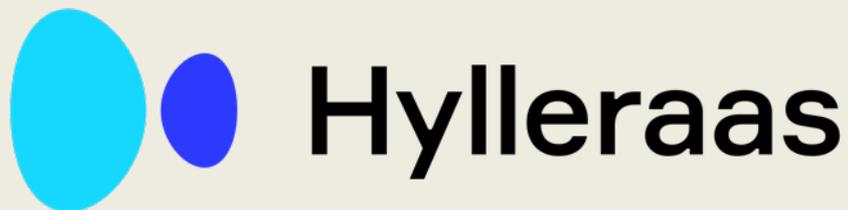


Hylleraas Centre for Quantum Molecular Sciences

Presentation for Scientific Advisory Committee

Radisson Blu Hotel Tromsø

28 October 2019



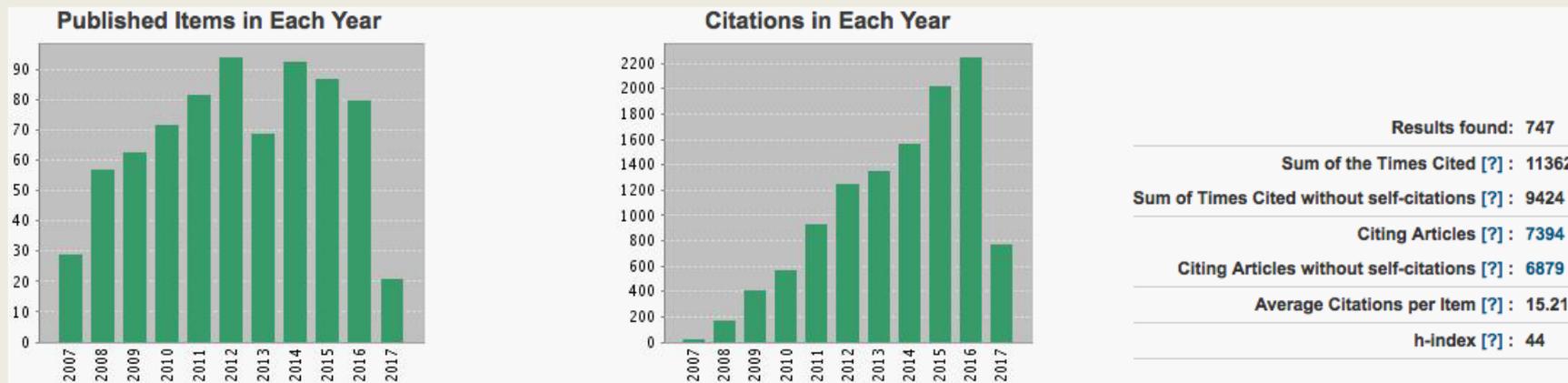
The Research Council
of Norway



Centre for Theoretical and Computational Chemistry

CTCC

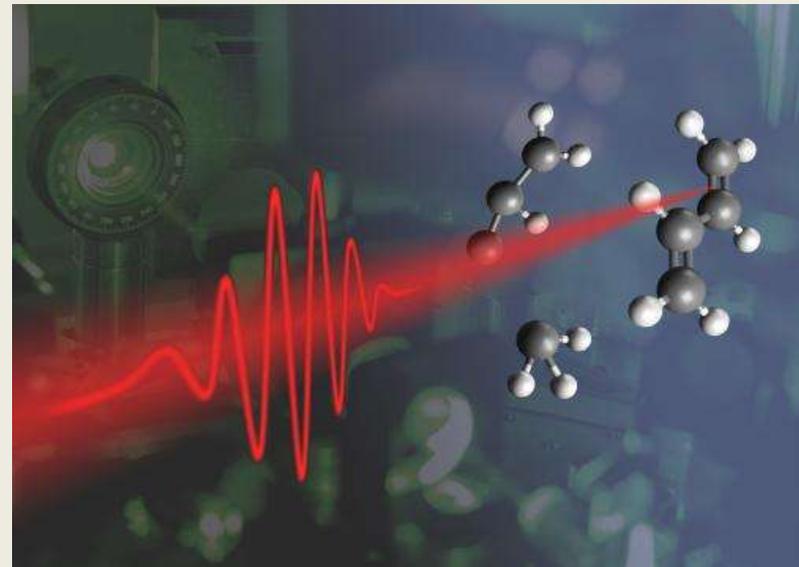
- Centre of Excellence 2007 – 2017 **shared between UiT and UiO**
- **Vision:** the CTCC will be a leading international contributor to computational chemistry by carrying out cutting-edge research in the field of **theoretical and computational chemistry** at the highest international level
- Integration of computation into **participating experimental groups**
- About 800 publications with 13000 citations in 150 journals



- 3 ERC Grants, 4 Young Research Talent Grants

Motivation

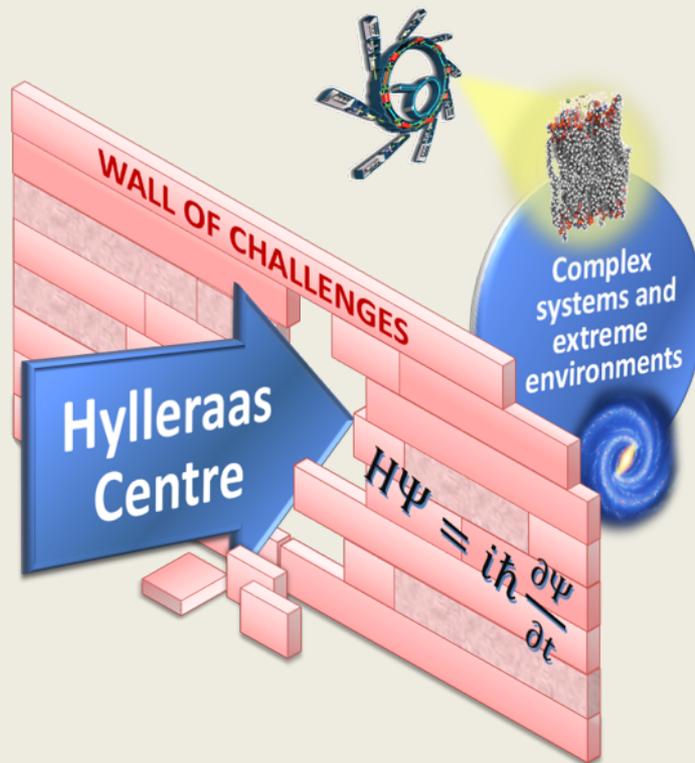
- **New experimental facilities revolutionize how we study matter**
 - unprecedented resolution in time and space



- **Revolution in computation needed to seize new opportunities**
 - we will develop, apply, and distribute the necessary computational tools

Challenges

- Millions of atoms in short laser pulses and strong fields
 - local and global processes occurring over short and long time scales
- Modeling of such processes poses a wall of challenges
 - forcing us to take fresh look at computation



TEAR
DOWN
THE
WALL!

Research Themes

Applications

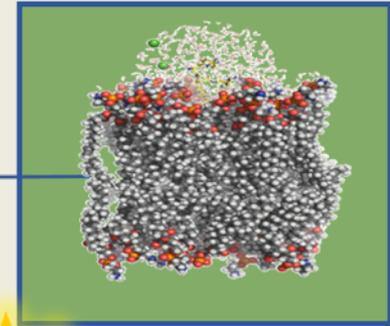
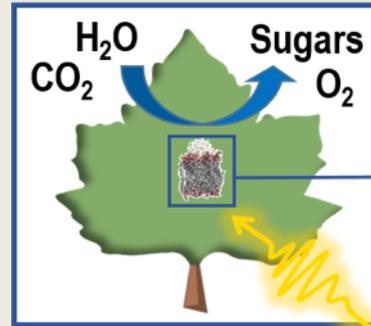
Matter ↔ Field

Matter

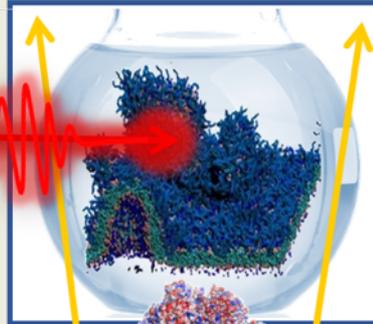
Novel Methods

RT5: Chemical Transformations

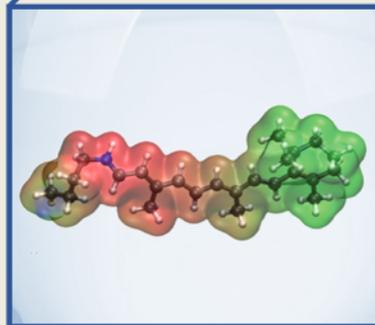
RT6: Multiphase Systems



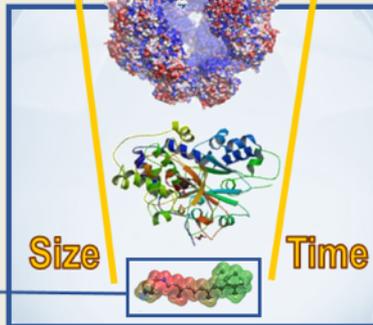
RT3: Spectroscopic Processes



RT4: Extreme Environments



RT1: Electronic Structure



RT2: Multiscale Modelling

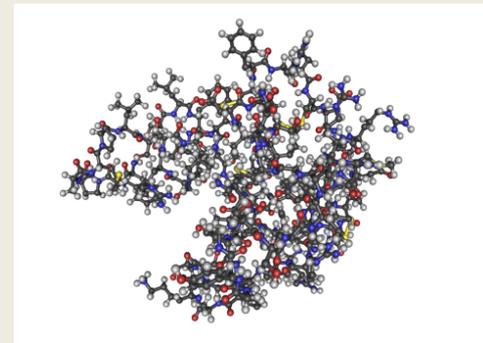
Iterative Feedback

RT1: Electronic Structure



Thomas Bondo Pedersen (UiO), Luca Frediani (UiT)

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.

