

Centre for Theoretical and Computational Chemistry

Trygve Helgaker

Department of Chemistry, University of Oslo

Holmen Fjordhotell

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Chemistry and computation

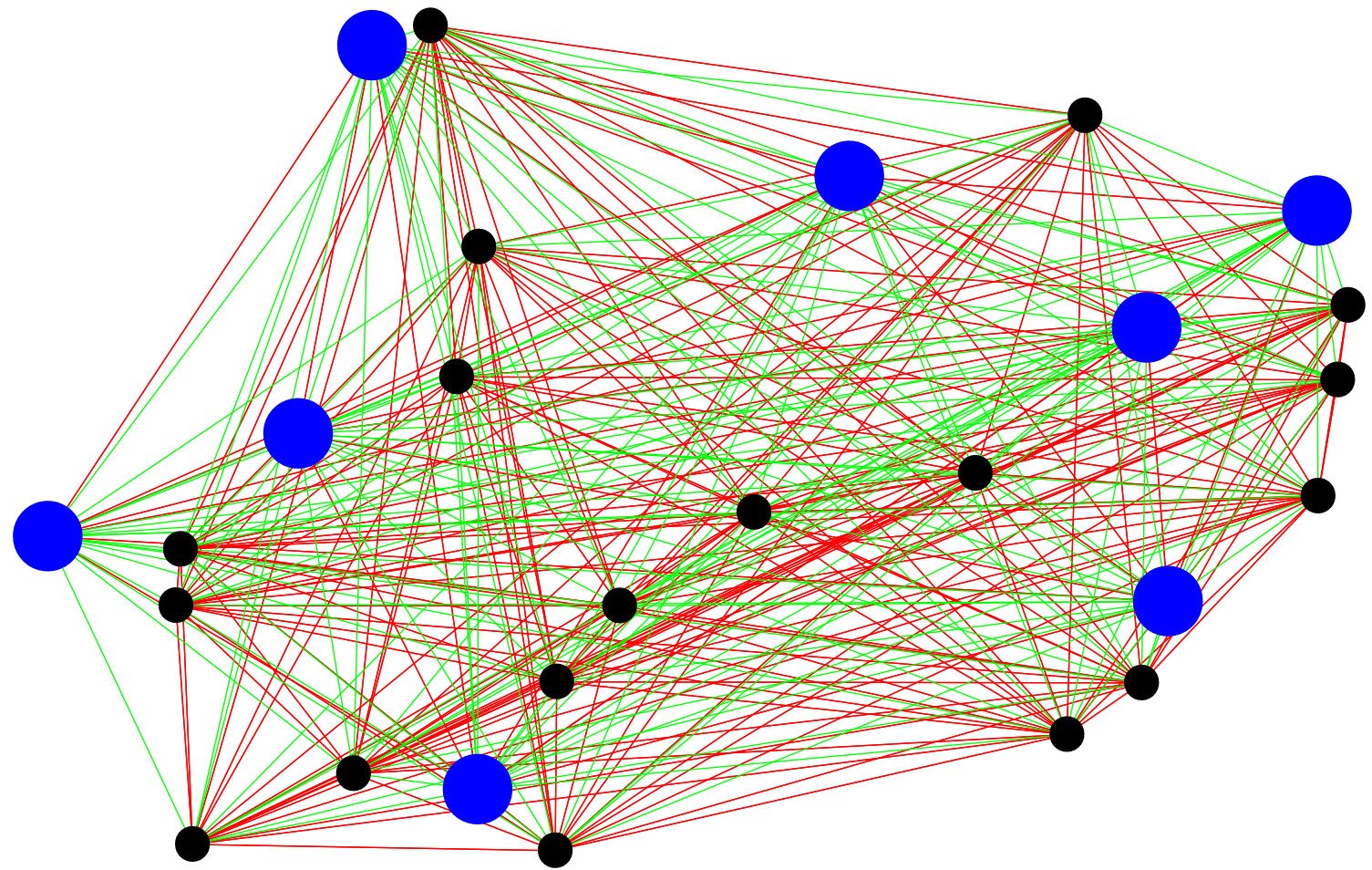
“Every attempt to employ mathematical methods in the study of chemical questions must be considered **profoundly irrational**. If mathematical analysis should ever hold a prominent place in chemistry—an aberration which is happily impossible—it would occasion a rapid and widespread degradation of that science.”

