

Hylleraas Centre for Quantum Molecular Sciences

Centre Director: Trygve Helgaker, UiO (2017–2022); Kenneth Ruud, UiT (2022–2027)

Host Institution: Department of Chemistry, University of Oslo

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Project Summary

The Hylleraas Centre for Quantum Molecular Sciences will make a decisive, timely contribution to the chemistry, physics and biology of molecules by developing an integrated multiscale approach for complex systems, emphasizing matter–field interactions. The emergence of advanced laser technology and fourth-generation light sources creates new opportunities and challenges that require major advances in the modelling of complex systems in extreme environments. The Hylleraas Centre will meet this challenge by developing novel computational methods that will allow us to treat systems containing thousands and even millions of atoms, by unravelling their response to short laser pulses and strong fields, and by exploring processes extending from attoseconds to microseconds.

The Hylleraas Centre gathers world-leading expertise in the domains of electronic-structure theory, multiscale modelling, computational spectroscopy, and the use of computation to understand and control complex chemical and biological systems. The centre is uniquely positioned to take the lead in the modelling and understanding of the new scientific frontiers that will be enabled by new experimental facilities.

Through an extensive incoming sabbatical programme, a generous visitors programme, focus bienniums, international workshops, conferences, outreach activities and seminar series, the Hylleraas Centre will create an internationally visible and attractive centre for the computational modelling and understanding of new chemistry at the frontiers of a wide range of scientific disciplines. Through the training of PhD students and postdocs, the establishment of national courses in theoretical chemistry and international winter schools, the Hylleraas Centre will educate a new generation of computational scientists skilled to address the new research frontiers. The centre will continue the PIs' longstanding efforts to improve gender balance in theoretical and computational chemistry.

Primary and Secondary Objectives of the Project

The primary objective of the Hylleraas Centre is to develop an integrated approach to the investigation of complex molecular systems in electromagnetic fields and extreme environments.

Secondary objectives are to 1) develop accurate, reliable, scalable electronic-structure methods for complex systems; 2) develop multiscale methods with quasi-atomistic/mesoscale resolution, spanning orders of magnitude in space and time; 3) develop novel multiscale methods for calculating and predicting new spectroscopies in strong fields and short pulses; 4) develop models and understanding of the squeezed chemistry of extreme magnetic fields and pressure; 5) develop new computational approaches to optimize and control chemical transformations; 6) understand the structure and dynamics of macromolecules at membranes and interfaces; 7) train a new generation of theoretical chemists; 8) establish national courses in theoretical chemistry; 9) provide new software to the international community at no cost.

Hylleraas Centre for Quantum Molecular Sciences

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

With the advent of powerful computers and the development of advanced computational methods, **first-principles calculations** of molecular electronic systems have become commonplace. Using advanced software such as our program DALTON [1], quantum-mechanical calculations are being routinely performed on systems containing hundreds of atoms by chemists in academia and industry, complementing or supplementing experimental work, with an accuracy that often rivals that of experimental measurements [2]. However, over the next decade, **new experimental facilities** such as the European Spallation Source, MAX IV Laboratory, and European XFEL will revolutionize the way we study matter, by enabling the use of intense laser fields in a wide frequency range and allowing ultrashort pulses to be generated, targeting increasingly complex chemical and biological systems. The rich experimental data brought forth by these fourth-generation light sources will, for instance, allow us to track the detailed course of chemical reactions and to follow the energy redistribution in biological systems; such knowledge will in turn enable us to control processes and generate new functionality [3]. This development offers new opportunities but also poses **new challenges for theory and computation**: To exploit fully the potential of the new infrastructures, computation is needed not only to simulate the **complex systems** themselves to complement experiment but also to interpret the new data, bearing in mind that these have been generated by little-understood **matter–field interactions**.

Simulations of complex systems require the treatment of phenomena that occur over widely different time and length scales. For a balanced description of such phenomena, **multiscale modelling** must be performed in a hierarchical manner, with a core treated quantum mechanically and its surroundings treated classically, at various levels of detail. The **Hylleraas Centre for Quantum Molecular Sciences**[†] will make a *decisive, timely contribution to chemistry by developing an integrated multiscale approach for complex systems, emphasizing matter–field interactions*, see Fig. 1. Our goal is to treat systems with thousands and even millions of atoms, including their interactions with short laser pulses and ultrastrong fields, in processes ranging from atto- to microseconds. With the new tools, we aim to study and uncover new phenomena, often in collaboration with experimentalists. We are well positioned to take on this challenge, possessing world-leading expertise in matter–field interactions, recently extended to multiscale modelling and computational chemistry by strategic group hirings.

Two examples from our own recent work [4, 5] illustrate how new tools for computational studies of matter–field interactions may provide crucial insight into natural phenomena in different areas of science, see Fig. 2. First, using our code LONDON [6], Helgaker and co-workers published in *Science* in 2012 the discovery of a new bonding mechanism, **paramagnetic bonding**, generated by the motion of the electrons in ultrastrong magnetic fields [4, 7]. As a result, chemistry is strongly affected,

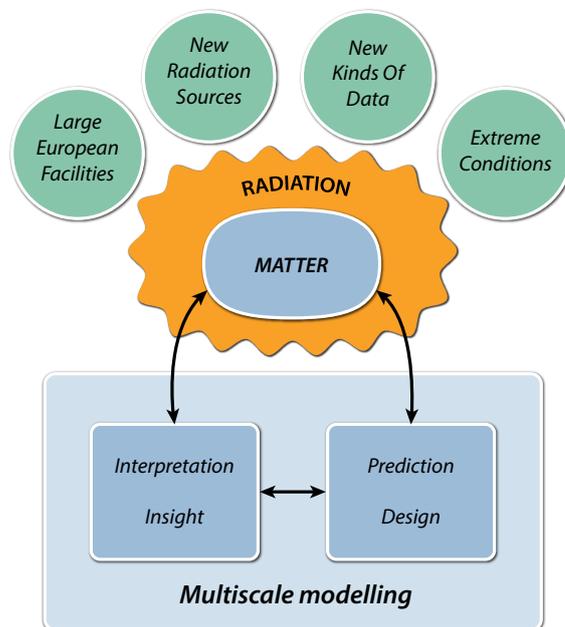


Figure 1: The Hylleraas Centre will make a *decisive, timely contribution to chemistry by developing multiscale methods for complex systems, emphasizing matter–field interactions*

[†]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).

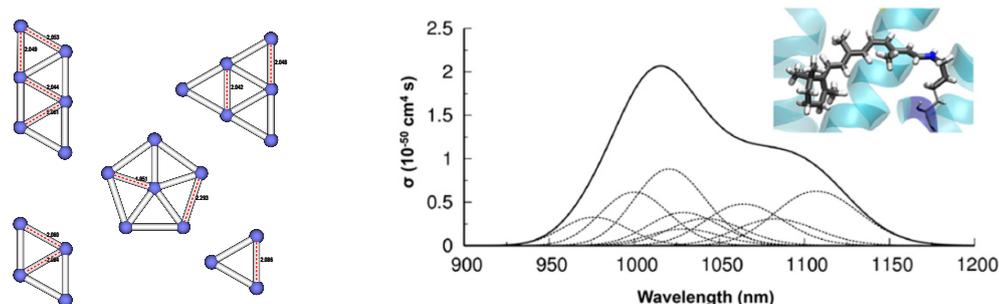


Figure 2: **New tools, new opportunities, new discoveries.** Left: Magnetically bound helium clusters in a field of 470 kT calculated with LONDON [7]. Rare-gas atoms bind in planar clusters constructed from triangular units, adopting a perpendicular orientation to the field. Right: Rhodopsin two-photon absorption cross section (full line) constructed from snapshot curves (dashed lines) obtained from DALTON calculations on the quantum region (inset) during multiscale dynamics [5]. The simultaneous absorption of two photons of wavelength 1020 nm (infrared, maximum of total curve) corresponds to absorption of a single photon of wavelength 510 nm (green).

giving rise to molecules that cannot exist on Earth but are predicted to exist on magnetic white dwarfs stars. Intriguingly, the effects of magnetic fields can be strongly enhanced in certain crystal impurities and experimental work has begun to detect paramagnetic bonding in such impurities [8]. Second, in 2015, the long-standing puzzle of **human infrared vision** was explained in a publication in *Proceedings of the National Academy of Sciences* by Cascella, in collaboration with experimental groups [5]. Combining classical simulations of proteins with quantum-mechanical calculations of two-photon absorption in rhodopsin performed using DALTON, the authors demonstrated that infrared vision arises from the simultaneous absorption of two infrared photons, whose total energy and absorption cross section are equal to those of a single visible photon and hence detectable by the eye.