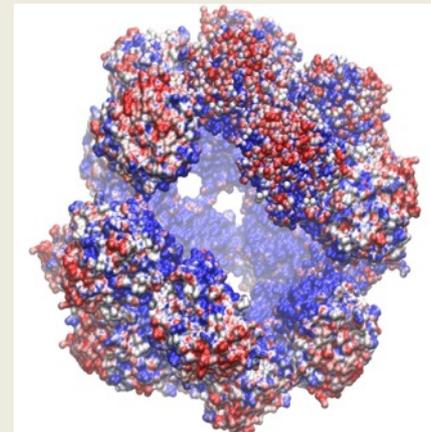
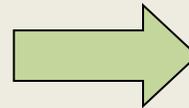
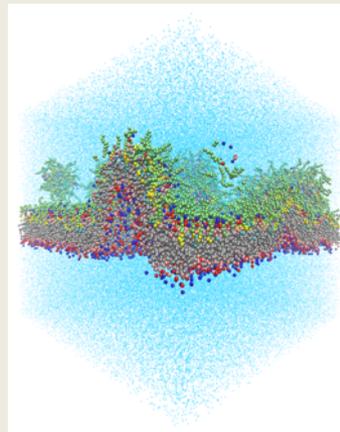
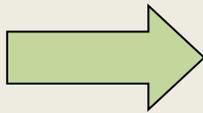
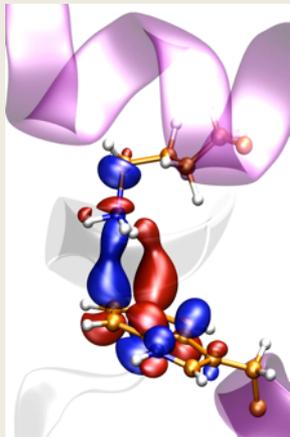


RT2: Multi-Scale Modelling



Michele Cascella (UiO), Bjørn Olav Brandsdal (UiT)

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.



all-atom

coarse-grained

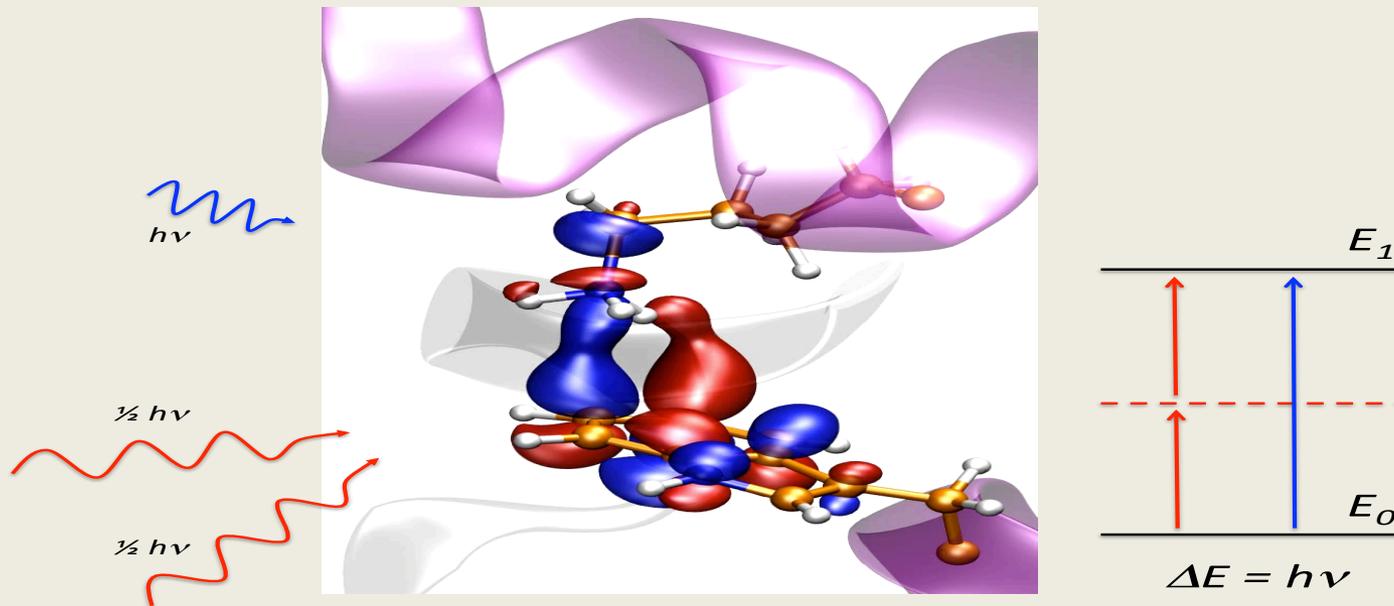
mesoscale

RT3: Spectroscopic Processes



Kenneth Ruud (UiT), Thomas Bondo Pedersen (UiO)

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.

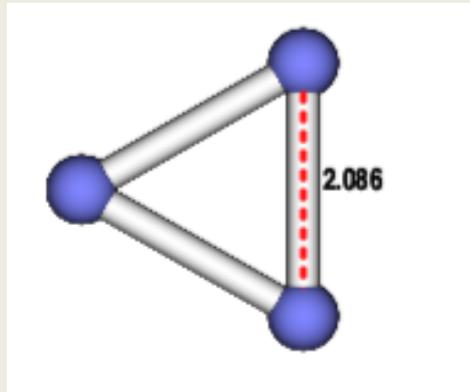


RT4: Extreme Environments



Trygve Helgaker (UiO), Kenneth Ruud (UiT)

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.

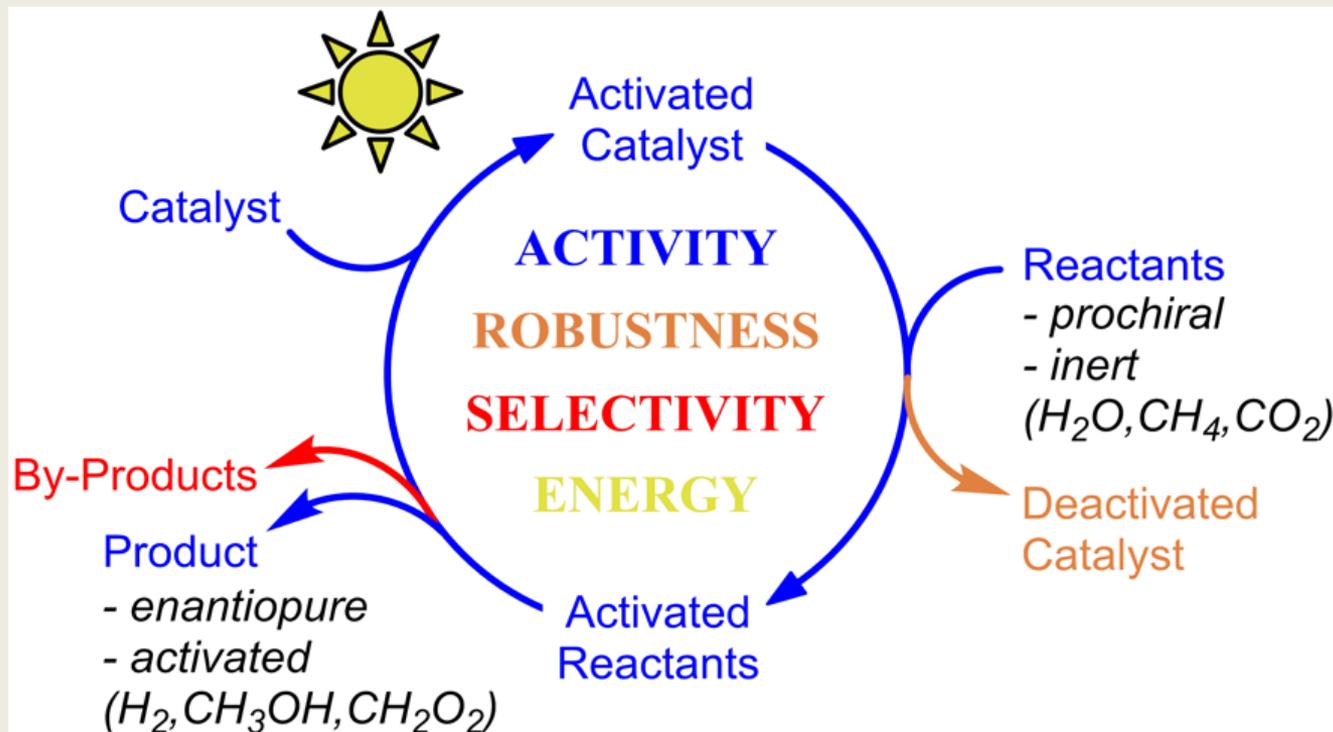


RT5: Chemical Transformations



Odile Eisenstein (UiO), Kathrin Hopmann (UiT)

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.

