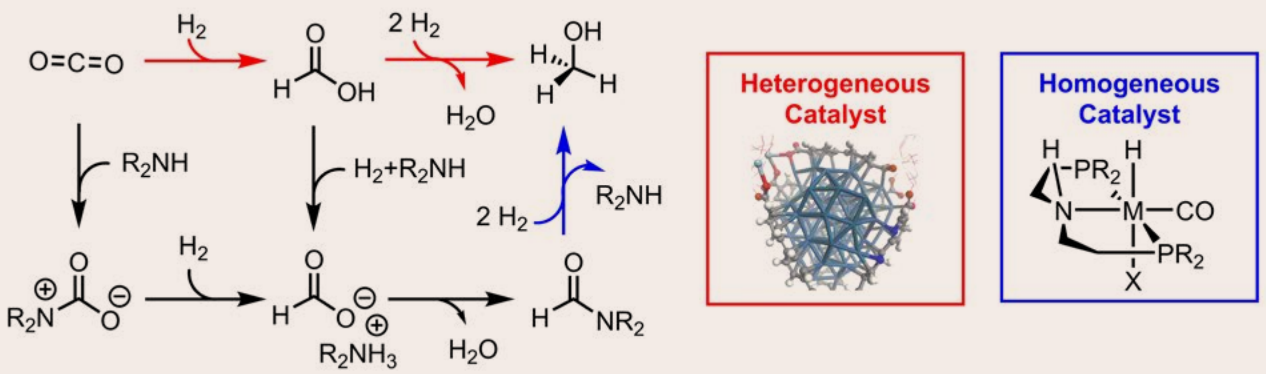


Figure 2: Reactions involved in the hydrogenation of CO$_2$ to methanol with the homogeneous and heterogeneous catalysts (M=Fe, Mo; X = H, CO). *Illustration: Ainara Nova*

Platinum nanoparticles supported on the UiO-67 MOF have also shown promise for the catalytic hydrogenation of CO$_2$ to methanol. However, the reaction mechanism and influence of the framework on the reaction were poorly understood. Nova studied this complex system in collaboration with the groups of Prof. Unni Olsbye at the University of Oslo and Prof. Egill Skúlason at the University of Iceland. This work was initiated by Researcher Torstein Fjermestad (now a Marie-Curie fellow in Italy) and continued by Harsha Pulami (PhD exchange student from the Skúlason group), both supported by the NordCO2 consortium.

Related to this topic, MSc student Robert Brevik is investigating the functionalization of the UiO-66 and -67 MOFs by Mg and Zn complexes, with the final goal of making nanoporous catalysts for the capture and conversion of CO2. These complexes activate the nodes of the MOFs by deprotonation of the bridging OH groups. The different configurations of the resulting products are being studied computationally by combining periodic calculations with single-node and full-cage cluster models (*figure 3*). The results of these computations are being exploited in the rational design of new materials. This work is a collaboration with the group of Prof. Karl-Petter Lillerud at the University of Oslo.

Base-metal catalysis

PhD student Julie Héron has been working on the computational modelling of the CuAAC reaction – a classic example of 'click chemistry', in which a copper catalyst enables the fast cycloaddition of an azide to an alkyne. The key features of the system studied by Héron include 1) a bimetallic core supported by a robust chelating ligand, reducing the number of possible reaction pathways, and 2) a non-symmetric P,N ligand, which allows for different electronic and steric effects at each metal centre. Héron combines state-of-the-art DFT methods with microkinetic models to understand the complex mechanism underlying this reaction. Of particular interest is the mechanism that assists the critical C–H activation step involved in the reaction. This work is done under the supervision of Balcells and in collaboration with the experimental group of Prof. T. Don Tilley at UC Berkeley (USA).

Under the supervision of Nova, PhD students Linn Berntsen and Julie Héron initiated a computational study on the mechanism of the Cu-catalysed arylation of hydantoins. This work is done in collaboration with the experimental group of Assoc. Prof. Alexander H. Sandtorv at the University of Oslo, who is co-supervising Berntsen in the development of the first catalytic process allowing for the selective N-3-arylation of unsubstituted hydantoins. The synthesis of these derivatives is relevant due to their presence in drugs and agrochemicals. The goal of this project is to improve both the efficiency and selectivity of the catalytic system.