These examples illustrate how molecular calculations can provide crucial insight into chemical, biological, and physical phenomena, replacing or complementing experiment under vastly different conditions: While magnetic bonding occurs in the fierce environment of white-dwarf atmospheres, two-photon activation of rhodopsin occurs in the delicate environment of the human eye. They also show how new tools (here first developed in our laboratory) may pave the way for new research and discoveries, in synergy with experimental work. *To enable and nurture such synergies in the future, the large investments in new facilities must be complemented by a substantial effort into the modelling of complex systems in extreme environments, as proposed for the Hylleraas Centre.*

Research

To reach our **primary objective** of developing an integrated approach to the investigation of complex molecular systems in electromagnetic fields and in extreme environments, we have identified

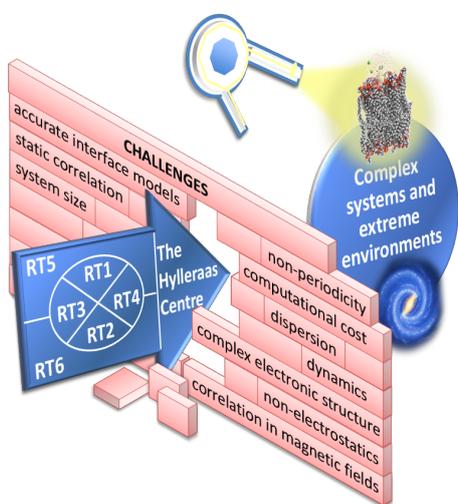


Figure 3: Research themes (RTs), research challenges, and overall objective of the Hylleraas Centre

two main challenges: (1) accurate and efficient modelling of complex systems in space and time; (2) understanding matter–field interactions and extreme environments. To address these, we have organized the work into six **Research Themes (RTs)**. The first challenge, accurate modelling of complex systems, is addressed in *RT1 (Electronic Structure)* and in *RT2 (Multiscale Modelling)*, whereas *RT3 (Spectroscopic Processes)* and *RT4 (Extreme Environments)* take on our second challenge regarding matter–field interactions. In *RT5 (Chemical Transformations)* and *RT6 (Multiphase Systems)*, complex systems will be studied computationally, often in collaboration with experimentalists, bringing our methodological advances to topical application areas of the new light sources. The results of all RTs will be successively merged into a unified

framework, covering the relevant time, length, and field scales. By 2027, the centre will have integrated the results of all RTs, creating a unified computational environment for modelling complex systems and processes in electromagnetic fields and extreme environments.

Our research programme can be successfully realized only through a concerted effort by a team of strongly motivated scientists with a common vision and complementary skills, led by a top international scientist with an extensive track record of research excellence and leadership. For the Hylleraas Centre, we combine the expertise of the groups of **Prof. Trygve Helgaker** at the University of Oslo (UiO) and **Prof. Kenneth Ruud** at UiT The Arctic University of Norway (UiT) in Tromsø. Both have extensive experience with molecular electronic-structure theory and matter–field interactions. In recent years, their groups have been strengthened by the hiring of several excellent young scientists, extending activities to complex systems, multiscale modelling, biological systems, and catalysis, the latter strongly boosted by the hiring of Prof. Odile Eisenstein. The establishment of the Hylleraas Centre, with **centre nodes in Oslo and Tromsø**, will ensure a targeted, concerted research effort towards complex systems and matter–field interactions that could not take place separately in the two groups, their combined thrust and expertise being a prerequisite for the success of the research programme. *Being shared by UiO and UiT, the centre will directly benefit two Norwegian universities and in this way have a greater impact on Norwegian chemistry as a whole.*

Below, we describe each RT in more detail, emphasizing steps that will be taken in the initial stages of the scientific activity of the centre. Each RT will be led by a **Principal Investigator (PI)** with extensive experience in the area, working closely with a co-leader from the other node.

RT1: Electronic Structure

To understand and predict quantum effects in complex systems and their interactions with external fields, we will develop accurate, scalable electronic-structure models, with emphasis on coupled-cluster theory and density-functional theory.

All research at the centre is based, directly or indirectly, on the methods of electronic-structure theory. As illustrated in Fig. 4, these methods fall into three classes: accurate but expensive **many-body methods** for dozens of atoms, affordable but less reliable methods of **density-functional theory (DFT)** for hundreds of atoms, and inexpensive but highly parameterized **semi-empirical methods** for thousands of atoms. In support of multiscale modelling in RT2, we will perform research in all three classes, emphasizing aspects relevant for complex systems and matter–field interactions. Our PIs have extensive experience with quantum-chemistry methods development, having contributed to several distributed programs, including DALTON [1], MOLCAS [10], and DIRAC [11].

The indisputable work-horse of electronic-structure theory is **Kohn–Sham DFT**. At the centre, DFT will be used not only in its usual computational role in RT5 and RT6, but also for multiphoton spectroscopic processes in RT3 (with the open-ended response code OPENRSP [12]) and for extreme environments in RT4 (with the magnetic-field code LONDON [13]). Such studies put new demands on DFT, which has been developed (often semi-empirically) to work well under normal conditions. High-order spectroscopic processes depend in a subtle, unknown manner on electron correlation;

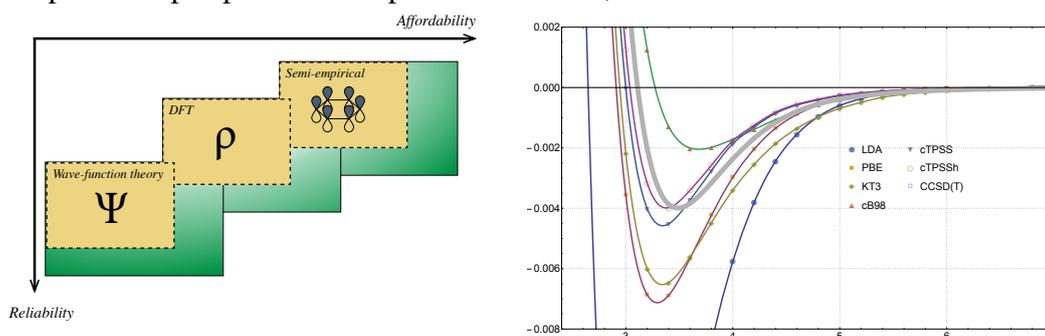


Figure 4: Left panel: Improved reliability and affordability of the three classes of electronic-structure methods. Right panel: Benchmarking of CDFT against CCSD(T) (broad grey curve) for the dissociation of magnetically bonded Ne_2 in magnetic field of 235 kT perpendicular to the molecular axis. The various exchange–correlation functionals exhibit widely different behaviours, the current-dependent cTPSS and cTPSSh functionals performing remarkably well [9].

in ultrastrong magnetic fields and under ultrahigh pressures, molecules are squeezed and bind in new manners. In such situations, DFT and our intuition are pushed out of their comfort zones and are likely to fail. For safe navigation, we must benchmark against methods that can be systematically refined towards the exact solution. The most successful such method is **coupled-cluster (CC) theory**.