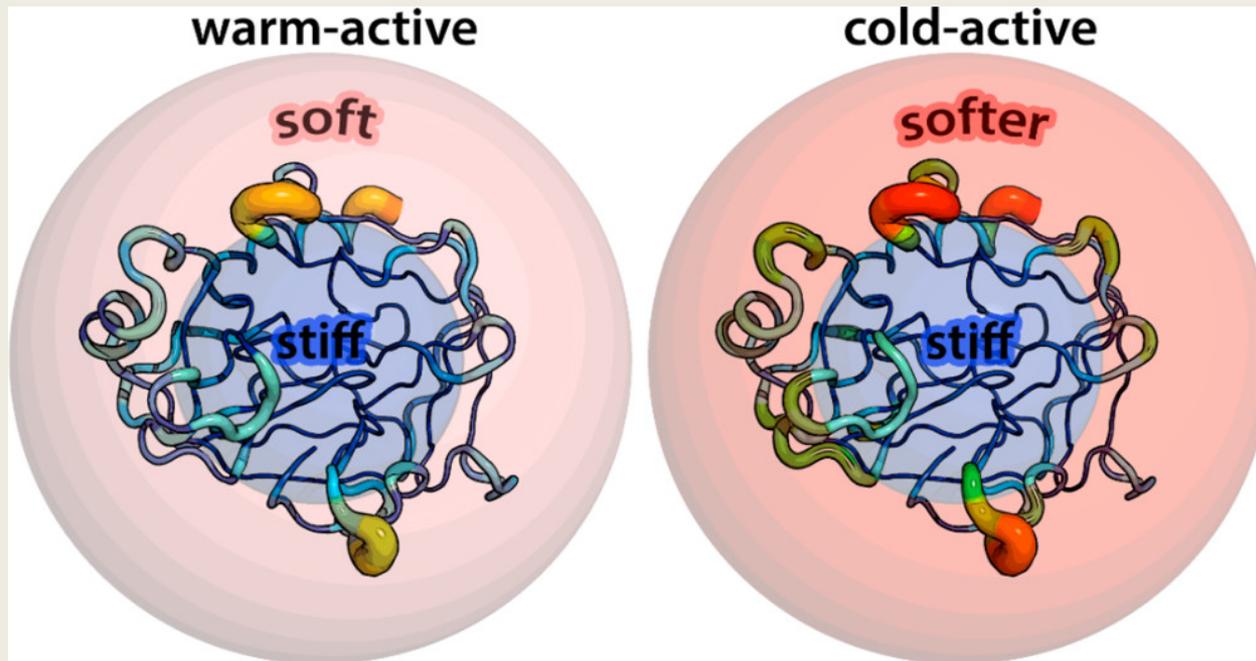


RT6: Multiphase Systems



Bjørn Olav Brandsdal (UiT), Michele Cascella (UiO),

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.



Research Themes

Applications

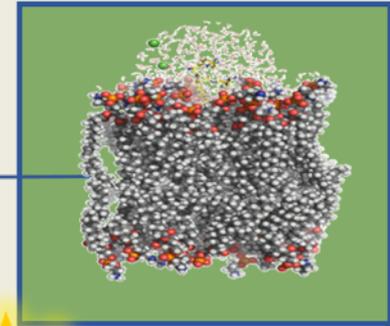
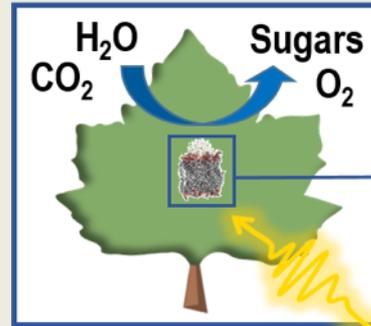
Matter ↔ Field

Matter

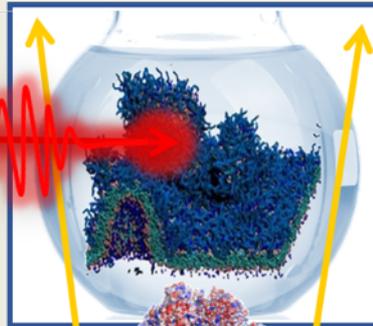
Novel Methods

RT5: Chemical Transformations

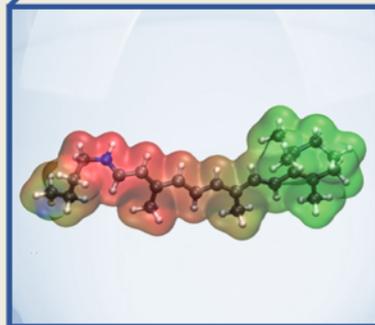
RT6: Multiphase Systems



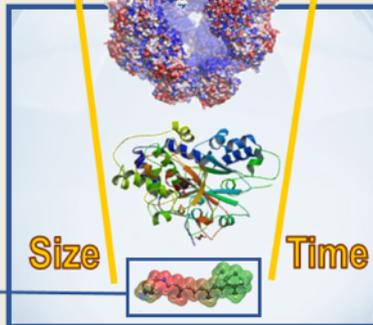
RT3: Spectroscopic Processes



RT4: Extreme Environments



RT1: Electronic Structure

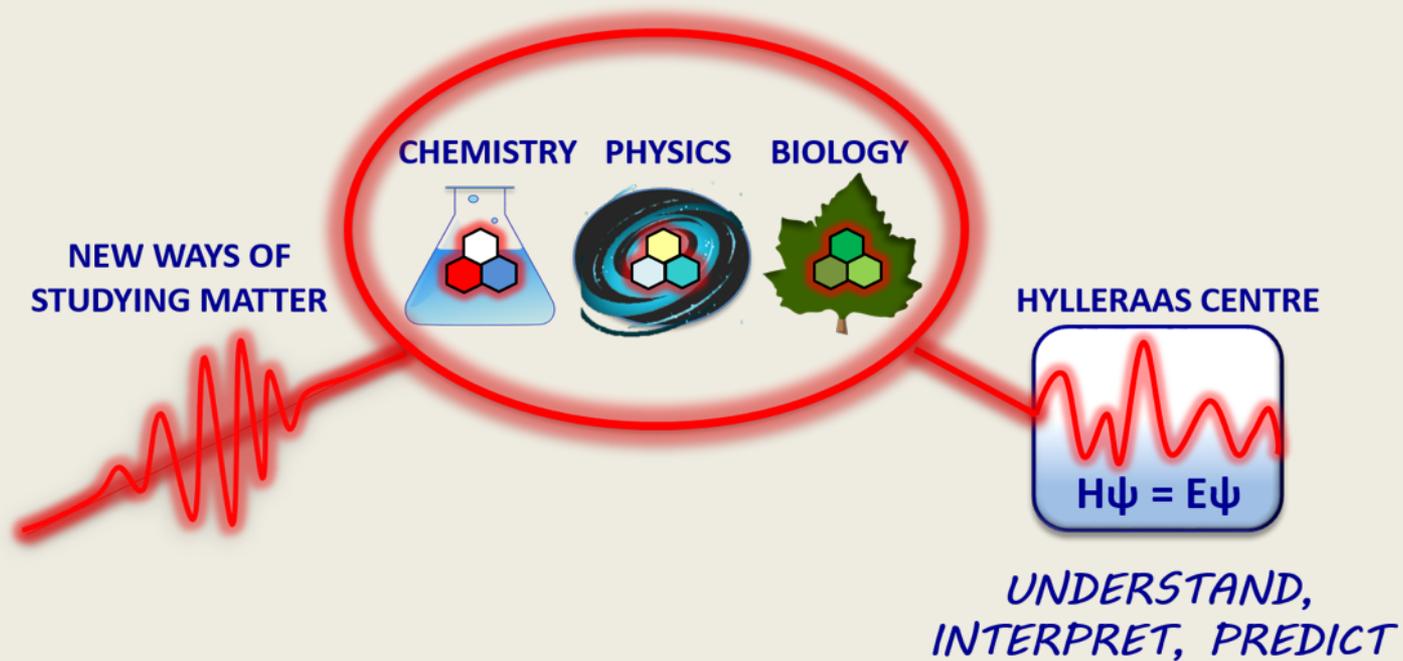


RT2: Multiscale Modelling

Iterative Feedback

Hylleraas Vision

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.



Hylleraas Members

position	total	Oslo	Tromsø	male	female	Norwegian	foreign
leadership and Pis	8	4	4	6	2	3	5
permanent researchers	5	3	2	5	0	1	4
non-permanent researchers	10	4	6	9	1	8	2
postdocs	9	6	3	6	3	2	7
PhD students	22	12	10	16	6	13	9
adjuncts	1	1	0	1	0	0	1
senior engineers	2	1	1	2	0	1	1
administration	2	1	1	1	1	1	1
	59	32	27	46	13	29	30
affiliates	6	4	2	6	0	6	0

For employees Norwegian website Search

Hylleraas Centre for Quantum Molecular Sciences
 UIO : University of Oslo and UiT : The Arctic University of Norway

Home Research topics News and events About **People**

People Norwegian

- Leadership and Administration
- Principal Investigators
- Adjuncts
- Affiliates
- Researchers
- Postdocs
- PhD Students
- Master Students
- Alumni
- Visitors
- Board of Directors
- Scientific Advisory Committee



Group photo (with several guests) at a meeting in Tromsø 2-4 October 2017. Photo: UIO. See the full format.