PhD student Ljiljana Pavlovic and Hopmann continued the collaboration with Prof. Paul Chirik (Princeton Univ, USA) [9] on Co-catalysed hydrogenations. Pavlovic is now investigating the mechanism of the Co-catalysed asymmetric hydrogenation of enamides developed by Chirik. Following the experimental and computational study of an Fe-catalysed carbenoid transfer reaction of vinyl sulfoxonium ylide in 2018 [10], Janakiram Vaitla and Hopmann were invited to write a perspective paper on the use of vinyl sulfoxonium ylide for synthetic purposes in 2019 [11].

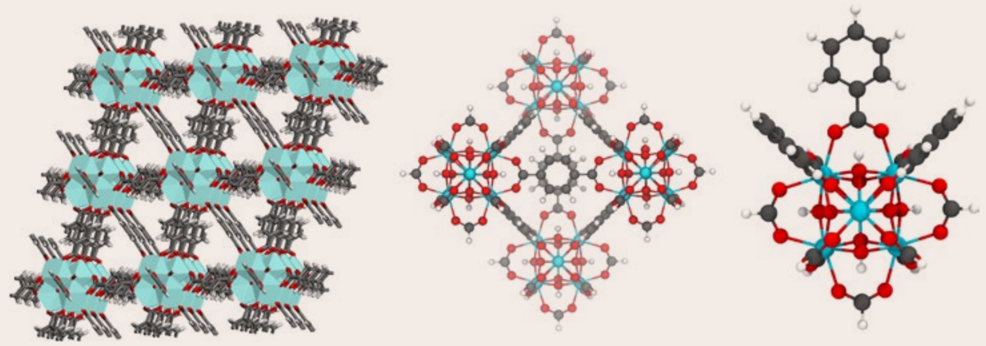


Figure 3: From left to right; periodic, full-cage and single-node cluster models used in the study of the UiO-66 and -67 MOFs functionalized by MgMe$_2$ and ZnMe$_2$. *Illustration: Robert Brevik*

Machine learning

Balcells initiated a project on machine learning (ML) applied to computational catalysis. The main goal of this project is to enable the exploration of large chemical spaces by means of ML models. A key advantage of these models, relative to DFT calculations, is their fast execution on a simple computer, like a laptop or a PC. A proof-of-concept was developed to prove the possibility of learning the H$_2$ activation barrier for thousands of derivatives of Vaska's complex. Deep neural networks yielded high accuracy, but Gaussian processes had the advantage of being trainable with smaller data sets. The models were complemented with circular fingerprints and gradient boosting algorithms with the aim of rationalizing the predictions. This work opened a new collaboration between the Hylleraas Centre and the Aspuru-Guzik group at the University of Toronto (Canada).

Structure and bonding from ^{13}C-NMR

In a long-standing collaboration with Profs. Christophe Copéret at ETH Zürich (Switzerland) and Richard A. Andersen at UC Berkeley (USA), Odile Eisenstein pursued her studies on the relationship between the chemical shift NMR tensor and electronic properties. The ^{13}C chemical shift tensors were used to get a detailed description of σ M– C$_{sp^3}$ bonds. It was shown that when an empty metal orbital is properly orientated relative to the M–C bond, the chemical shift tensor of C$_{sp^3}$ acquires significant anisotropy. This anisotropy indicates that the M–C bond has also some π-character perpendicular to the most deshielded component of the tensor. The π-character accounts for the directional C–H bond activation at the C$_{sp^3}$ yielding the double M=C bond. This character was found experimentally and computationally in numerous unsaturated metal-alkyl complexes and is prevalent in all unsaturated d^0 early transition metal complexes. A later study showed that it is also found in several unsaturated late transition metal complexes [12]. Following this JACS publication, a perspective on the topic of NMR chemical shift tensors related to structure and bonding in catalysis was published in the *Accounts of Chemical Research* [13].

Relativistic and dynamic effects in NMR simulations of transition-metal complexes

The recognition that NMR spectroscopy is an indispensable structural tool in the modern analytical arsenal of chemists and structural biologists has led to an increased activity in the computation and simulation of NMR signatures for large molecular species in solution. In 2015, Abril Castro came to Oslo for an internship visit as part of her PhD training in Spain with Prof. Marcel Swart. During her visit, she worked on ^{31}P NMR chemical-shift calculations in a trans-platinum(II) complex in aqueous solution, benefiting from complementary expertise in Oslo and Tromsø in calculations of electronic-structure theory, response theory, and dynamics. Together with Helgaker, Cascella, Michal Repisky, and Heike Fliegl (now at the Karlsruhe Institute of Technology), Castro was able to simulate the ^{31}P NMR chemical shift in good agreement with experimental values; published in 2019 [14] and elaborated in a Highlight in this report.