August Comte, 1748–1857

“The underlying physical laws necessary for the mathematical theory of a large part of physics and **the whole of chemistry** are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble.”

P. A. M. Dirac, 1902–1984

Quantum mechanics and the many-body problem



The electronic computer—the quantum chemist's tool

- The solution came in an unexpected manner, with the emergence of the computer
- ENIAC (Electronic Numerical Integrator and Computer) (1946)
 - the first large-scale electronic digital reprogrammable computer
 - 30-ton collection of 19 000 vacuum tubes (357 multiplies per second)



- four of the six main programmers of ENIAC

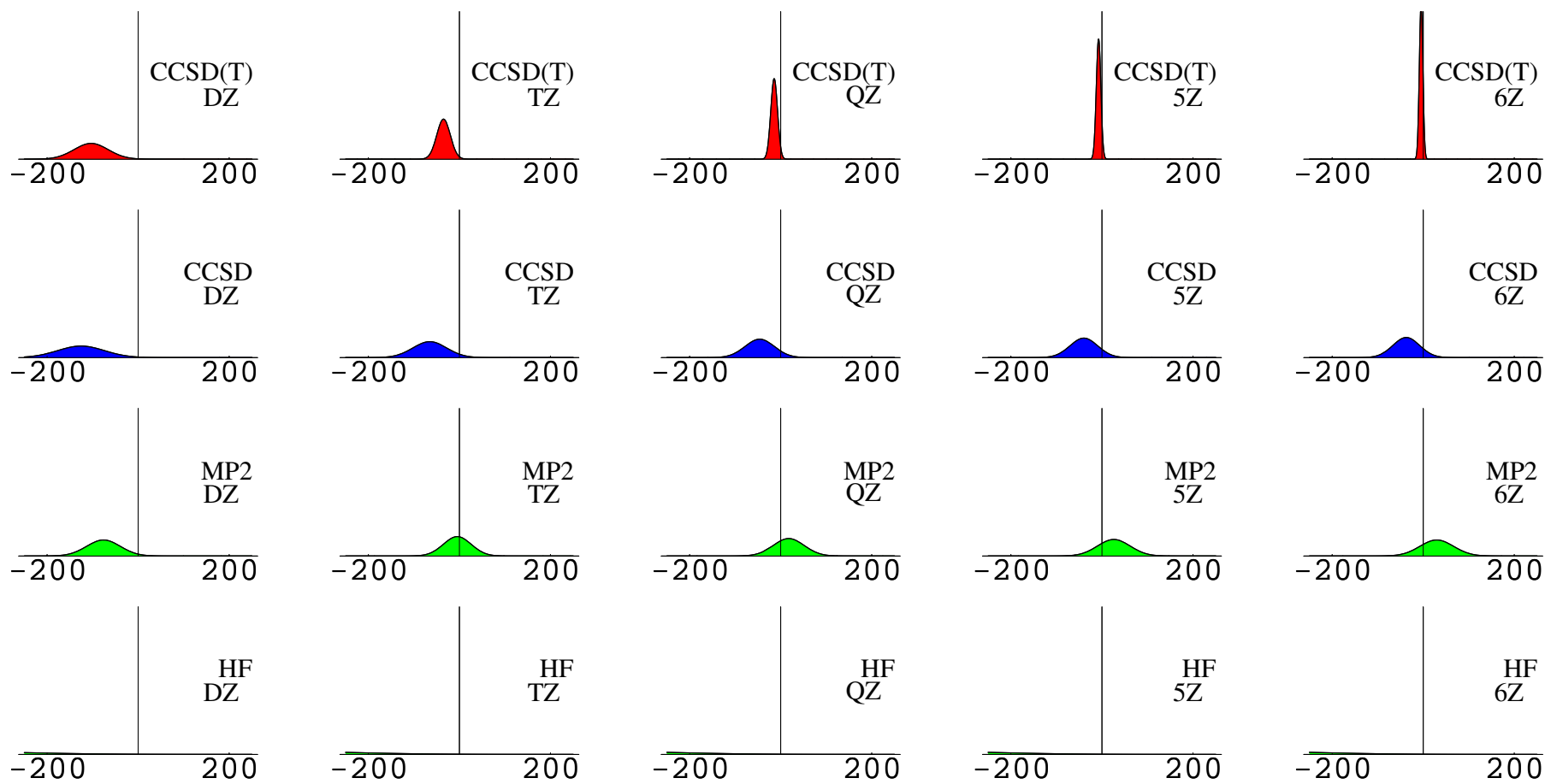
The electronic computer—the quantum chemist's tool