Group Photo May 2019



Publications — Web of Science

42
2019

64
2018

18
2017

Export Data: Save to Excel File

Total Publications

124 Analyze



2000

2019

h-index

9

Average citations per item

2.95

Sum of Times Cited

366

Without self citations

301

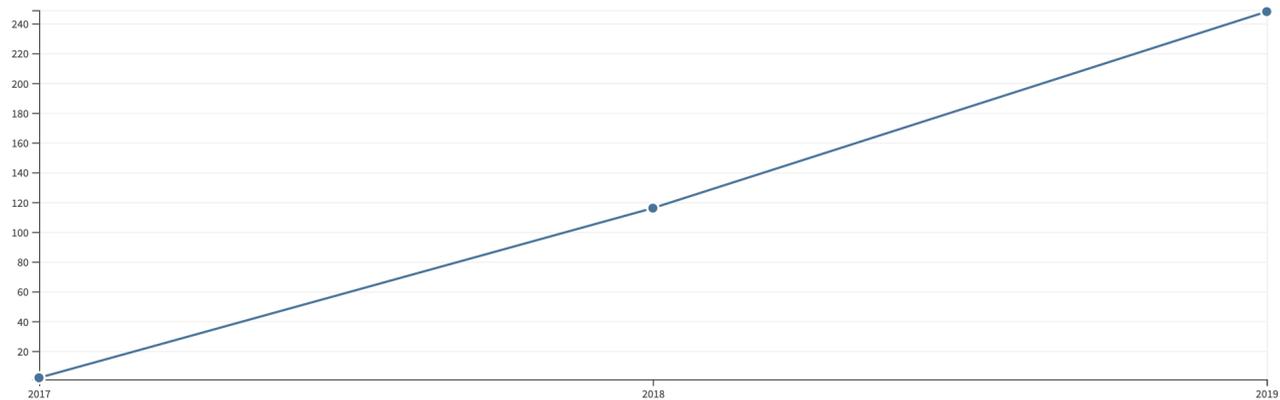
Citing articles

316 Analyze

Without self citations

274 Analyze

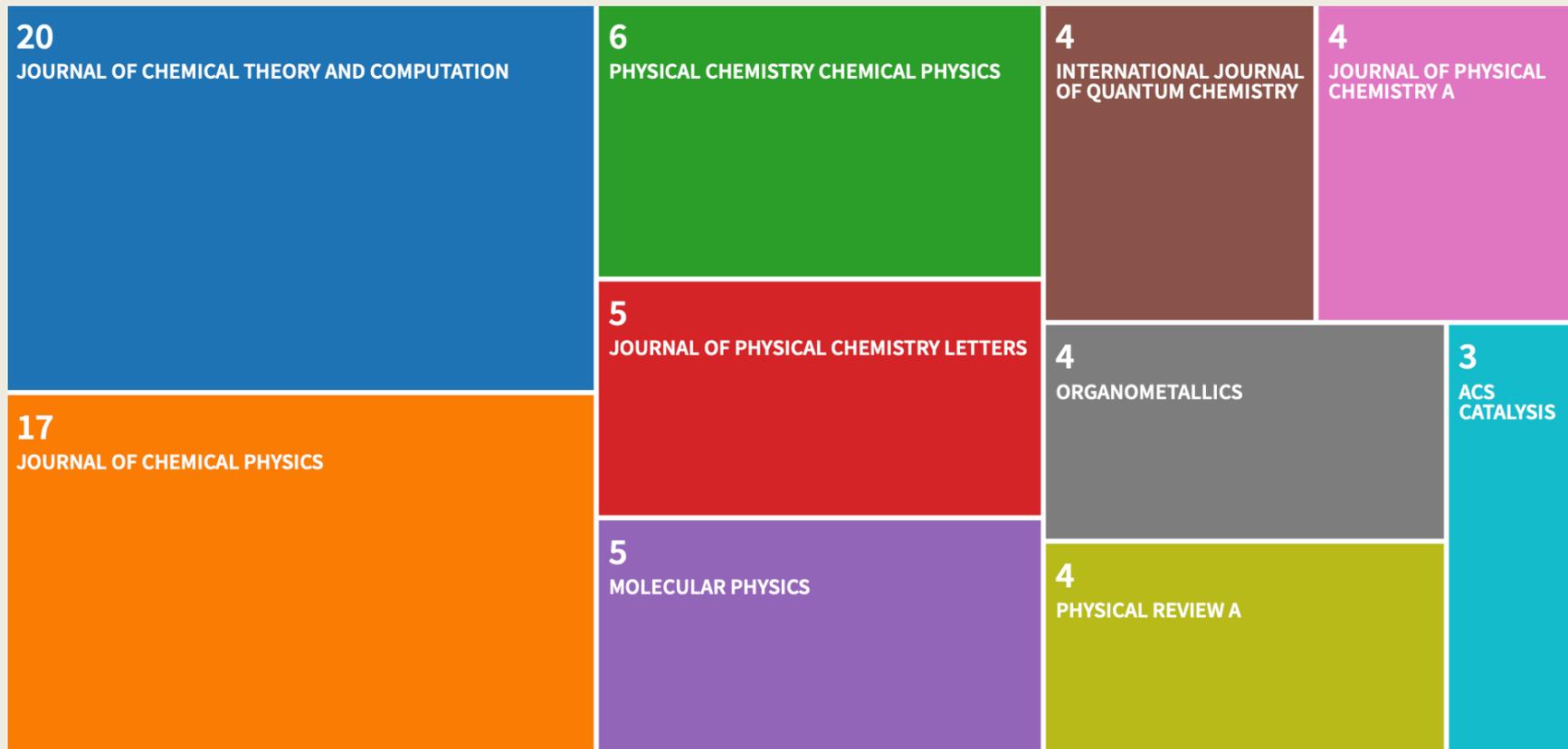
Sum of Times Cited per Year



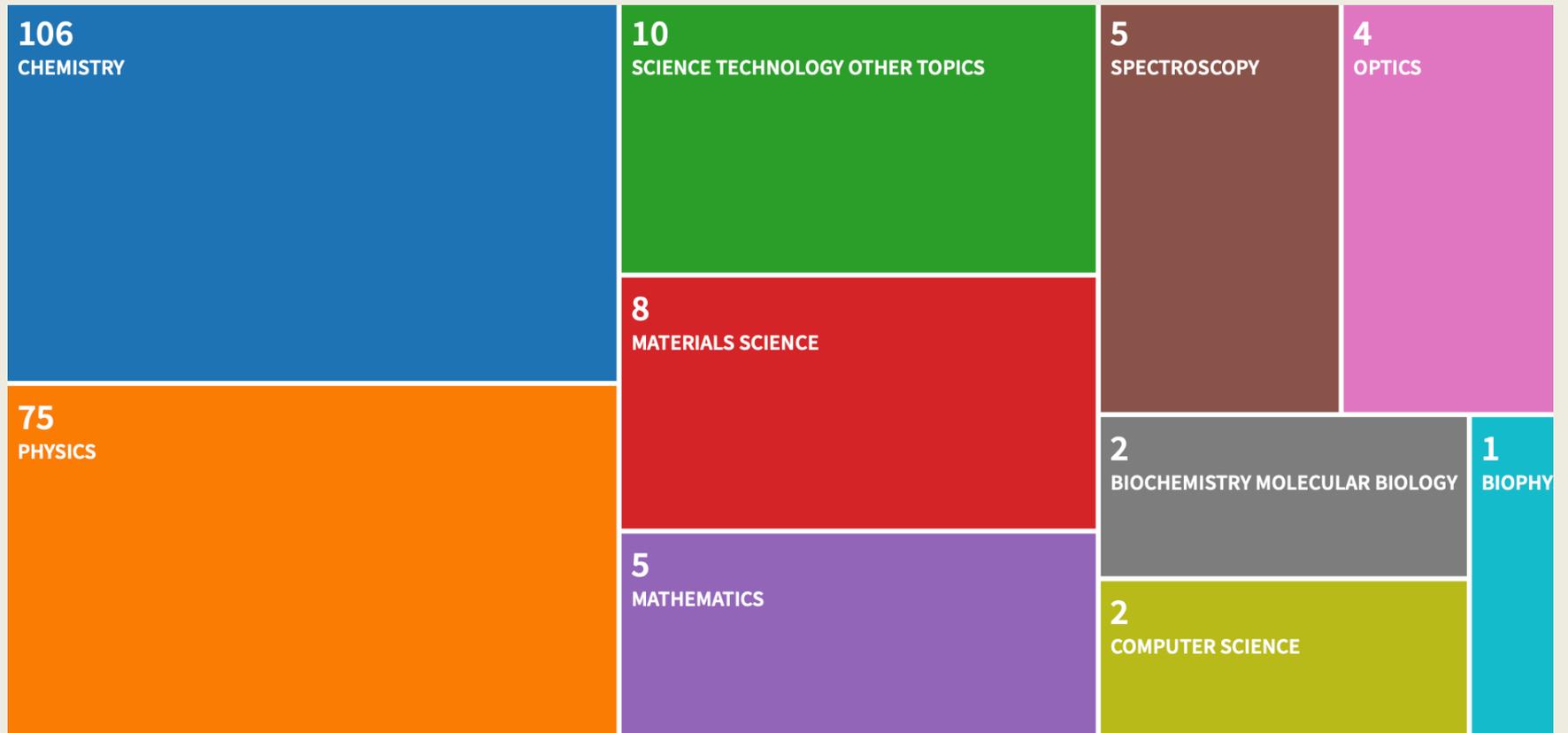
Publications by institution



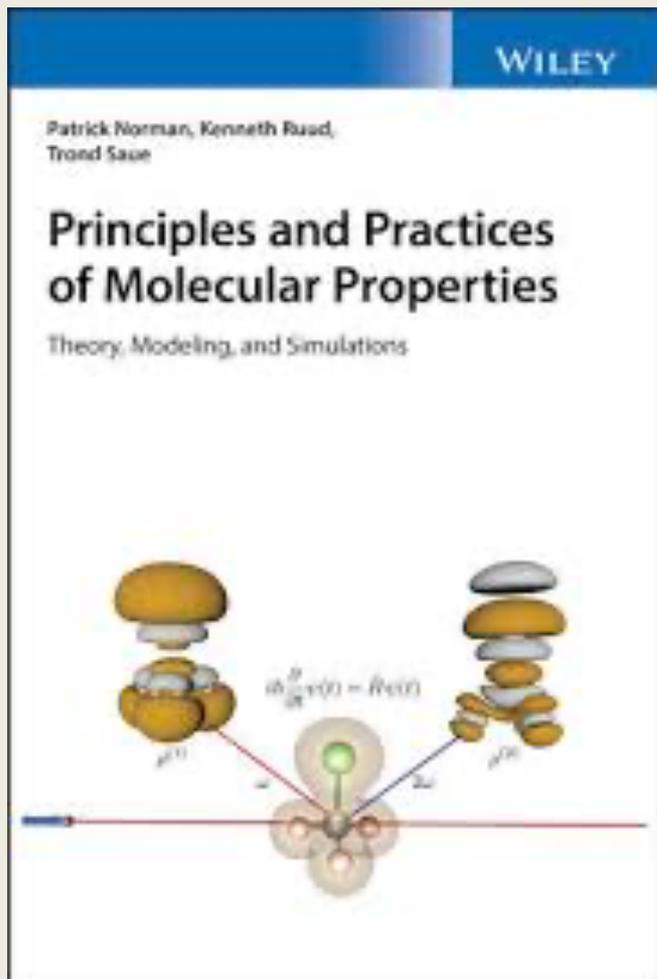
Publications by journals



Publications by areas



Monographs



Principles of Density-Functional Theory

Trygve Helgaker
Department of Chemistry, University of Oslo, Norway

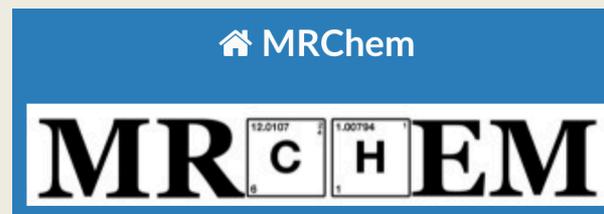
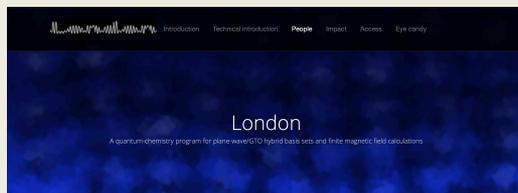
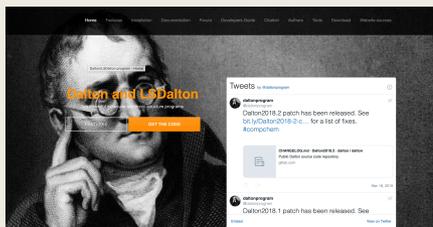
Poul Jørgensen
Department of Chemistry, University of Aarhus, Denmark

Jeppe Olsen
Department of Chemistry, University of Aarhus, Denmark

October 14, 2019

Program Development

- We contribute to several program packages
 - Dalton and associated packages
 - open source distribution
 - two senior engineers



High-Performance Computing

UNINETT

figma2

Services

Access

Support