The need to combine full four-component relativistic quantum-chemical

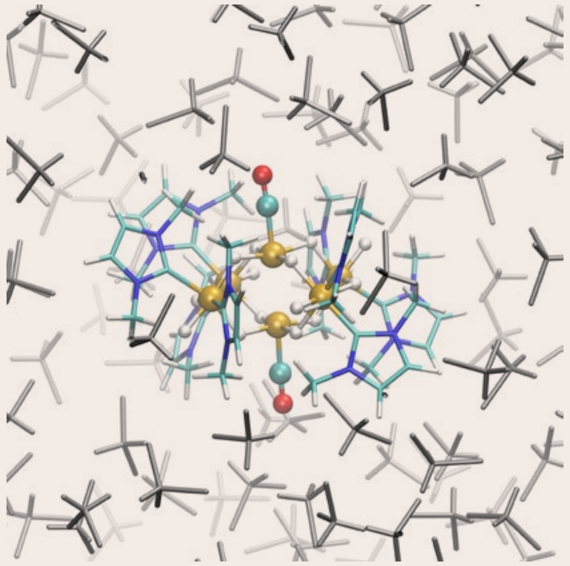


Figure 3: Structure of the iridium polyhydride $[Ir_6(IMe)_8(CO)_2H_{14}]^{2+}$ cluster surrounded by dichloromethane solvent molecules. *Illustration: Abril C. Castro*

methods and ab-initio molecular dynamics simulations for a proper determination of the NMR parameters is apparent. The robustness of the methodology was demonstrated for the ^{1}H-NMR chemical shifts in a gold complex by Nova in collaboration with Hylleraas affiliate Prof. Mats Tilset [15]. In the case of the iridium polyhydride $[Ir_6(IMe)_8(CO)_2H_{14}]^{2+}$ cluster (*figure 3* ↑), the calculation provided a new strategy to assign hydride positions not located by X-ray studies, as shown by Castro and Balcells in collaboration with Prof. Robert H. Crabtree (Yale).

Au(III) catalysis

The interest in Au(III) chemistry has recently increased significantly due to the isolation of many intermediates that are well known for Au(I) but elusive for Au(III). The isolation and characterization of an η^3-allyl intermediate was reported in 2019 by the group of Tilset. In collaboration with Nova, the chemical properties of this compound were determined in solution [15]. The strong asymmetry of the (tpy)Au(III)-allyl complex yielded an NMR spectrum that was interpreted by variable temperature NMR and DFT calculations as resulting from a rapid diastereomeric interconversion between various forms of this species.

Outlook

RT5 focus is the computational modelling and analysis of chemical reactions. While this goal has been maintained for some years, the tools are evolving very rapidly, an evolution strongly catalysed by the environment provided by the Hylleraas Centre. In strong synergy with the other RTs, higher levels of modelling have been implemented and this trend should and will get stronger. The need to combine complementary methods developed and/or used at the Hylleraas Centre was apparent in the study of the ^{31}P NMR chemical shift in a platinum complex, but this is far from the only case, as indicated in the reports from the other RTs.

Research topics for next years will naturally follow those presented here. In particular, the influence of solvents will be modelled with molecular dynamics methods, making studies of reactions involving alkali and alkaline-earth ions possible. For instance, a study of the Grignard reaction in tetrahyrofuran has been initiated with ab initio molecular dynamics (AIMD) methods. Another focus area will be modelling and development of asymmetric transformations with CO2, for which accurate methods are needed to model small energy differences. Computation of NMR signatures (chemical shifts in particular) will be carried out and their relation to structures and interactions (halogen bonds, for instance) will be pursued.

The RT5 toolbox will be also expanded by adding machine learning methods and there is currently an initiative to use this approach for fostering inter-RT collaborations, together with the UiO Department of Mathematics. The use of periodic models, and their combination with large clusters, is also expected to increase in connection with our work on nano-porous materials.

People, mobility and training

In January 2019, Abril Castro started her MSCA-IF Fellowship at the Hylleraas Centre, to work on the project *Relativistic and Dynamic effects in Computational NMR Spectroscopy of transition-metal complexes* (ReaDy-NMR), under the supervision of Michele Cascella and Trygve Helgaker. Her ongoing project involves a close collaboration with Balcells, Repisky, and Nova. In October 2019, PhD student Cuong Dat Do joined the research team of RT5 at UiT. His project focuses on asymmetric CO_2-incorporating reactions. Experimental postdoc Janakiram Vaitla left the UiT team for a permanent position as Assistant Professor at IIT Dehli, India, at the end of 2019.