For the spectroscopic studies in RT3, the DFT-based response framework of OPENRSP will therefore be extended to CC theory, going significantly beyond the state of the art for property studies. For magnetic-field studies in RT4, the open-shell functionality of LONDON will be extended to equation-of-motion CC (EOM-CC) and to multiconfiguration self-consistent-field (MCSCF) theories. Today, LONDON boasts the only existing implementation of **current-density-functional theory (CDFT)** for molecules in magnetic fields, but improved exchange–correlation functionals are needed. In the absence of experimental data, the development of these will be guided by CC theory, see Fig. 4.

Two recently initiated projects aim to extend the applicability of CC theory significantly. Kvaal’s ERC-StG project *Bivariational Approximations in Quantum Mechanics and Applications to Quantum Chemistry* aims at a convenient formulation of multi-reference CC theory, exploring the **bivariational principle** as a flexible alternative to the standard variational principle. Pedersen’s Research Council of Norway Researcher Project (RCN-RP) *Coupled-Cluster Methods for Periodic Systems* aims to enable high-accuracy studies of condensed-phase systems by **exporting CC theory to periodic systems**, with Wannier functions expanded in Gaussians for computational scalability. In RT1, we will leverage these projects to guide development of density functionals and semi-empirical methods.

For large systems, we will continue ongoing work on **linear-scaling methods** in LSDALTON [1]. Our recently developed code MRCHEM [14] for basis-set-free DFT calculations using **multiwavelets** is inherently linear scaling and will be extended to large systems, while also providing useful basis-set-limit results for RT3 and RT4. For even larger systems, semi-empirical methods such as **density-functional tight binding (DFTB)** will be implemented and reparameterized for our purposes. For heavy atoms, **relativity** is crucial: two- and four-component methods will be implemented in LONDON and the efficient relativistic DFT code RESPECT [15] will be extended to the condensed phase.

Objectives:	extend reliability, applicability, and affordability of electronic-structure methods
Beyond the State of the Art:	bivariational principle for multireference systems, CC theory for condensed phase and for high-order spectroscopies, relativistic DFT for condensed phase, CDFT for molecules in magnetic fields, multiwavelets for basis-set limit results and multiscale modelling
Challenges:	high cost of CC theory, description of static correlation and correlation in magnetic fields
Collaborators:	J. Gauss (Mainz), P. Jørgensen (Aarhus), R. Lindh (Uppsala), Trond Saue (Toulouse), J. Toulouse (UPMC, Paris), D. Tozer (Durham)
Theme Leaders:	T. B. Pedersen (UiO, leader), L. Frediani (UiT, co-leader)

RT2: Multiscale Modelling

To model large-scale systems and the effects of complex environments, we will develop multiscale tools coupling quantum/atomistic models to coarse-grain/mesoscale schemes, spanning several orders of magnitude in space and time.

New developments in experimental techniques allow complex phenomena and processes to be resolved in both space and time. The dimensionality of the processes that can be investigated *span several orders of magnitude*, from fast highly localized chemical reactions occurring on the picosecond timescale and localized to a few nanometers, to large-scale diffusional processes extending beyond micrometers and milliseconds. Although all systems obey the same fundamental principles of quantum mechanics, phenomena at different resolutions *do not require descriptions at the same level of detail* [16]: Whereas spectroscopic properties require a quantum-mechanical description, molecular localization may be described even without atomistic resolution. Multiscale modelling ensures a balanced treatment of phenomena at different scales, see Fig. 5 [17].

In RT2, detailed representations based on electronic-structure methods, including those developed in RT1, will be embedded in a multiscale hierarchy of progressively coarser descriptions of the en-

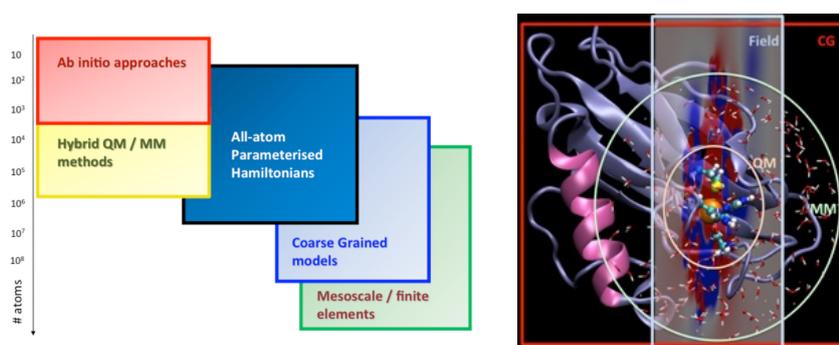


Figure 5: Left panel: multi-scale methods and their range of applicability; right panel: properties and phenomena that can be investigated by different methods.

vironment: **QM/QM, QM/MM, QM/PCM** [18, 19]. These models will give accurate descriptions of the dielectric response of the environment, taking also into account steric effects, thus providing crucial enabling tools for the research in RT3–RT5, while also contributing to RT6. The development of embedding schemes for multidimensional vibrational spectroscopy has recently received RCN-RP support (Ruud) and will be vigorously pursued in RT2.

At the other end of the scale, we will work on multi-resolution atomistic/coarse-grained/mesoscale simulations, developing, in particular, the **hybrid particle–field molecular-dynamics self-consistent-field (MD-SCF) method** [20]. This method describes particle–particle interactions by coupling the individual particles to an external potential dependent on the density. In this manner, intermolecular forces can be calculated in linear time, allowing simulations of quasi-atomistic resolution at scales that are today *hardly accessible even on the most powerful massively parallel architectures*. In RT2, we will extend the MD-SCF method to biological systems and biomaterial interfaces. Seed funding has been obtained from the *H2020 Marie Skłodowska-Curie Action (MSCA)* by Bindu and Cascella. All multiscale and multiresolution methods will be integrated in codes developed at the centre; in collaboration with Prof. G. Milano, our MD-SCF developments will also be incorporated in the OCCAM code. In the long term, we seek a unifying description connecting all resolutions up to the mesoscale.

Objectives:	explicit treatment of the environment, coupling to external electromagnetic fields, accurate coarse-grained models for biological systems
Beyond the State of the Art:	polarizable (density) embedding techniques for spectroscopic applications, hybrid particle–field MD-SCF models for biological systems
Challenges:	dielectric and non-electrostatic environmental response, transferability of coarse-grained potentials
Collaborators:	J. Kleinjung (Crick Institute, London), J. Kongsted (Southern Denmark), G. Milano (Salerno), J. M. H. Olsen (Southern Denmark)
Theme Leaders:	M. Cascella (UiO, leader), B. O. Brandsdal (UiT, co-leader)

RT3: Spectroscopic Processes

To model interactions between complex systems and electromagnetic fields made accessible through fourth-generation light sources, we will develop novel multiscale models for calculating and predicting new spectroscopies.