International

Outreach

Search

Search

About

Services

UNINETT Sigma2 AS manages the national infrastructure for computational science in Norway, and offers services in high performance computing and data storage.

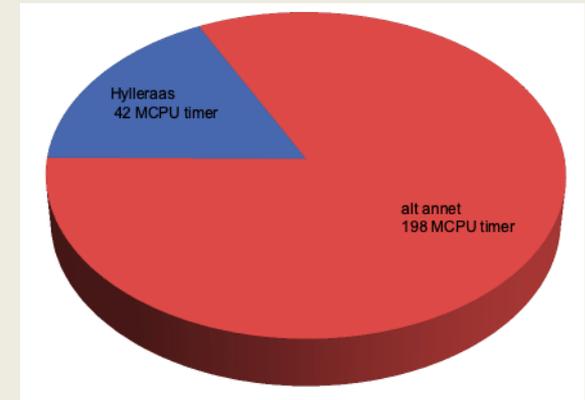
[See our services](#)

Shortcuts

- ▶ [Hardware Live status](#)
- ▶ [Metacenter opslog](#)
- ▶ [Procurements](#)
- ▶ [Research Data Archive](#)
- ▶ [Training](#)
- ▶ [User documentation](#)

Get access

- ▶ [Apply for HPC resources](#)
- ▶ [Apply for storage resources](#)
- ▶ [Apply for AUS resources](#)
- ▶ [Apply for user accounts](#)



News

HPC and storage resources allocated to our researchers

The allocation period 2019.2 starts today, 1 October. Almost 2000 researchers affiliated to nearly 400 research projects are now granted allocations on the national e-infrastructure resources.

[Read more »](#)

Invitasjon til oppstartsmøte for HPC Referansenettverk

Sigma2 har gleden av å invitere til oppstartsmøte i forbindelse med etablering av Referansenettverk for HPC i Norge.

Re

Inte

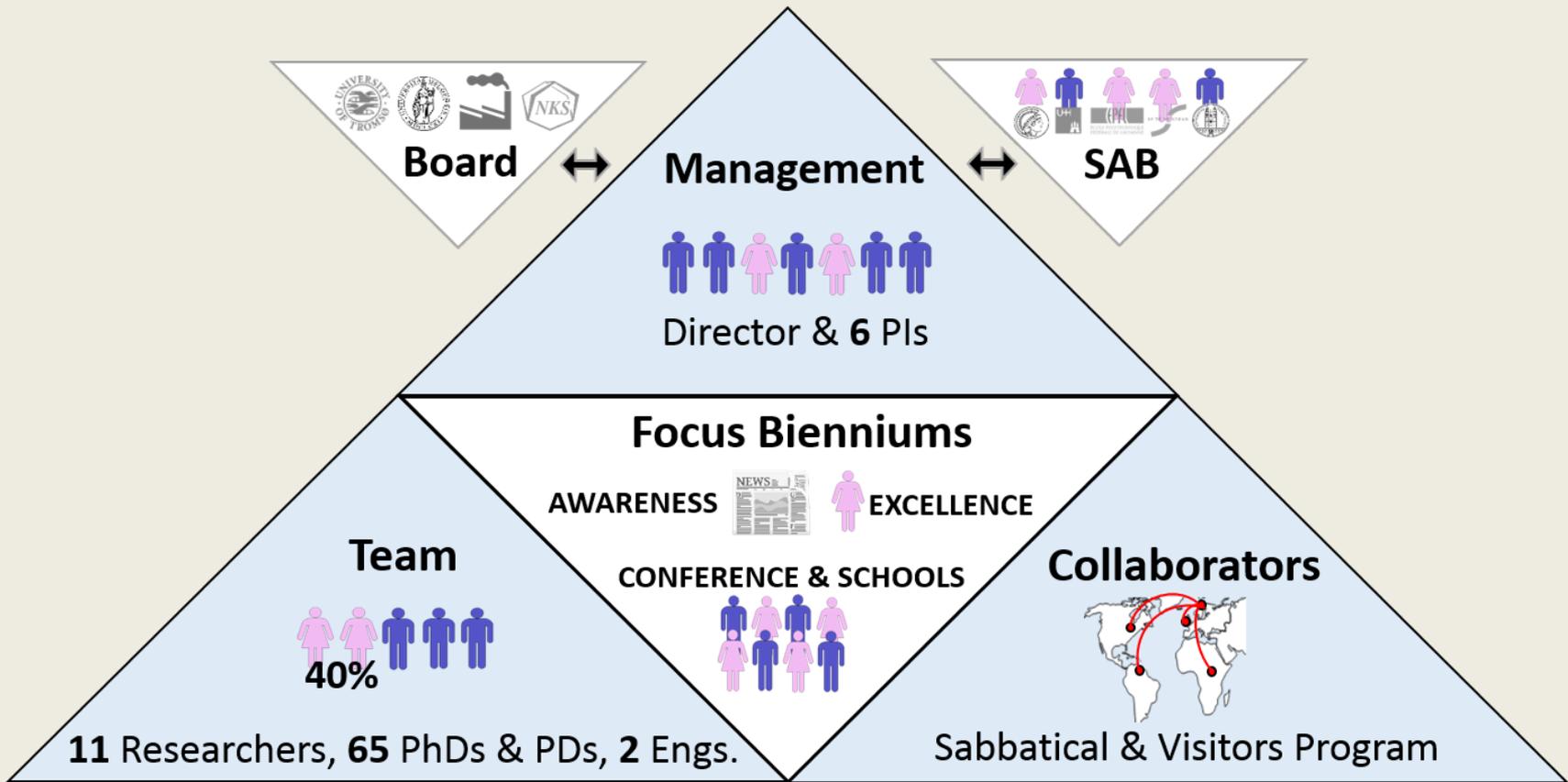
Sigm

Acce

Re

Resource	Job types	Memory	Cores/Node
Abel	P S L	60/1024	16/32
Stallo	P S L	32/128	16/20
Vilje	P L	32	16
Fram	P L	64/512	32