As part of PhD exchanges, Irene Casademont came to UiO from University of the Basque Country for three months in 2019; Harsha Pulumati from University of Iceland for three weeks and Juan Ángel de Gracia Triviño from Stockholm KTH for three months. Dr. Aleix Comas-Vives from Autonomous University of Barcelona came to UiO for two days.

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RT6

Multiphase Systems

Principal investigators:
Bjørn Olav Brandsdal and
Michele Cascella

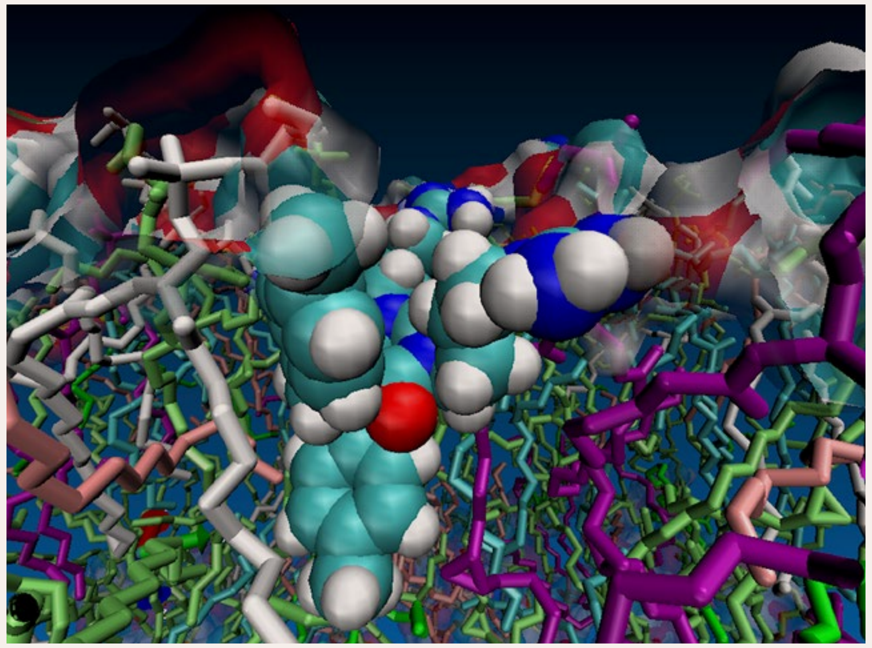
The RT6 team applies computer simulations to important problems in chemistry, biology, and physics. Activities in 2019 have focused on antimicrobial resistance, temperature dependence of chemical rates, aggregation of charged surfactants and lipids.

Antimicrobial resistance

Antimicrobial resistance is emerging and spreading globally, threatening the ability to treat common infections, leading to prolonged illness and treatment. Together with researchers in the DigiBiotics project, where Bjørn Olav Brandsdal and Kenneth Ruud are PIs, we have explored novel compounds as potential antimicrobial agents, inspired by arctic marine natural products. Membrane-active compounds are of particular interest, as these are believed to have a mode of action that prevents resistance to occur. Cellular membranes are complex structures that separate the contents of all cells from the outside environment, consisting mainly of amphiphilic lipids. They contain a great variety of different lipids and different regions may adopt various fluid and solid phases, where the former is biologically most relevant.

The interaction between a series of short cationic antimicrobial peptides has been examined using a combination of molecular dynamics simulations and NMR [1]. Here, the simulations reveal that these compounds undergo significant structural rearrangements upon binding to a membrane model when compared with their solution structures. These observations are in agreement with experimental data from NMR. Furthermore, free energy calculations show that the driving force for membrane association is a combination of hydrophobic and electrostatic interactions.

In parallel, two different membrane models have been constructed and equilibrated by extensive molecular dynamics simulations. The first model mimics E. coli, while the second mimics a mammalian membrane. Analysis of both models reveal that they are stable and that the simulations capture the physical properties of these membranes. The project has now entered into a production phase, where the membrane models are exposed to antimicrobial compounds in various concentrations. Preliminary studies of a test library of compounds with known activities have been initiated and show that the active compounds associate to the membrane surface, followed by an almost complete burial (*figure 1* ↑).



↑ **Figure 1:** Molecular dynamics snapshot of active compound entering the membrane.

In addition to the atomistic molecular dynamics simulations mentioned above, we have also developed a new pharmacophore model to predict the activity of compounds against resistant strains of *Staphylococcus aureus*. A new parameter that reflects the hydrophobicity of the antimicrobial agents is shown to have a strong predictive power for a test set of approximately 100 compounds with known activity [2] (*figure 1* ↑).