The detection of **response of matter to electromagnetic radiation** in different frequency ranges, from the high-energy, strongly perturbing X-ray regime to the more subtle interactions in the radio- and microwave region, is one of the most important tools for unravelling the structure and properties of molecules. Such responses can also be used to induce and control chemical reactions through, for example, photocatalytic and optogenetic processes. At the same time, the response of individual molecules can be strongly **altered by complex surroundings**—in surface-enhanced spectroscopies, for example, plasmonic resonances can greatly enhance the intensity of scattered light, allowing for single-molecule imaging and spectroscopy. With recent advances in laser optics and spectroscopy, we can in contrast design spectroscopic processes that allow us to see past the complexity: A non-linear process such as second-harmonic generation, for instance, is **interface specific**, being impervious to an isotropic surrounding. As reactions and processes often occur at interfaces, surfaces, and membranes, these regions are of great importance in chemistry and biology, and non-linear spectroscopy

is a powerful method for studying such processes *in situ*. The analysis of the experimental observations is difficult and would benefit from the availability of theoretical data. However, the reliable calculation of non-linear responses from complex interfaces is currently not possible.

In RT3, we will develop methods that can accurately and reliably describe **advanced spectroscopic processes of complex systems**. With our code OPENRSP, we have developed a state-of-the-art approach to calculate non-linear electronic and vibrational responses of any order [12], allowing

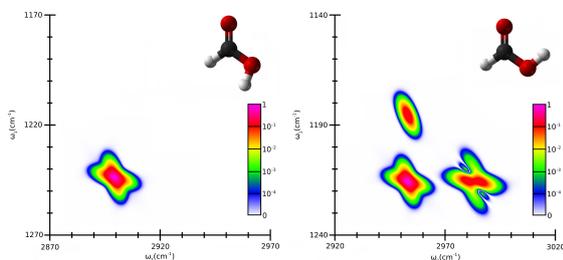


Figure 6: Doubly-vibrationally enhanced four-wave mixing spectrum involving the vibrational modes ν_2 and ν_5 of the two conformers of formic acid calculated analytically using OPENRSP and WILSON, illustrating the strong dependence of the spectra on molecular conformation through vibrational anharmonicities.

us to study anharmonic vibrational spectra [21], high-order multiphoton processes [22], and excited-state properties [23] in a unified framework. To calculate multidimensional spectra from *ab initio* data, we have developed the program WILSON [24]. Used in tandem, these two programs allow us to explore the powers of such techniques for conformational studies, see Fig. 6.

Our goal is to apply these methods to identify secondary structures of biomolecules in their native environment. In the Hylleraas Centre, we will therefore take these open-ended methods from the realm of individual molecules to complex heterogeneous systems, extending the multiscale methods of RT2 to response theory, building on an RCN-RP grant recently awarded to Ruud, going significantly beyond the state of the art. The development of a CC extension to OPENRSP in RT1 will allow us to benchmark our DFT and DFTB results with respect to the treatment of electron correlation, while basis-set limits will be established by combining the MRCHEM code with OPENRSP.

Fourth-generation light sources provide both **high-intensity laser fields and ultrashort pulses**. Femto- and attosecond pulses induce fast non-equilibrium processes of the electrons that cannot be treated perturbatively. To describe such processes, we will develop *models for describing dynamics at different time scales*, including real-time methods at the two- and four-component relativistic levels [25], to study, for instance, X-ray pulses that interact with the core electrons, for which relativistic effects are large. We will also extend these real-time relativistic methods to include nuclear motion—allowing, for instance, for the direct calculation of light-induced spin crossover processes, where light is used to control the magnetic properties of materials. Using developments from RT4, we will extend the capabilities of LONDON to investigate the effects of laser pulses in the presence of strong magnetic fields, allowing us to investigate systems that today cannot be addressed computationally.

Objectives:	modelling of non-linear, interface-specific, and time-resolved spectroscopies of complex systems
Beyond the State of the Art:	open-ended response theory for multidimensional spectroscopies in complex environments, spectroscopic responses at surfaces and interfaces, two- and four-component Ehrenfest dynamics for chemical transformations
Challenges:	reliable surface/interface models, dynamics, non-electrostatic contributions
Collaborators:	J. Kongsted (Southern Denmark), V. Malkin (Slovak Academy of Sciences), P. Norman (KTH, Stockholm), J. M. H. Olsen (Southern Denmark)
Theme Leaders:	K. Ruud (UiT, leader), T. B. Pedersen (UiO, co-leader)

RT4: Extreme Environments

To understand the exotic, squeezed chemistry of extreme magnetic fields and pressure, computational models will be extended to large systems with inclusion of dynamics, and spectra of astrophysical relevance will be calculated.

On Earth, chemistry is governed by Coulomb interactions, the effect of magnetism being weak and subtle. Elsewhere, the situation is different—on many white dwarf stars, for example, magnetic forces compete with electric forces, setting up an exotic chemistry of egg-shaped atoms that interact in unexpected ways [26, 27]. Apart from shedding light on a fascinating chemistry that cannot be

experienced directly, the study of **chemistry in ultrastrong magnetic fields** thus has relevance in astrophysics. Following the serendipitous first observation of molecules on *nonmagnetic* white dwarf stars in 2013 [28], we will simulate spectra of H_2 for their detection on *magnetic* white dwarfs, in collaboration with astrophysicist J. S. Heyl at the University of British Columbia, with whom an application for Hubble observation time will be made. If successful, it would be the first glimpse of chemistry in an environment where electric and magnetic forces compete. However, demands are high in terms of the accuracy required and the number of states, field strengths, and field orientations that must be addressed, see Fig. 7. For sufficient accuracy, (anisotropic) basis sets must be designed, benchmarked against the basis-set limit established with the MRCHEM multiwavelet code of RT1.

Responding to our work on the magnetic bond, Murdin *et al.* [8] noted that, in semiconductor impurities, the dielectric constant of the material and effective mass of the electron combine to enhance the effective strength of the magnetic field for the impurity relative to that experienced by a free molecule. The effects of ultrastrong fields may therefore be studied inside impurities, at laboratory

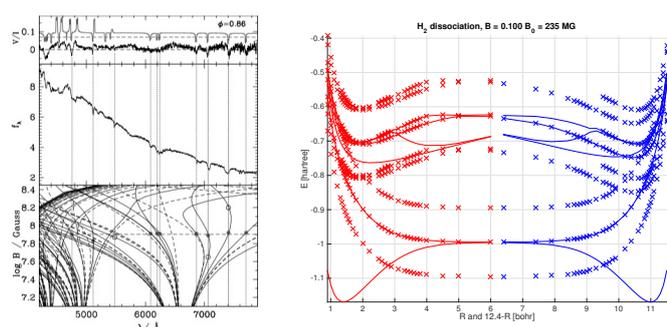


Figure 7: Left panel: Alignment of calculated and observed Lyman lines of the H atom in the spectrum of the magnetic white dwarf PG 1015+014 identifies the field strength at different stellar orientations [29]; Right panel: FCI/cc-pVTZ energy curves of the lowest states of H_2 at about the same field strength. Red curves (left half) are energies in the perpendicular orientation plotted against bond distance R ; blue curves (right half) are energies in the parallel orientation plotted against $12.4 - R$. Crosses indicate triplet states.

field strengths, *prompting speculation that magnetic bonding may be observed under laboratory conditions*, with far-reaching implications. This observation provides compelling motivation for extending our study to large systems. Combining LONDON with multiscale methods, we will study **magnetic enhancement effects** in large systems and its effect on bonding. Moreover, for a broader picture of chemistry, **molecular dynamics** in a magnetic field will be developed. Although the Born–Oppenheimer approximation is still valid for fields up to 10^5 T as considered here, a non-adiabatic Lorentz correction [30] to the forces must be calculated. LONDON is the only code capable of performing gauge-invariant FCI [4],

CCSD(T) [31], and CDFT [9, 32] calculations in magnetic fields; its extension to large systems, multiscaling and dynamics goes well beyond the state of the art, allowing new phenomena to be studied.