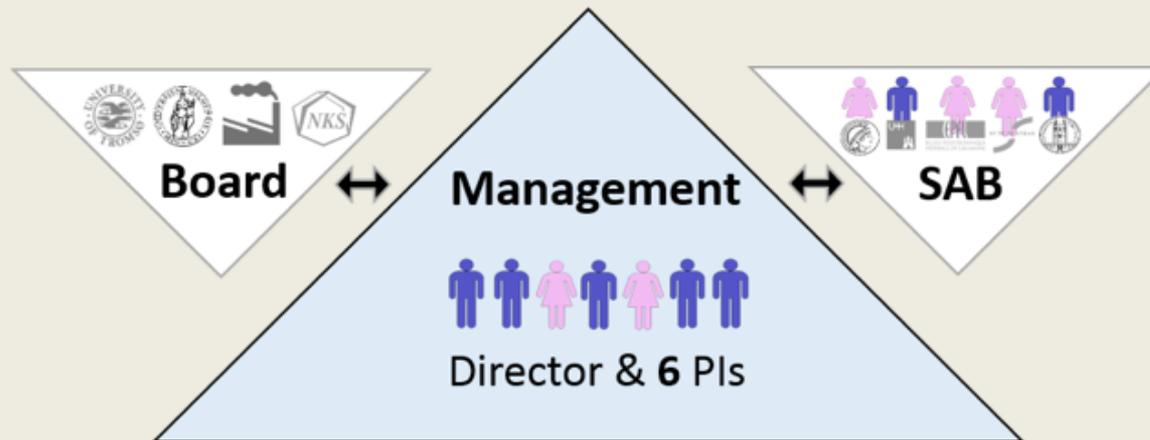
Organization



Outreach	Dissemination	Events	Training
<p>10 HYLLERAAS DAYS</p>	<p>80 VIDEOS >2000 BLOGS&TWEETS</p>	<p>SOFTWARE 600 ARTICLES</p>	<p>4 CONFERENCES 40 SYMPOSIA</p>
		<p>SCHOOLS NATIONAL PHD COURSES</p>	<p>MENTOR PROGRAM</p>

Leadership & Management

- **Director**
 - appointed in an 80%–20% position at the two universities
 - responsibility for all activities and fulfillment of scientific ambitions
- **Management Team of Director, PIs, and two YRP representatives**
 - oversees all research, training, outreach, and dissemination
 - responsibility to allocate resources among RTs
 - identify new projects and promote synergies
 - meet regularly by video conferencing
- **Administration**
 - Heads of Office in Oslo and Tromsø



Boards

- Board of Directors
- Scientific Advisory Committee



Jo Døhl (chair)

Head of Department
Dept. Chemistry
UiO



Camilla Brekke

Professor
Dept. Phys. Tech.
UiT



Nathalie Reuter

Professor
Dept. Bio. Sciences
UiB



Atle Jensen

Professor
Dept. Mathematics
UiO



Kajsa Rytberg-Wallgren

VP Innovation
Yara International



Chantal Daniel (chair)

Professor
Université de Strasbourg



Serena DeBeer

Professor
MPI Mülheim



Ursula Röthlisberger

Professor
EPF Lausanne



Markus Reiher

Professor
ETH Zürich

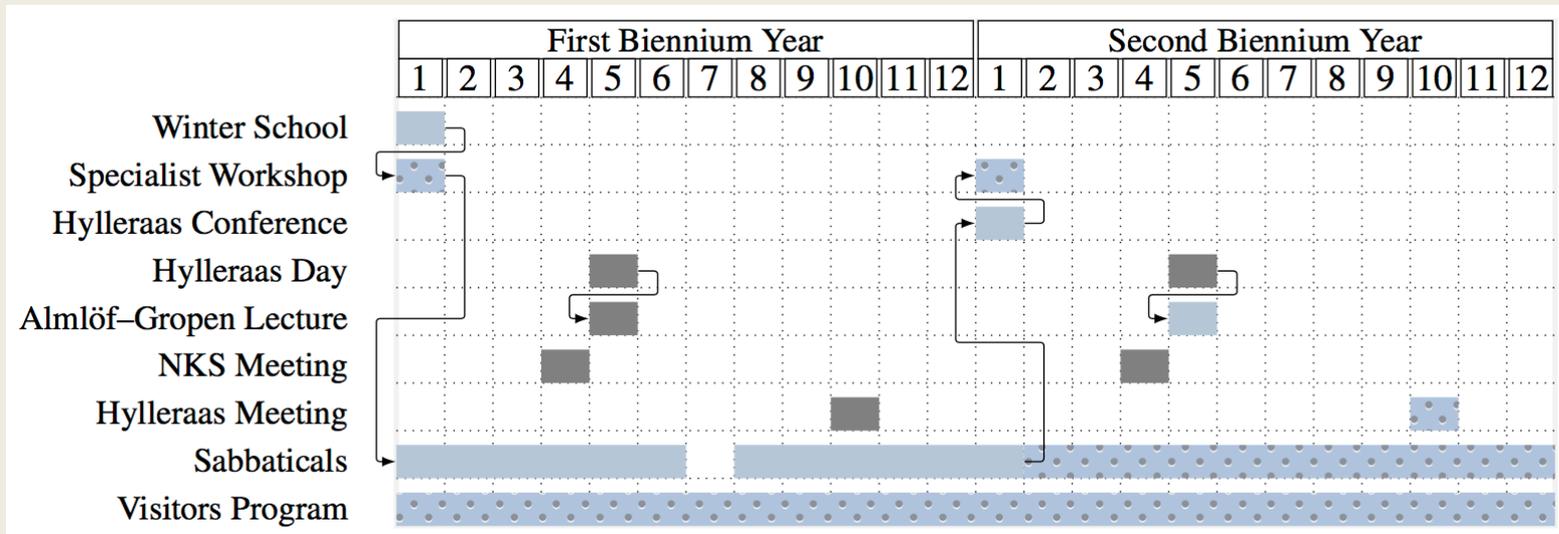


Peter Schmelcher

Professor
Universität Hamburg

Regular Events

- **Weekly seminar series**
 - video transmitted and recorded
- **Biannual Centre Meetings**
 - one internal and one with Norwegian Chemical Society
- **Almlöf–Gropen Lecture**



Meetings and conferences organized

- **CTCC Final Meeting – Hylleraas First Meeting**
 - Clarion Hotel the Edge, Tromsø, October 2–4 2017 (70)
- **Adventures from Numerical Quantum Chemical Methods to Biological Systems and Beyond**
 - Norwegian Academy of Science and Letters, Oslo, January 15–17 2018 (70)
- **Mathematical Methods in Quantum Chemistry**
 - Mathematisches Forschungsinstitut Oberwolfach, Germany March 18–24 2018 (45)
- **Atoms, Molecules, and Materials in Extreme Environments**
 - Norwegian Academy of Science and Letters, Oslo, June 4 – 6 2018 (50)
- **16th International Congress of Quantum Chemistry**
 - Le Palais d'Europe, Menton, France, June 18–23 2018 (500)
- **Do Electron Current Densities Determine All There is to Know?**
 - Holmen Fjordhotell, Asker, July 9–13 2018 (15)
- **Annual Meeting of Division for Quantum Chemistry and Modelling at 21st National Meeting of Norwegian Chemical Society**
 - Norway Trade Fairs, Lillestrøm, October 16–18 2018 (36)
- **Molecular Response Properties winter school**
 - Haraldvollen, Bardufoss, January 14–19 2019 (56)
- **Hylleraas Spring Meeting**
 - Haraldvollen, Bardufoss, May 13–14 2019 (40)
- **10th Congress of International Society for Theoretical Chemical Physics**
 - Clarion Hotel the Edge, Tromsø, July 11–17 2019 (500)
- **Chemistry 2019 – On Hassel's shoulders**
 - Norwegian Academy of Science and Letters, Oslo, November 1–2 2019 (80)



Mobility Programme

- **Mobility Programme**

- glue of the centre and key to success
- initiate and maintain collaborations
- flexible, generous, non-bureaucratic
- cannot be obtained in any other manner



- **Sabbatical Visitors**

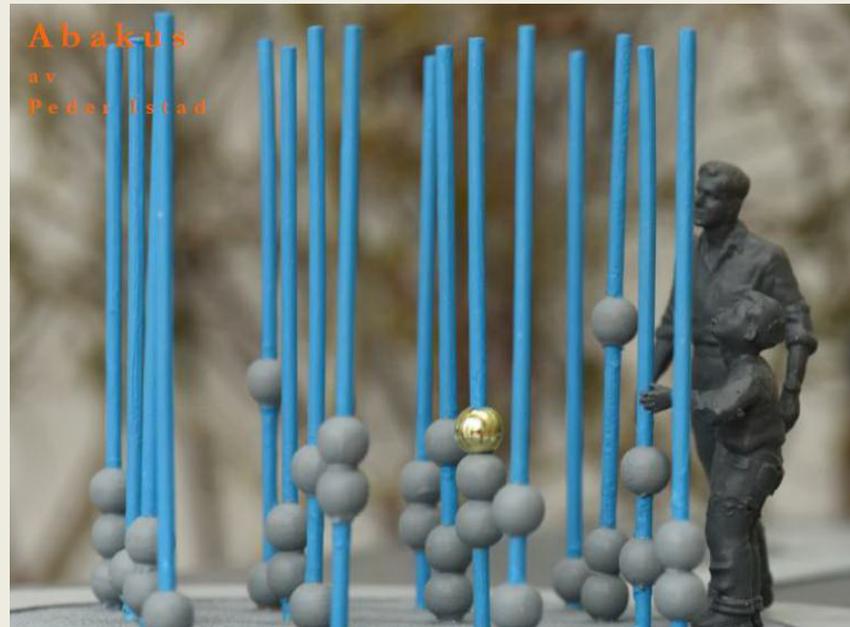
- three or more months at centre
- one full year offered to prominent female scientist at each Biennium

- **Incoming and Outgoing Visitors**

- incoming and outgoing visits
- each PhD student should spend three months abroad

Outreach

- **Almlöf–Gropen Lecture**
 - targeting scientific community
- **Hylleraas Day**
 - targeting general audience
- **Popular Science Articles**
 - all members at least one article
- **Social Media**
 - Facebook, Twitter, YouTube
 - recorded seminars



Engerdal kommune gratulerer Hylleraas Centre

Av: [Gerd Øverstad Galten](#) | Emneord (los) [forsiden](#)

Under Engerdalsdagene 4. august 2017 åpner Engerdal kommune et kunstverk, laget av Peder Istad, i Baggroa til minne om Egil A. Hylleraas. Derfor er det ekstra hyggelige å lese at hans arbeid med den moderne kvantefysikken, nå har fått sin renessanse ved at Hylleraas Centre ved Universitetet i Oslo er blitt tildelt 150 mill.