Temperature dependence of catalytic rates

A large part of the activity in 2019 has been to understand temperature dependence of catalytic rates, with focus on which structural modifications are required for enzymes to maintain high catalytic activity at temperatures close to the freezing point of water. The universal fingerprint of enzymes adapted to cold is a reduction of the activation enthalpy and more negative activation entropy. According to transition state theory, the reduction of the activation enthalpy renders the catalytic rates less sensitive to temperature. How this is achieved is still largely unknown, but previous computer simulations indicate that tuning of the protein surface mobility is involved.

The chemical reaction is described using the Empirical Valence Bond (EVB) method originally developed by Prof. Arieh Warshel, where the reaction is described using valence bond structures. This method gives the activation free energy, and by performing the calculations at 5–8 different temperatures, a computational Arrhenius plot can be constructed. Each temperature requires up to 150 independent simulations to achieve the required accuracy. It therefore depends on specialized software for setting up, running and analysis of the data. A major update to our software was released in 2019 [3], which now also allows us to predict how point mutations affect both the catalytic reaction rates and thermal stability of enzymes. The latter has been implemented using free-energy perturbation protocols. The aim is to use these techniques to disentangle the mutations that affect the catalytic rates from those that provide stability.

The concept of enthalpy–entropy compensation observed in temperature adaptation of enzymes was examined for several enzymes in 2019. Multiple sequence alignments of psychrophilic and mesophilic enzymes revealed

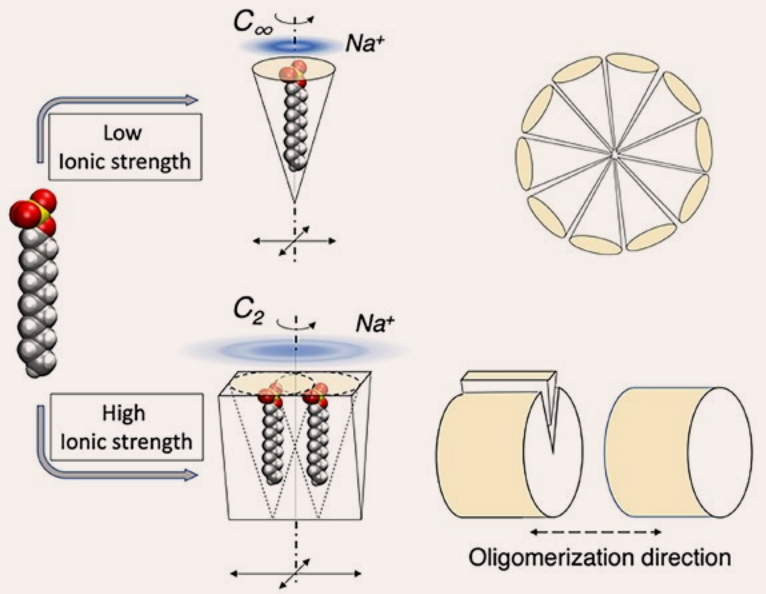


Figure 2: Mechanism of SDS self-assembly. Salt-induced changes in the symmetry of the aggregating unit lead to different global shapes for the micelles.

characteristic motifs located in protein surface loops, and we examined the effect of a number of designed surface mutations of psychrophilic and mesophilic elastases on the temperature dependence of the catalysed peptide cleavage reaction [4]. The results from analysing 14 mutant enzyme variants show that substitution of psychrophilic loop residues into the mesophilic enzyme consistently changes both the activation parameters and loop flexibilities towards the former, and vice versa for opposite substitutions. These findings represent a major step forward towards rational engineering of cold-active enzymes.

Another system we have studied is cold- and warm-active endonucleases, which catalyse the hydrolysis of phosphodiester bonds in DNA [5]. Firstly, the reaction mechanism was examined using DFT calculations on a cluster model. These calculations gave support for a concerted mechanism, but failed in providing quantitative agreement with experimental barriers – that is, based on the functional used for the DFT calculations, a variation of 7–8 kcal/mol in the activation free energy was observed. Parameterisation of the EVB reference reaction was instead based on experimental data and quantitative agreement with experimental activation free energies, enthalpies and entropies for both the cold- and warm-active endonuclease. It should be noted that the $\Delta G^\ddagger$ is very similar for the two enzymes, but with a difference of about 8 kcal/mol in $\Delta H^\ddagger$ (8 and 16 kcal/mol) and $T\Delta S^\ddagger$ (−8 and 0 kcal/mol). These calculations add further support to the idea that surface regions distant to the active site are involved in tuning the temperature dependence of the enzymatic catalytic rates. The functional dependencies observed in this study is now under investigation using projector-based embedding.