There is an intriguing connection between ultrastrong magnetic fields and **ultrahigh pressure**: both squeeze matter, creating highly complicated, electronic systems, challenging our understanding of chemistry and our computational models. For instance, under high pressure, helium has an hcp crystal phase; in ultrastrong magnetic fields, it forms magnetically bonded structures suggestive of a hexagonal 2D crystal lattice, see Fig. 2. Recently, materials have been studied at pressures up to 400 GPa, revealing a chemistry with novel structural, electronic, and magnetic properties, challenging our intuition [33]. Noting that ultrahigh pressure poses challenges similar to those of an ultrastrong magnetic field, in both cases related to **electron confinement**, we will develop and adapt the methods of electronic-structure theory to explore both phenomena.

Objectives:	chemistry and bonding in ultrastrong magnetic fields and under ultrahigh pressure
Beyond the State of the Art:	spectra of molecules in magnetic white dwarfs, molecular dynamics in magnetic fields, electron confinement and electron correlation in extreme environments
Challenges:	sufficient accuracy of calculated spectra, large system size needed for enhancement, response of environment to the external field, non-adiabatic force corrections in molecular dynamics
Collaborators:	J. Gauss (Mainz), J. S. Heyl (British Columbia), M. R. Hoffmann (North Dakota), P. Schwerdtfeger (Massey), S. Stopkowicz (Mainz), A. Thirumalai (DigiPen, Redmond)
Theme Leaders:	T. Helgaker (UiO, leader), K. Ruud (UiT, co-leader)

RT5: Chemical Transformations

To control the reactivity and energy transfer of complex chemical transformations, we will develop new computational protocols based on state-of-the-art electronic-structure and multiscale methods.

Chemistry is the science of matter and its transformation. Ideally, **chemical transformations** should yield the desired products at minimum energy consumption and waste generation. Catalysts are essential to achieve this goal, see Fig. 8. *To understand and to control chemical transformations and catalytic processes are key to developing sustainable energy technologies.* Computation is a valuable tool for understanding chemical transformations [34, 35]. However, synergy between experiment

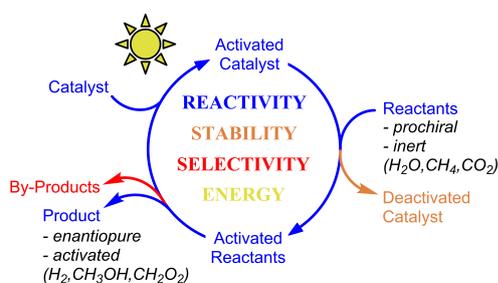


Figure 8: Key concepts of catalysis and chemical transformations

and computation is often hampered by lack of detailed experimental data and incomplete theoretical exploration of the chemical systems. The improved resolution of new light sources will allow exploration of key steps on the time scale of chemical processes, producing a wealth of new experimental data. A complete understanding of these processes will require theoretical analysis with adequate protocols and methods. To match these experimental developments, we will improve the theoretical description by *combining state-of-the-art electronic-structure and multiscaling methods with new techniques for automatic reaction-space exploration* such as the Global-Reaction-Route-Mapping (GRRM) method [36]. Electronic, vibrational, and NMR data generated using, for instance, the relativistic methods of RT1 and the functionality of OPENRSP will be employed for direct comparison of theoretical predictions and experimental observations, facilitating the understanding of current systems and the development of improved catalysts.

Fourth-generation light sources will open two highly challenging avenues of research, for which novel computational strategies must be developed—namely, the **control of chemical reactivity** and the **control of energy transfer**. The control of reactivity, stability, and selectivity by structural elements, pressure, fields, or pulses is the holy grail of catalytic design. To make breakthroughs in reaction control, we will develop computational strategies incorporating the methods of RT1–RT3 for an accurate treatment of molecules and their reaction pathways in complex environments and in the presence of fields, spurring new experimental work by our collaborators. Second, chemical transformations for sustainable energy technologies or for the transformation of unreactive molecules such as CO₂ into added-value chemicals will not only require an understanding of energy conversion and transportation in the reactive system itself but also of the **transfer of energy to the environment**. The most efficient conversion mechanisms in nature use complex interactions with the environment to convert, for instance, solar light into chemical energy. The design of such processes is a formidable task, requiring an understanding of electronic correlation, of conversion of energy into vibrational degrees of freedom at the femtosecond scale, and of energy dissipation at longer time scales.

Combining reaction-space exploration with methods for multicomponent reactions and matter-field interactions emerging from RT1–RT3, we will be able to analyse systems currently beyond reach and to design novel, efficient catalysts, initially benefiting from two *RCN Young Research Talent (YRT)* grants (Hopmann, Nova) and one *MSCA Career Integration Grant (CIG)* (Balcells).

Objectives:	complex reactions related to sustainable use of resources, water oxidation, CO ₂ conversion, CH activation, asymmetric induction
Beyond the State of the Art:	accurate calculations of multicomponent chemical systems with complex electronic structures including the role of the environment
Challenges:	optimal representation of strong and weak interactions for multicomponent chemical systems whose electronic structure can vary widely during thermal or photochemical multistep reactions
Collaborators:	C. Copéret (ETH Zürich), R. Crabtree (Yale), N. Hazari (Yale), S. Maeda (Hokkaido), C. Raynaud (Montpellier), E. Le Roux (Bergen), T. Skrydstrup (Aarhus), M. Tilset (UiO)
Theme Leaders:	O. Eisenstein (UiO, leader), K. Hopmann (UiT, co-leader)

RT6: Multiphase Systems

To unravel the statistical laws of complex systems, we will develop novel computational protocols to study the structure and dynamics of macromolecules and their interactions with membranes and interfaces.

Biological systems have developed an impressive array of complex functional structures, such as molecular machines, which drive living processes and hold the key to revolutionizing energy sustainability [37]. Biological functions are the result of a complex interplay through a dynamic network of crowded macromolecules. Intriguingly, large-scale, slow biological events that occur on micrometer and millisecond scales are triggered and regulated by local, fast biochemical events like ligand binding or enzymatic reactions occurring on nanometer and pico/nanosecond scales—for example, as in G protein-coupled receptor signalling cascades.

Multicomponent biological structures arise in **multiphase environments**—in fact, subcellular processes hardly ever occur at random locations in the cell but are usually compartmented at specific membranes such as the endosome, the endoplasmatic reticulum, or the plasma membrane. To model such complex systems and extract information relevant to experiment, we must draw on the tools of RT1–RT4. In particular, we must go beyond the current description of biological membranes as a periodic lipid bilayer made up of a few chemical components.