Almlöf–Gropen Lecture

2008 Prof. Björn Roos
University of Lund, Sweden:
Multiconfigurational quantum chemical methods and heavy element chemistry

2009 Prof. Tom Ziegler
University of Calgary, Canada:
Analyzing complex electronic structure calculations on large molecules in simple chemical terms

2010 Prof. Michele Parrinello
ETH Zürich, Switzerland:
Through mountains and valleys with metadynamics

2011 Prof. Pekka Pyykkö
University of Helsinki, Finland:
Relativity and chemistry: some recent results

2012 Prof. Harry B. Gray
Caltech, 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



© Prof. Jack Simons delivering the Almlöf-Gropen lecture 2017 at the Department of Chemistry, University of Oslo

Almlöf–Gropen Lecturer 2017: Professor Jack Simons

The Wonderful World of Molecular Anions

Professor Jack Simons, University of Utah, was the first Almlöf-Gropen Lecturer at the Hylleraas Centre, presenting

Metal of the International Academy of Quantum Molecular Sciences (1993) and the Joseph O. Hirschfelder Prize in



© Prof. Walter Thiel delivered the Almlöf-Gropen lecture 2018 at the Department of Chemistry, University of Oslo

Almlöf–Gropen Lecturer 2018: Professor Walter Thiel

Chemistry with the Computer

In his lecture, Walter Thiel discussed the current status and prospects of

Hylleraas Day

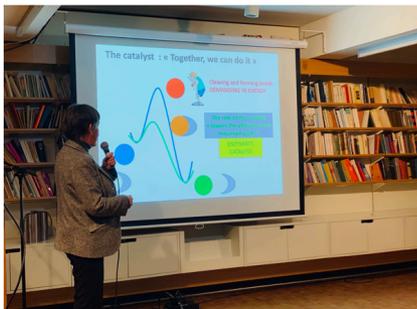
Hylleraas Day 2018 at the Litteraturhuset in Oslo



The first Hylleraas Day was held at the Litteraturhuset in Oslo on 19th November 2018. Following an introduction by the Hylleraas Communication Officer Elina Melteig, members of the Hylleraas Centre gave four short popular talks, covering different aspects of the research at the centre:

- Professor Trygve Helgaker: Utenomjordisk kjemi
- Professor Kennet Ruud: Relativt god kjemi
- Professor Odile Eisenstein: Bærekraftig kjemi via modellering
- Professor Bjørn Olav Brandsdal: Kuldetilpasninger

These presentations were followed by a lively forum, with questions from the audience.



Hylleraas day 2019

The Hylleraas centre will present the life and science of the Norwegian research pioneer Egil Hylleraas, followed by short popular-scientific accounts of the research activity of the centre.

Time and place: Sep. 21, 2019 12:15 PM–2:30 PM, [Tromsø Museum](#)

Program

12.15: *Egil Hylleraas — A Pioneer of Computational Quantum Mechanics.*

Presented by: *Trygve Helgaker, University of Oslo*

The Norwegian physicist Egil A. Hylleraas (1898–1965) performed a number of pioneering computational studies in the early days of quantum mechanics, including accurate calculations on helium (confirming the validity of quantum mechanics for two particles) and the first calculation of the cohesive energy of a crystal. Many techniques introduced by Hylleraas are in use today. In this talk, an overview is given of the life and career of Hylleraas, the founding father of quantum chemistry in Norway.

13.00 Short break, with free coffee and cake

13.15: Science at the [Hylleraas centre](#)

- *Trygve Helgaker (UiO):* Ekstreme magnetfelt — kjemiens forvandling
- *Kenneth Ruud (UiT):* Relativt god kjemi
- *Bjørn Olav Brandsdal (UiT):* Kuldetilpasninger
- *Ainara Nova (UiO):* Can we transform carbon dioxide into something useful?

Young Researchers

- Total of 23 PhDs and 34 postdocs to be trained
 - 18 PhDs and 18 postdocs funded from basic RCN and UIO/UiT funding
 - the remaining to be externally funded grants
- Important elements for young PhDs and PDs
 - biennial PhD courses offered to all Norwegian Universities
 - PhD training organized as research school
 - a generous visitors and sabbatical program
 - career development plans
 - mentoring program
- Young researchers are important at the Hylleraas centre
 - excellent young people will generate their own projects



The Research Council
of Norway

Career Development Program

- **We have initiated project for improved career development**
 - Career Development Program (CDP) — Michele Cascella & Kathrin Hopmann
 - Karriereutviklingspilotprogram (KUPP 2018) at University of Oslo
 - Two full-day meetings
 - Elements of CDP will be introduced in the second half of 2019
- **Three phases of career development**
 - **onboarding**: introduction to centre of newcomers
 - **ongoing**: support for success in your work at the centre through ownership
 - **outgoing**: preparation for the next step — inside or outside of academie
- **Set up Young Researcher Parliament**
 - two representatives at all MT meetings
 - take part in all centre activities and initiate own actions

Female Centre Membres

- **Field dominated by men**

- 25–30% female enter the field
- little national recruitment



Prof. II
CTCC

- **CTCC**

- four female adjunct professors
- talented female postdocs
- FemEX conference series



Young
Research
Talents
CTCC

- **Hylleraas Centre**

- 2 of 6 PIs are women
- female sabbatical visitors
- mentor program
- aiming for 40%–60% balance



Principal
Investigators
Hylleraas

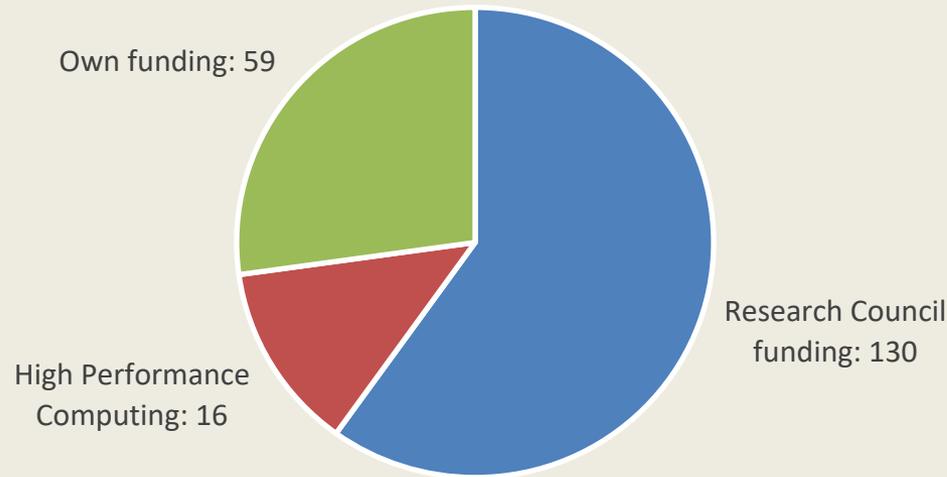
Did You Think?

- Exhibition in Tromsø
 - Kathrin Hopmann,
 - Karen Dundas



Funding over 10 years

- **Basic funding: 205 MNOK** = 130 (RCN) + 16 (HPC) + 37 (UiO) + 22 (UiT)
 - UiO = 37 MNOK = 20 MNOK + 6 PhDs
 - UiT = 22 MNOK = 1/3 of 65 MNOK



- **External funding:**
 - more than 100 MNOK so far secured for the first five years
 - 33.6 + 29.1 + 21.9 + 13.0 + 8.9

Cost Items Basic Funding

Cost Item	annual cost / MNOK
directors & adjunct PI (50%)	2.7
heads of office & communication officer	1.5
PhDs and postdocs	10.5
mobility	3.0
regular events	0.7
expenditure	0.6
HPC	1.6
	20.6

salary PhDs and postdocs: $10.5 = 4.5 \text{ (RCN)} + 3.7 \text{ (UiO)} + 2.3 \text{ (UiT)}$

Personnel on RCN basic funding

UiO	Centre Director	Trygve Helgaker	100
	Head of Office	Jan Ingar Johnsen	100
	Communication officer	Elina Melteig	20
	Principal investigator	Odile Eisenstein	50
	Researcher	David Balcells	100
	PhD student	Julie Héron	100
UiT	Head of Office	Stephanie Hansen	50
	Researcher	Peter Wind	30
	Postdoc	Lukas Konecny	100
	Postdoc	Magnus Olsen	100
	PhD student	Marc Joosten	100

In-kind contributions

UiO	Principal investigator	Michele Cascella	50
	Principal investigator	Thomas B. Pedersen	50
	Researcher	Simen Kvaal	100
	Adjunct Professor	Andrew Teale	20
	Software Engineer	Simen Reine	100
UiT	Deputy Director	Kenneth Ruud	100
	Principal investigator	Bjørn-Olav Brandsdal	50
	Principal investigator	Luca Frediani	50
	Principal investigator	Kathrin Hopmann	100
	Researcher	Bin Gao	100
	Software Engineer	Michal Repisky	100

In-kind contributions: 96 MNOK

5 PIs and 1 Associate Professor (50% positions)
normal teaching duties except directors
2 senior engineers (100% positions)

Externally Funded Projects

- **External projects are essential for our research programme**
 - externally funded projects complement internally funded projects
 - designed with respect to potential for cross-links and synergies
 - needed to meet our deliverables training (PhD and postdocs)
- **Responsibility of Management Team & RT Leaders**
 - all members expected to apply for funding
- **Target for external funding**
 - ERC, MSCA, RCN, CAS, TFS