Our studies of temperature dependence of catalytic rates open the possibility to use EVB calculations as a tool in rational enzyme engineering. Bjarte Lund Aarmo has successfully produced six enzymes in the laboratory. Based on EVB simulations, tailor-made variants will be studied theoretically and experimentally in 2020.

Aggregation of multiphase systems

The year 2019 saw the establishment of collaboration with other theoretical and computational groups with the idea of exploiting the multiscale methodologies developed in RT2 – in particular, the hybrid particle-field-molecular dynamics (hPF-MD) method to understand the aggregation properties of charged surfactants.

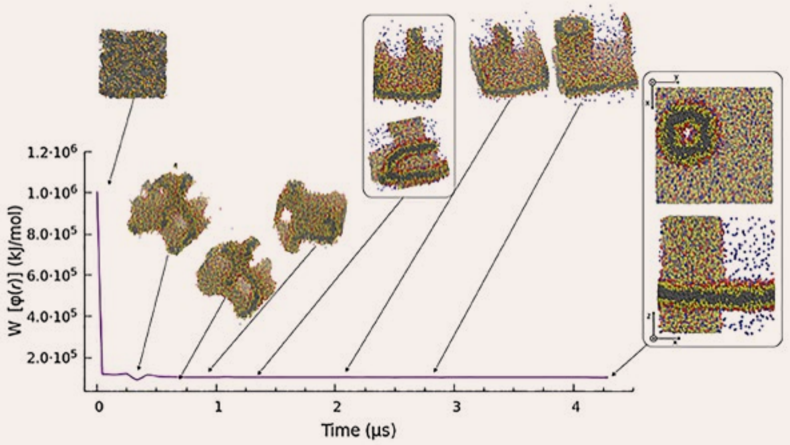


Figure 3: Formation of Lipid A mixed lamellar/cubic phase in a 30%/70% lipid/water mixture. *Reprinted from Ref. [7], Copyright (2020), with permission from Elsevier.*

Sodium dodecyl surfate (SDS) is one of the most studied amphiphiles due to its wide array of applications in science and industry, finding such diverse uses as a detergent in tooth paste or shampoo and as an extraction tool for protein and DNA. SDS provides an archetypical example of the complexity of predicting how surfactants aggregate in water. Despite its simple molecular structure, SDS micelles respond in a complex way to different concentrations – at low concentrations, SDS assembles into regular small spherical micelles 2–3 nm in radius; at increased concentrations, SDS micelles undergo a morphological transition into cylindrical structures spanning lengths on the order of 100–1000 nm. Moreover, such transitions can be drastically enhanced by the presence of a significant excess of salts in the solution.

Surfactant aggregation is usually rationalized in terms of optimal packing of molecular shapes, but the presence of long-range electrostatic interactions severely challenges such interpretation.

Combining data from small-angle neutron scattering (SANS) and small-angle X-ray scattering (SAXS) experiments with hPF simulations, we were able to show that the morphological transition from spherical to cylindrical shapes is accompanied by a change in the localization of the bound counterions on the solvent-accessible surface of the micelles. Using a simple toy model of a charge bound to two poles, we demonstrated how differently the counterions may prefer to bind to either individual SDS molecules or to SDS dimers under the different experimental conditions. In the second case, self-assembly of surfactants occurs not by aggregation of individual, cylindrically-symmetric molecules, but by aggregation of supramolecular lower-symmetry units (*figure 2*). This symmetry breaking is ultimately responsible for the appearance of the tubular aggregates observed in experiment.

This study was initiated by visiting PhD student Ken Schäfer (Johannes Gutenberg University, Mainz) and made possible by a collaboration with the group of Hylleraas affiliate, Assoc. Prof. Reidar Lund [6]. The computational–experimental collaboration between the groups of Cascella and Lund is currently being expanded towards other surfactants and to systems of biological relevance such as phospholipid bilayers and bacterial membranes.

Cell-wall modelling

As a first step to build large-scale models of the bacterial cell wall, we developed a hPF model of Lipid A, the lipophilic component of lipopolysaccharides (LPS), the chemical moiety characterizing the outer leaflet of the outer membrane of Gram-negative bacteria. The model, developed in collaboration with the groups of Prof. Giuseppe Milano (Yamagata University, Japan) and Prof. Thereza A. Soares (Federal University of Pernambuco, Recife, Brazil), accounts for different acylation states; it is able not only to reproduce with good accuracy the structural properties of constituted Lipid A bilayers (in comparison with all-atom simulations) but also to predict the formation of complex lamellar/hexagonal or lamellar/cubic phases at specific concentrations of Lipid A in water (*figure 3 previous page* ←). The work, recently accepted for publication [7], forms the base for future investigations both on the phase behaviour of simpler Lipid A derivatives and on the biophysics of LPS.

