

Hylleraas Centre for Quantum Molecular Sciences

Kjemibygningen / "Chemistry Building" UiO. 22. Juni 2018

Trygve Helgaker and Kenneth Ruud

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New Tools, Opportunities and Discoveries

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Innholdsfortegnelse

Motivation

Challenges

Research

Leadership

Organization

Hylleraas Centre

Objectives

Research

Themes

Staff

Focus Bienniums and Regular Events

Funding over 10 years

Expenses over 10 years (MNOK)

10-Year Budget

Agenda

Motivation

Challenges & Research

Leadership

Focus Bienniums & Regular Events

- **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

Objectives

- **Primary Objective**

- Develop an integrated approach to the investigation of complex molecular systems in electromagnetic fields and extreme environments

- **Secondary Objectives**

- Develop accurate, reliable, scalable electronic-structure methods for complex systems
- Develop multiscale methods with quasi-atomistic/mesoscale resolution, spanning orders of magnitude in space and time
- Develop novel multiscale methods for calculating and predicting new spectroscopies in strong fields and short pulses
- Develop models and understanding of the squeezed chemistry of extreme magnetic fields and pressure
- Develop new computational approaches to optimize and control chemical transformations
- Understand the structure and dynamics of macromolecules at membranes and interfaces
- Train a new generation of theoretical chemists
- Establish national courses in theoretical chemistry
- Provide new software to the international community at no cost

“As far as the laws of mathematics refer to reality, they are not certain; and as far as they are certain, they do not refer to reality.”

— Albert Einstein

“The cosmos is within us. We are made of star-stuff. We are a way for the universe to know itself.”

— Carl Sagan



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