The Research Council
of Norway



New Projects since 1st October 2017

- **A Topological Approach to Density-Functional Theory (topDFT)**
 - ERC Consolidator Grant 2018–2023, Teale, 2 MEuros
- **The Nordic Consortium for CO₂ Conversion (NordCO₂)**
 - NordForsk Nordic University Hub Grant, 2018–, Hopmann, Nova and Cascellaa
- **Evolutionary Principles of Biocatalysts from Extreme Environments**
 - RCN FRIPRO ToppForsk, 2018–2023, Brandsdal, 12.5 + 17.4 MNOK
- **Multi-Resolution Methods for Soft-Matter Systems**
 - DFG Collaborative Research Centre TRR 146, 2018–2023, Cascella and Gauss
- **Digital Discovery of Antimicrobial Molecules from Marine Artic Resources with reduced Risk of Triggering Resistance**
 - RCN Digital Life Programme, 2018–2023, Svendsen, Ruud and Brandsdal
- **A Posteriori Error Estimates for Coupled-Cluster Theory**
 - Peder Sather Centre for Advanced Study, Berkeley 2018–2019, Faulstich, Kvaal and Lin
- **Error Estimates for Coupled-Cluster Methods, Ground and Excited States**
 - RCN YRT, 2019–2022, Laestadius 8MNOK
- **Magnetic Chemistry**
 - RCN FRIPRO, 2019–2022, Helgaker, 10MNOK
- **Optical Probe Sensors at Biological Environments,**
 - SiU Russia Cooperation Programme, 2018–2020, Ruud, Beerrepot, Frediani and Helgaker,
- **Attosecond Quantum Dynamics Beyond the Born–Oppenheimer Approximation**
 - Centre for Advanced Study (CAS), 2021–2022, Kvaal and Pedersen
- **Cooperation Towards a Sustainable Chemical Industry (CO₂PERATE)**
 - H2020 MSCA-ITTN, Hopmann, Frediani, Nova, Balcells, aand Cascella

External Projects

Project		RT	Project leader	2017	2018	2019	2020	2021	2022	
Molecular spin frustration	RCN YRT	RT4	Erik Tellgren	2,1	1,8	0,2			<	4,1
Coupled cluster methodes for periodic systems	RCN FRIPRO	RT1	Thomas B. Pedersen	2,0	2,2	0,8				5,0
Rational catalyst design for transforming CO2	RCN YRT	RT5	Ainara Nova	1,9	2,4	1,9	0,2			6,4
Eeny, meeny, miny, moe	RCN	RT5	Kathrin Hopmann	0,2	0,3					0,5
Stochastic methods for molecular chiroptical properties	RCN Mobility	RT3	Roberto Di Remigio	0,5	0,9	1,0	0,8			3,2
New dimensions in theoretical multiphoton spectroscopy	RCN	RT3	Kenneth Ruud	0,9	3,4	1,7	0,4			6,4
Response theory for advanced spectroscopic experiments	RCN Mobility	RT3	Magnus Ringholm		0,6	0,9	1,0	0,7		3,2
Evolutionary principles of biocatalysts from extreme environments	RCN Toppforsk	RT6	Bjørn Olav Brandsdal		0,5	3,0	3,3	3,1	1,9	11,8
Magnetic chenistry	RCN FRIPRO	RT4	Trygve Helgaker			0,8	3,5	3,7	2,0	10,0
Error estimates for coupled-cluster methods, ground states and excited states	RCN YRT	RT1	Andre Laestadius			0,1	2,1	2,4	2,4	7,0
DigiBiotics	RCN	RT3	John S. Svendsen			1,2	1,2	1,2	1,4	5,0
Hydrogen bond strengths for large molecules	RCN YRT	none	Heike Fliegl	1,3	0,7					2,0
The chemistry of CO2 activation and fixation	RCN FRIPRO	none	Einar Uggerud	2,8	3,3	2,4	0,4			8,9
				11,7	16,1	14,0	12,9	11,1	7,7	73,5
Bivariational approximation in quantum mechanics and applications to qauntum chemis	ERC StG	RT1	Simen Kvaal		3,9	2,8	2,2			8,9
Hybrid particle-field approach including electrostatics for large-scale simulations of bi	MSCA IF	RT2	Kolli / Cascella		0,7					0,7
Computational modelling and design of sustainable catalysts for water oxcdiation	FP7 CIG	RT4	Balcells / Helgaker		0,5					0,5
Spectra of molecules in strong magnetic fields	MSCA IF	RT4	Sen / Tellgren		0,9		1,1			2,0
Relativistic and dynamic effects in computational NMR spectroscopy of transition-met	MSCA IF	RT3	Castro / Caascella			1,2	0,6			1,2
Cooperation towards a sustainable chemical industry	MSCA ITN	RT5	Kathrin Hopmann							0,0
					6,0	4,0	3,3			13,3
Catalysts for homogeneous conversion of CO2	TRS	RT5	Kathrin Hopmann	4,2	4,5	4,1	2,1			14,9
Optical probe sensors at biological environments	DIKU	RT3	Kenneth Ruud		0,4	0,7	0,8			1,9
Molecules in extreme environments	CAS	RT4	Trygve Helgaker							
Do electron current densities determine all there is to know?	YoungCAS	RT4	Andre Laestadius							
Multi-resolution methods including quantum chemistry	CRC TRR DFG	RT2	Cascella / Gauss							
Nordic consortium for CO2 conversion	NordForsk	RT5	Kathrin Hopmann	2,6	6,6	6,3	2,8	1,9	1,2	21,4
Attosecond quantum dynamics beyond the BO approximation	CAS	RT1	Pedersen / Kvaal							
				6,8	11,5	11,1	5,7	1,9	1,2	38,2
				18,5	33,6	29,1	21,9	13,0	8,9	125,0

Centre For Advanced Study (CAS)

Centre for Advanced Study
at the Norwegian Academy of Science and Letters

- *Molecules in extreme environments*
 - T. Helgaker
 - 2017–2018 (10 ½ months)
- *Do electron densities determine all there is to know?*
 - André Laestadius
 - 2018 (one week)
- *Attosecond quantum dynamics beyond the Born–Oppenheimer approximation*
 - Simen Kvaal, Thomas Bondo Pedersen
 - 2021–22 (10 ½ months)



Key Performance Indicators after 4 (10) [so far] Years

- **Publications:**
 - 260 (500) [140] articles, 750 (6000) [360] citations
- **Grants:**
 - on average two [4] RCN FRIPRO running at any given time
 - 2 (4) [none] to pass first stage ERC grants
 - 1 (3) [1] MSCA-ITN and 3 (8) [2] MSCA-IF grants with score above 85%
 - total income of 15 (45) [35] MNOK
- **Students:**
 - 7 [4] (23) PhD students and 14 [10] (34) postdocs
- **Events:**
 - 2 [1] (4) Winter Schools, 3 [1] (10) Specialist Workshops
 - 1 [4] (4) Conferences, 8 (20) [3] Centre Meetings
 - 4 [0] national PhD course, each given 1 (3) times
- **Gender Balance:**
 - 30% [21%] female members at all times and 40%–60% balance after 10 years

Egil A. Hylleraas (1898–1965)

- **Egil Hylleraas — a pioneer of computational quantum mechanics**
 - confirmed validity of quantum mechanics for more than one particle (1929)
 - predicted the stability of hydrogen anion, later detected on the Sun (1930)
 - first quantum-mechanical study of a molecular crystal LiH (1930)
 - introduced many now-standard techniques of quantum chemistry

The image is a composite graphic with a light green background. At the top center, there is a complex mathematical equation involving multiple integrals and partial derivatives, representing the Schrödinger equation for a two-particle system. Below the equation, the text "mit der Nebenbedingung" is written. To the left, there is a small black and white portrait of a young man in a suit and tie. In the center, the name "Egil A. Hylleraas" is written in a cursive script. Below the name, the text "a pioneer of computational quantum mechanics" is written in a bold, sans-serif font. At the bottom center, there are two small circular portraits: one of a woman and one of a man in a suit. On the right side, there is a large, semi-transparent portrait of an older man with a friendly expression, smiling.

Information about Hylleraas Centre

For employees Norwegian website

Hylleraas Centre for Quantum Molecular Sciences

UiO · University of Oslo and UiT · The Arctic University of Norway

Home Research topics News and events About People



Hylleraas

Our research

We develop and apply methods to simulate complex molecular systems interacting with fields and radiation.

Events

25 [Advanced experimental optical spectroscopy](#)
Jan. 3:00 PM, Tomsk State University
[Add to calendar](#)

26 [Advanced experimental optical spectroscopy](#)
Jan. Tomsk State University
[Add to calendar](#)

27 [Advanced experimental optical spectroscopy](#)
Jan. Tomsk State University
[Add to calendar](#)

[→ All events](#)

People

- Leadership and Administration
- Principal Investigators
- Researchers
- Postdocs
- PhD Students

Vacancies

- [Postdoctoral Research Fellowships in Theoretical Chemistry](#)
Hylleraas Centre for Quantum Molecular Sciences -
The Faculty of Mathematics and Natural Sciences
Deadline: Thursday, October 31, 2019
- [Postdoctoral Research Fellowships in Theoretical Chemistry/Applied Mathematics](#)
Hylleraas Centre for Quantum Molecular Sciences -
The Faculty of Mathematics and Natural Sciences
Deadline: Sunday, November 17, 2019



Hylleraas

Annual report 2018
Report title here

 **UiO · University of Oslo**

 **Norwegian Centre of Excellence**
The Research Council of Norway

Hylleraas Vision

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.