Funding / personnel

A postdoctoral position is announced and will be filled in 2020 (funding from DigiBiotics) to work on membrane simulations and antimicrobial resistance.

The work on temperature dependence of chemical reaction rates will be continued for the next years by senior researcher Geir Villy Isaksen, postdoctoral fellow Bjarte Aarmo Lund, Prof. Johan Åqvist (20% position). In addition, Ryan Wilkins started as a PhD student at the end of November 2019 and Bente Sirin Barge will start in January 2020. The project will hire one more PhD student and one three-year postdoctoral fellow in 2020. These positions are all financed through the Toppforsk grant Brandsdal received in 2018.

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> “What hold the countless atoms and molecules together in the large complexes we call matter are nothing but electrical forces – in a sense, everything is electricity. I know this sounds weird – but you get used to the idea, it eventually becomes natural. But don’t show this to anybody – lest they think I have become a bit odd.”

Egil A. Hylleraas (1898–1965),
in letter to his brother Ottar Andersen in 1927

Hylleraas members

Leadership and Principal Investigators

Trygve Helgaker
Director
Professor
UiO

Kenneth Ruud
Deputy Director
Professor
UiT

Michele Cascella
Principal Investigator
Professor
UiO

Bjørn Olav Brandsdal
Principal Investigator
Professor
UiT

Odile Eisenstein
Principal Investigator
Professor
UiO

Luca Frediani
Principal Investigator
Assoc. Professor
UiT

Thomas Bondo Pedersen
Principal Investigator
Professor
UiO

Kathrin Hopmann
Principal Investigator
Assoc. Professor
UiT

Researchers

Gustav Baardsen
UiO

David Balcells
UiO

Maarten Beerepoot
UiT

Torstein Fjermestad
UiO

Bin Gao
UiT

Jógvan Magnus Haugaard Olsen
UiT

Geir Isaaksen
UiT

Stig Rune Jensen
UiT

Simen Kvaal
UiO

Andre Laestadius
UiO

Ainara Nova
UiO

Thomas Håbu Qureishy
UiO

Sangita Sen
UiO

Erik Tellgren
UiO

Peter Wind
UiT

Gabriel Adolfo Gerez Sazo
UiT

Postdocs


Tilmann Bodenstein
UiO


Diego García-López
UiT


Bjarte Aarmo Lund
UiT


Abril Carolina Castro Aguilera
UiO


Marius Kadek
UiT


Roberto Di Remigio
UiT


Lukas Konecny
UiT

PhD Students


Tor Arne Heim Andberg
UiT


Victoria Ariel Bjørnestad
UiO


Manuel Carrer
UiO


Jon Austad
UiO


Sigbjørn Løland Bore
UiO


Cuong Dat Do
UiT


Magnar Bjørgve
UiT


Anders Brakestad
UiT


Karen Oda Hjort Dundas
UiT

PhD Students


Karolina Solheimslid Eikås
UiT


Håkon Emil Kristiansen
UiO


Ljiljana Pavlovic
UiT


Fabian Maximilian Faulstich
UiO


Morten Ledum
UiO


Birta Ravdna Sarre
UiT


Audun Skau Hansen
UiO


Laura Liikanen
UiT


Samiran Sen
UiO


Julie Héron
UiO


Sverre Løyland
UiO


Lluis Artus Suarez
UiO


Joakim Samuel Jestilä
UiO


Benedicte Ofstad
UiO


Ryan Scott Wilkins
UiT


Marc Joosten
UiT


Marc Obst
UiT

Master Students

Uthman Seyi Abdulyaqeen
UiT

Bente Sirin Brage
UiT

Eirill Strand Hauge
UiO

Einar Aurbakken
UiO

Robert Brevik
UiO

Oda Hovet*
UiO
**co-supervision with Dr. Nikolina Sekulic, NCMM*

Bastian Skjelstad
UiO

Affiliates

Tor Flå
Professor
UiT

Reidar Lund
Assoc. Professor
UiO

Einar Uggerud
Professor
UiO

Ute Krengel
Professor
UiO

Mats Tilset
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UiO

Inge Røeggen
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Adjunct Professor