We will in RT6 address **bacterial antimicrobial resistance**, one of the biggest threats to public health [38]. Drug-resistance mechanisms have evolved independently in different bacterial strains and may involve macromolecular complexes such as multidrug efflux pumps. The dimensionality of these transporters is such that only models beyond the state of the art can give a comprehensive

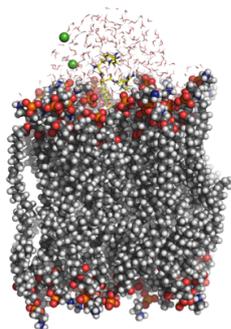


Figure 9: A cationic antimicrobial peptide attached to a bacterial membrane model, as observed in MD simulations.

description of their mechanisms. Moreover, the peculiar composition of the outer bacterial membranes provides a promising target for the development of specific antibiotics [39], see Fig. 9. The study of **membrane polymorphism** under different conditions will involve vastly different time and length scales. Using multiscale methods—in particular, the MD-SCF method of RT2—we will develop protocols for an *atomistic description of molecular interactions that trigger biological function* (molecular recognition, enzymatic catalysis) and for a *mesoscale description of molecular phenomena that generate macroscopic complex responses*. By combining large-scale simulations with the spectroscopic tools developed in RT2 and RT3, we will be able to identify key fingerprints for optically active compounds in different multiphase environments. Finally, we will use our multiscale tools to investigate biointeractions of nanomaterials, describing, in particular, protein and polymer coating of nanoparticles, important for the development of antifouling, biocompatible materials.

The integration of structural, dynamical and spectroscopic calculations will put us in an excellent position to provide computational protocols to complement data coming from experimental facilities: fourth-generation light sources are heralded as capable of elucidating the statistical laws that govern macromolecular systems through the use of time-resolved soft X-rays; free-electron lasers, cryo-electron microscopy, and novel neutron scattering equipment promise to give new insights into large membrane-associated systems, their dynamics, and structural aggregation.

Objectives:	macromolecular complexes, protein–membrane interactions, molecular adsorption and transport
Beyond the State of the Art:	correct stoichiometry of lipid membranes, system-dependent curvature at interphases, signal propagation at multiple scales
Challenges:	non-covalent interactions, size of systems, diffusional processes, interface dynamics, molecular crowding, treatment of both periodic and non-periodic systems of (bio)chemical relevance
Collaborators:	F. Fraternali (King’s College, London), P. Ruggerone (Cagliari), T. A. Soares (UFPE, Recife), J.-S. Svendsen (UiT)
Theme Leaders:	B. O. Brandsdal (UiT, leader), M. Cascella (UiO, co-leader)

Ambition, Impact, and Feasibility of Research

Complex systems and multiscale modelling are important current areas of research in chemistry. Our contribution will be unique by including advanced methods for describing matter–field interactions, an area in which we have world-leading expertise. This **ambition** is further strengthened by the integrated approach to complex systems: At the finest level, our quantum description extends to all (core and valence) electrons, with an explicit treatment of electron correlation and the option for a full relativistic treatment; at the coarsest level, we develop a hybrid particle–field model for mesoscale simulations in biology. On the shortest time scale, we explore electron dynamics in attosecond pulses; on the longest time scale, we study large-scale conformational changes extending to microseconds.

Timeliness relative to emerging experimental facilities ensures an **impact** extending far beyond the centre itself, in research and in industry. This impact is strengthened by the dissemination of the methods developed to the community through **software distribution**, at no cost, for use in chemistry, physics, astrophysics, and biology. The research is **ambitious**, going **beyond the state of the art** in several areas—for example, we will study spectroscopic processes at interfaces and surfaces by combining the unique methodology in OPENRSP with multiscale methods; likewise, the unique methodology in LONDON is combined with multiscale methods to study magnetic enhancement.

Many members of the proposed centre have already secured external funding that works towards the goals of the centre (see Table 1); based on their track records, we are confident that they will continue to secure individual funding. Nevertheless, the **feasibility** of the proposed research programme is critically dependent upon our ability to create synergies across individual research interests and expertise, working together as a team towards the common vision for the centre. Indeed, the creation of such a shared research focus and commitment is the most important **added value** of the establishment of the Hylleraas Centre. The mechanisms that will be put in place to achieve this goal are described in the Organization Section.

The centre funding will enable us to **draw on the best international research** of relevance to the centre, through flexible visitor and sabbatical programmes, in a manner that cannot be achieved through individual grants. Second and more importantly, the centre funding will make it possible to **integrate activities and complementary expertise across our chosen RTs**, creating the synergies that are needed to go significantly beyond the state of the art. Third, together with the in-kind contributions, the centre funding will guarantee a **sustained base level of PhD students and postdocs**, needed to realize our long-term ambitions. The students and postdocs will play an important role in developing research at the interfaces between the RTs, ensuring coherence and convergence towards our goal of modelling complex systems in electromagnetic fields and extreme environments. At the centre, they will receive world-class training in an important emerging research and innovation area, putting them in a good position to take a future lead, in industry and research, in the new opportunities offered by controlling light–matter interactions.

Relationship to Centre for Theoretical and Computational Chemistry

The Hylleraas Centre builds on the Centre of Theoretical and Computational Chemistry (CTCC), a Centre of Excellence (CoE) established by the RCN in 2007, which has successfully reached its ambition to integrate computation into its participating experimental groups. Emerging experimental techniques and facilities mandate a strong, concerted effort to model complex systems in extreme fields and environments. The theoretical competence of the CTCC and the recent strategic additions to the groups at UiO and UiT—in particular, in computation and multiscale modelling—have put the proponents of the Hylleraas Centre in a unique position to move the state of the art in modelling such systems and also to establish multiscale modelling on a par with electronic-structure theory in Norway. With its strong emphasis on multiscale modelling and matter–field interactions, made possible by our own recent research and recent hirings, the Hylleraas Centre differs fundamentally from the CTCC.

Organization

The Hylleraas Centre will be organized as a project at the Department of Chemistry, UiO, and operated as a CoE consortium with nodes at UiO and UiT. In recognition of their theory groups as being world leading, both institutions have made significant recent investments by increasing the permanent staff by two positions in each group.

Leadership and Management: The **Director**, appointed full time at the Centre in an 80%–20% position at the two universities, has responsibility for all centre activities—in particular, the fulfilment of its scientific ambitions. One PI, from the opposite node of the director, will act as a **Deputy Director**, assisting the director, especially in matters concerning his/her node. The **Management Team**, consisting of the director and the PIs, oversees all research, training, outreach, and dissemination, with responsibility to allocate resources among the research themes, to identify new projects (and contribute to acquiring funding to realize these projects when necessary), and promote synergies among the centre members. Each research theme is headed by a **Theme Leader** and a co-leader, one from each node, with responsibility for research, proposals, and hiring in that theme. For an efficient day-to-day management, one **Head of Office** is recruited at each node. The centre is governed by a **Board of Directors** with representatives of each university, industry, and of Norwegian computational scientists: Jo Døhl (chair, Head Dept. Chem., UiO), Prof. Nathalie Reuter (Dept. Mol. Bio., UiB), Prof. Atle Jensen (Dept. Math., UiO), Prof. Fred Godtlielsen (Pro-Dean, Faculty Science and Techn., UiT), and Kajsa Rytberg-Wallgren (Vice President Innovation, Yara International). The board is responsible for strategy in matters of research, training, outreach, and budget.

Director: In its first five-year period, the centre will be directed by Prof. Trygve Helgaker (UiO, 308 publications, 18996 not-self citations, H-index 69); in the second period, by Prof. Kenneth Ruud (UiT, 296 publications, 8624 not-self citations, H-index 53), who will also act as Deputy Director in the first period. Both have directed the Centre of Excellence CTCC (Ruud 2007–2013, Helgaker 2013–2017); both are **ERC grant winners**. With their outstanding track records in research and leadership, as documented by their attached CVs, they are well suited to lead the Hylleraas Centre.