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KTH, Sweden

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> “It is chemistry, brother, chemistry! There is no hope for it, your reverence, you must make way for chemistry!”
>
> “But you must understand, my dear fellow, that it’s not just me; we’re all rather confused, and all because of your sciences. As long as there were still atoms, the five senses, the four elements, well, it all fitted together somehow. For there were atoms in the ancient world too. But when we heard that you had discovered the ‘chemical molecule’, ‘protoplasm’, and God knows what, we all had out tails between our legs. There was a terrible confusion among us and, indeed, an upsurge of superstition and gossip …”
>
> *from The Brothers Karamazov (1880),*
> *by Fyodor Dostoevsky (1821–1881)*

Publications 2019

Publications 2019

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Funding and Staff Report

Total Revenue and Expenditure

(in man-years)

Funding (in NOK thousand)	2019
Basic funding as agreed in the Centre contract	
Funding from Research Council (CoE grant)	**15 439**
Funding from home institutions	**7 609**
Total basic funding	**23 048**

Additional funding from external projects	
Research Council funding	**11 977**
International funding	**2 570**
Public funding	**749**
Private funding	**4 296**
Total additional funding	**19 592**

Total funding	**42 640**

Staff Report 2019

(in man-years)

	2019
Professors and researchers	**16.0**
PhD students	**20.3**
Postdoctoral fellows	**9.0**
Visiting researchers	**3.5**
Administrative and technical staff	**3.6**
All staff	**52.5**

Being located 1150 km apart, the two nodes of the Hylleraas Centre are critically dependent on good communication. All Friday seminars utilize video conferencing, for example.

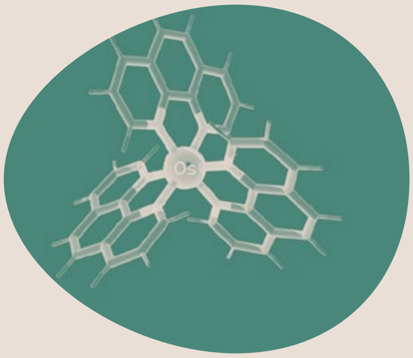
Here Sigbjørn Løland Bore is about to give a presentation in Oslo on September 6, 2019, with the audience in Tromsø visible on the screen behind him. Chairman is David Balcells.

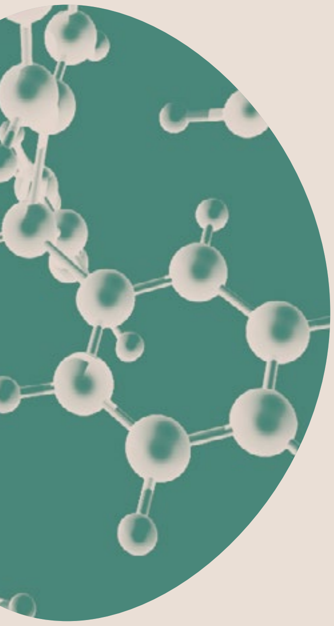
Photo: Trygve Helgaker

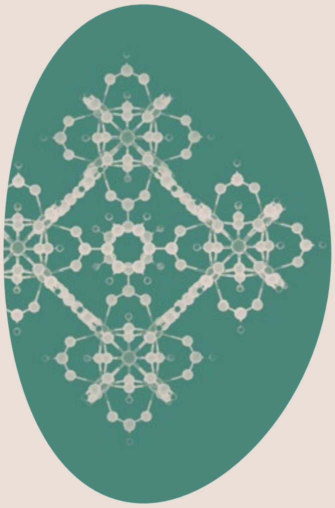
> “When you ask what are electrons and protons I ought to answer that this question is not a profitable one to ask and does not really have a meaning. The important thing about electrons and protons is not what they are but how they behave – how they move. I can describe the situation by comparing it to the game of chess. In chess, we have various chessmen, kings, knights, pawns and so on. If you ask what a chessman is, the answer would be that it is a piece of wood, or a piece of ivory, or perhaps just a sign written on paper, or anything whatever. It does not matter. Each chessman has a characteristic way of moving and this is all that matters about it. The whole game of chess follows from this way of moving the various chessmen.”

Paul Dirac (1902–1984)
in a public lecture given at the 1955 Indian Science Congress in Baroda, India

Design: Anagram Design







Hylleraas contact information

web pages: hylleraas.no
email: post@hylleraas.no

Postal address Oslo:

Hylleraas Centre
Department of Chemistry
University of Oslo
P. O. Box 1033 Blindern
N-0315 Oslo
Norway

Postal address Tromsø:

Hylleraas Centre
Department of Chemistry
UiT The Arctic University of Norway
P. O. Box 6050 Langnes
N-9037 Tromsø
Norway