Scientific Advisory Committee: A scientific advisory committee of five prominent scientists including experimentalists will give advice regarding research directions, management, and funding. Its members are Prof. Chantal Daniel (Université de Strasbourg, quantum-chemistry computation), Prof. Serena DeBeer (Max-Planck-Institut für chemische Energikonversion, Mülheim, X-ray spectroscopy), Prof. Markus Reiher (ETH Zürich, quantum-chemistry theory), Prof. Ursula Röthlisberger (École polytechnique fédérale de Lausanne, multiscale modelling), and Prof. Peter Schmelcher (Universität Hamburg, laser physics). The committee, whose expertise covers all research directions at the centre, will be consulted annually and meet biennially.

Team: The team is built around a core of three tenured professors at UiO (Cascella, Helgaker, Pedersen) and three at UiT (Brandsdal, Frediani, Ruud), who will contribute their research fully to the centre, see Table 1. Prof. Eisenstein, who is currently hired as adjunct professor (20%) at UiO, will in the Hylleraas Centre take on a full professorship but without teaching and administrative duties (i.e., 50% position). In addition, the initial team will consist of eleven researchers, three of whom are permanently hired at their institutions and one in a 20% adjunct position (Teale). Importantly, the team also includes one senior engineer at each node.

Expertise: We possess world-class expertise in quantum chemistry, electronic-structure theory, molecular properties and spectroscopic processes (Frediani, Gao, Helgaker, Pedersen, Ruud), recently extended to computational chemistry (Eisenstein, Hopmann), multiscale modelling and complex systems (Brandsdal, Cascella), and mathematical physics (Kvaal). The quality of our team can be judged by the fact that it includes *all three ERC chemistry grant winners in Norway* (Helgaker, Kvaal, Ruud), *all but one of the five RCN Young Research Talents (RCN-YRT) chemistry grant winners* (Fliegl, Hopmann, Nova, Tellgren), *one MSCA Career Integration Grant (MSCA-CIG) winner* (Balcells), *one*

Table 1: Leadership, research and technical staff at the Hylleraas Centre

	name	title	aff	role	RT1	RT2	RT3	RT4	RT5	RT6	ext funding	nat.	m/f
perm. faculty	Trygve Helgaker	Professor	UiO	dir ^a	✓		✓	✓			ERC-AdG	NO	m
	Kenneth Ruud	Professor	UiT	PI ^a	✓	✓	✓	✓			ERC-StG, RP ^b	NO	m
	Bjørn Olav Brandsdal	Professor	UiT	PI		✓			✓	✓		NO	m
	Michele Cascella	Assoc Prof	UiO	PI		✓			✓	✓		IT	m
	Odile Eisenstein	Professor	UiO	PI			✓		✓	✓		FR	f
	Kathrin Hopmann	Researcher	UiT	PI			✓		✓	✓	YRT ^c	DE	f
	Thomas Bondo Pedersen	Assoc Prof	UiO	PI	✓		✓	✓			RP ^b	DK	m
	Luca Frediani	Assoc Prof	UiT		✓	✓	✓			✓		IT	m
	Bin Gao	Researcher	UiT		✓	✓	✓					CH	m
	Simen Kvaal	Researcher	UiO		✓	✓	✓	✓			ERC-StG	NO	m
temp. faculty	David Balcells	Researcher	UiO				✓		✓	✓	MSCA-CIG	ES	m
	Heike Fliegl	Researcher	UiO			✓			✓		YRT ^c	DE	f
	Stig Rune Jensen	Researcher	UiT		✓			✓				NO	m
	Hima Bindu Kolli	Researcher	UiO			✓				✓	MSCA-IF	IN	f
	Ainara Nova	Researcher	UiO				✓			✓	YRT ^c	ES	f
	Magnus Ringholm	Researcher	UiT			✓	✓					NO	m
	Andrew Teale	Adj Prof ^d	UiO		✓		✓	✓			RS URF ^e	UK	m
	Erik Tellgren	Researcher	UiO		✓			✓			YRT ^c	SE	m
admin.	Stig Eide	Head of Office	UiT									NO	m
	Jan Ingar Johnsen	Head of Office	UiO									NO	m
techn.	Simen Reine	Sr. Engineer	UiO									NO	m
	Michal Repiský	Sr. Engineer	UiT									SK	m

^aKenneth Ruud will initially act as a deputy director and take over as director in 2022; ^bRCN FRIPRO Researcher Project Grant; ^cRCN FRIPRO Young Research Talents Grant; ^d20% adjunct position; ^eRoyal Society University Research Fellowship

MSCA Individual Fellowship (MSCA-IF) winner (Bindu), and one Royal Society University Research Fellowship (RS URF) winner (Teale). In addition, Pedersen and Ruud each hold an *RCN Researcher Project (RCN-RP)* grant and three members have this year passed to the second stage of their ERC Starting/Consolidator applications. The broadness of our interests can be seen from the fact that eight of the twelve grants are for theoretical, methodological work, while four are for computational work. We are young (all but two under 50 years of age), international (twelve non-Norwegian members of nine nationalities), and with a broad network (having graduated from twelve different institutions).

Principal Investigators: PIs have been selected based on their ability to lead the RTs at the centre. *Helgaker* and *Ruud* will naturally lead the pivotal RT3 and RT4 on matter–field interactions; likewise, *Eisenstein* is a natural choice for RT5 on chemical transformations. These three researchers have outstanding track records that perfectly match these RTs. *Pedersen* has an accomplished track record in electronic-structure theory and methods development, having contributed significantly to several software packages, both academic and commercial. His contributions span from novel formulations of time-dependent CC theory to efficient implementations of multiconfigurational methods, making him ideally suited for RT1. Early-career researcher *Cascella* has a broad background in multiscale modelling, having developed and applied several integrated models at *ab initio*, QM/MM, atomistic, and coarse-grained scales, making him an ideal choice for RT2. *Brandsdal* has extensive experience in the application and development of methods for chemical reactivity (QM/MM, EVB, MD) and molecular recognition (MD-based free-energy methods) of biological systems and also in their experimental characterization, making him well suited to lead RT6. Early-career researcher *Hopmann* was chosen as an additional PI, due to her expertise in advanced quantum-chemical modelling of complex catalytic reactions (awarded with an RCN-YRT grant) coupled with a broad experience in spectroscopy. These qualifications make her an excellent co-leader of RT5, where novel methods for prediction of spectral properties are integrated with advanced studies of chemical transformations.

Among the non-PI members, *Frediani* has been selected to co-lead RT1, being in charge of the MRCHEM multiwavelet development at UiT and having a solid background in continuum solvation methods for molecular properties and heterogeneous environments. ERC grant winner *Kvaal* has a strong background in mathematical physics, quantum mechanics, many-body theory, coupled-cluster theory, fundamental DFT and CDFT. To allow him full attention to his ERC-StG project on the bi-variational principle, he will initially not take a leadership role at the centre.

Structure, Physical Organization, and Size of Centre: The Hylleraas Centre will be located at the Department of Chemistry of each participating institution, with no need for significant extra infras-

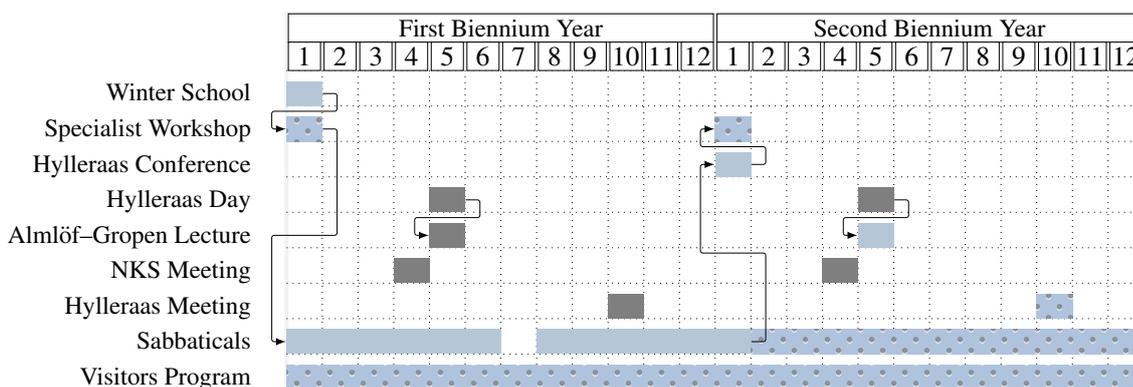


Figure 10: Structure of a Hylleraas FBI. Curly arrows indicate events held back-to-back, grey indicates general centre activities, steel blue activities dedicated to the FBI, whereas the cross-hatched areas indicate activities in both categories.

structures or equipment. At each node, all centre members will be located in close proximity, in their current premises but with sufficient adjacent room for expansion. Both nodes will be equipped with dedicated video conferencing equipment, for group meetings, seminars, and other shared activities. Including PhD students, the centre will initially consist of about 45 members.

Research Collaboration: The centre depends heavily on research collaboration to reach its goals, taking advantage of the complementary skills of its members and its extensive international network. As seen from Table 1, each PI contributes to at least two RTs; moreover, each RT is a collaboration between the two nodes. Seminars, including those of the **weekly seminar series**, will be broadcast to both nodes by video conferencing. Two **Centre Meetings** will be organized yearly, one in partnership with the Norwegian Chemical Society, disseminating the research at the centre to the Norwegian chemical community. These meetings will provide a venue for PhDs and postdocs to present their recent research in terms of contributed talks, engage them in scientific discussions through poster sessions, and expose them to topical lectures by international experts.

Focus Bienniums: To bring freshness, inspiration, and international visibility to the centre, all RTs except RT1 and RT2 will have a **Focus Biennium (FBI)** dedicated to their activities, beginning with RT3 in 2019. In each FBI, an international **Winter School** will be held back-to-back with a **Specialist Workshop** in the first biennium year, while a **Hylleraas Conference** with about 100 participants will be held in the second, see Fig. 10. Leading experts in the field of the FBI will be invited to all events, as teachers or as speakers. The school will be an integral part of the training of students and postdocs at the centre: The first week of the school will remain the same in all bienniums, covering electronic-structure theory (RT1) and multiscale modelling (RT2) taught by centre members, while the second week will be dedicated to biennium topics. Our members have long experience with the organization of schools and meetings—the centre leader has, for instance, organized a two-week international summer school together with P. Jørgensen and J. Olsen of Aarhus University biennially since 1990.

International Orientation and Mobility: To attract the best international expertise, we will run a broad **Sabbatical Programme**, coordinated with but not exclusive to FBI activities. Potential sabbatical visitors will be identified and invited to spend three months or more at the centre, with at least one full year offered to a prominent female scientist in each biennium. An extensive **Visitors Programme** will enable members to initiate collaborations and reinforce established ones, creating a highly international, dynamic research environment for students and postdocs. Our permanent faculty are entitled to a sabbatical year every five (UiT) or seven (UiO) years; these will be used strategically to strengthen research at the centre. PhD students will be strongly encouraged to spend at least three months abroad. As part of the Career Development Plan discussed below, research visits to relevant international research laboratories will be defined for all postdocs.

Training: The centre will establish national biennial PhD courses in theoretical and computational chemistry, offered to all Norwegian universities. We will organize PhD training as a research school,

providing each PhD student with a Supervisory Committee of three members and at least two from the Hylleraas Centre. All academic staff will teach PhD courses and be engaged in master, PhD, and postdoc training; apart from Helgaker, Ruud, and Eisenstein, all will perform undergraduate teaching duties. The sabbatical and visitors programmes together with the FBI events will ensure that the young researchers are exposed to the research frontiers and receive training of the highest quality.

Career Development: To prepare the young researchers for careers as scientific or industrial leaders, a mentorship programme will be set up and detailed in a **Career Development Plan**. We will encourage participation in courses that provide transferable skills relevant to academia and industry such as ethics, communication, scientific writing, leadership, business creation, and entrepreneurship, as offered by the Research Leadership Programme at UiO and the High North Academy at UiT.

Outreach and Dissemination: Scientific results and other centre information will be disseminated through the following channels: peer-reviewed articles, conference presentations, annual reports, web pages, blogs, and popular science articles. Software will be maintained, developed, and distributed under the leadership of Sr. Engrs. Dr. Reine and Dr. Repiský, ensuring an extensive impact on the academic and industrial community at large. Social media (Facebook, Twitter, YouTube) will be used to promote centre activities such as software tutorials, new results, popular talks, or didactic videos. Our video-conference facilities allow us to stream and record seminar presentations of a broad interest. Annually, an open **Hylleraas Day** for science outreach will be hosted, targeting young people, and a prominent scientist will be invited to deliver the **Almlöf–Gropen Lecture**, initiated by CTCC in 2008, intended to be broadly accessible and promote the field to the scientific community.

Gender Balance: The centre will work towards improving gender balance in theoretical chemistry by making all efforts to ensure female applicants to all positions, by having at least 30% female members including students, by offering a mentoring programme for female members to provide (academic and non-academic) career advice with attention paid to career hurdles for female researchers, and by organizing seminars with focus on gender balance and implicit bias. In each FBI, an internationally recognized female scientist will work at the centre, acting as a role model and mentor for female members. In all outreach and dissemination activities, we will pay attention to gender balance. The centre will support the conference series **Female excellence in theoretical and computational chemistry (FemEx)**, established by the CTCC and now adopted as a regular international conference [40].

Funding: Internally funded projects will be complemented by externally funded projects that support the goals and vision of the centre. All projects will be designed and evaluated with respect to their potential for cross-links and synergies. Members are expected to apply for funding—our ambition is to have at least two FRIPRO grants running at all times. We will seek to participate in H2020 projects that allow for a tight interaction with researchers or industry using the new experimental facilities. To strengthen PhD training, we aim to coordinate an MSCA Innovative Training Network (MSCA-ITN).

Key performance indicators to measure centre success after four and ten years

The primary success criterion after 4 (10) years will be scientific impact as demonstrated by 160 (500) publications in international journals with more than 750 (6000) citations and an H-index of 12 (40).

All chemists in Norway that have received an ERC grant are members of the proposed centre: Helgaker (AdG, 2010), Ruud (StG, 2011), Kvaal (StG, 2014). Building on this record, we expect 2 (4) ERC grant applications (two Advanced Grants and two Starting/Consolidator Grants) to pass the first evaluation stage. We will use MSCAs to strengthen centre activities by submitting at least 1 (3) MSCA-ITN and 3 (8) MSCA-IF applications with a score above 85%. Our target is to have on average two RCN FRIPRO grants running at any given time, which will give an expected income from new external projects of 15 (45) MNOK. Given that our primary activity is basic science, many H2020 programmes are not well suited. Nevertheless, we will seek strategic partnerships with the intention

of involvement in projects in the H2020 programme directed towards societal challenges and/or future and emerging technologies. Our ambition is that at least one application to other funding instruments in H2020/FP9 than the excellence programme is evaluated with a score above threshold for funding.

In terms of training, we will have graduated 7 (23) PhD students and trained 14 (34) postdocs, organized 2 (4) winter schools, 3 (10) specialist workshops, 1 (4) conferences and 8 (20) Hylleraas Centre meetings. We will also have established four national PhD courses, each given at least 1 (3) times. We aim to have at least 30% female members at all times and a 40%–60% gender balance after 10 years.

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