- Over the last 50 years, computers have developed in a spectacular fashion,
 - Moore's law: the capacity of computers double every two years, at no extra cost
 - computers are now 10000 more powerful than one generation ago



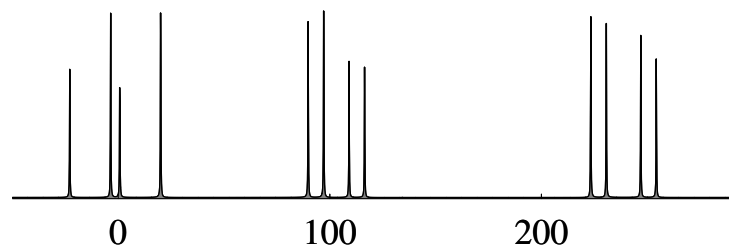
- With this amazing tool at their disposal, chemists have diligently developed new computational techniques: quantum chemistry
 - the development of refined models of chemical electronic systems
 - their solution using advanced methods of numerical analysis
 - their implementation on the latest computer hardware
- The exact solution is beyond reach but can be approached systematically
 - the “insoluble” problem is being solved every day—by nonspecialists!

Atomization energies (kJ/mol)

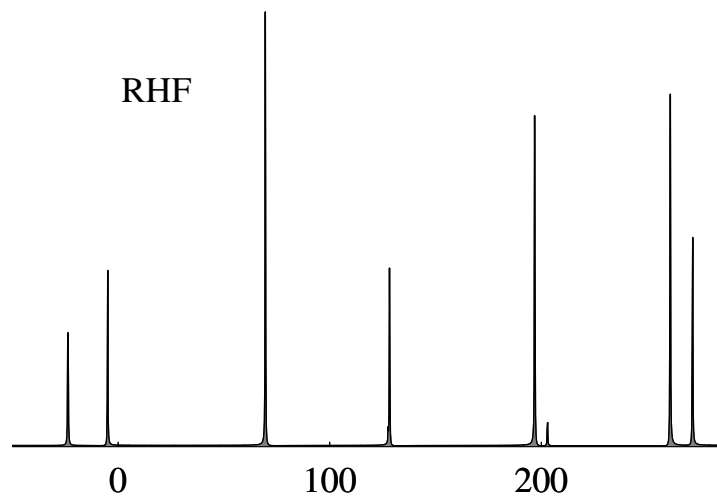


200 MHz NMR spectra of vinyl lithium

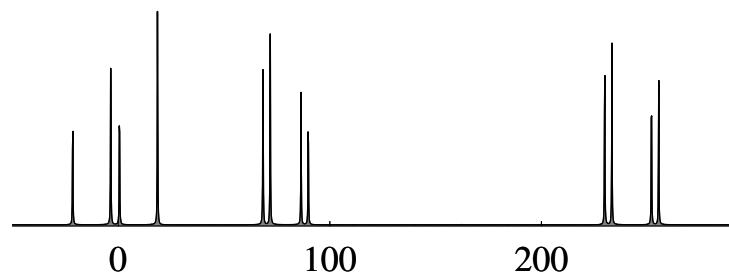
experiment



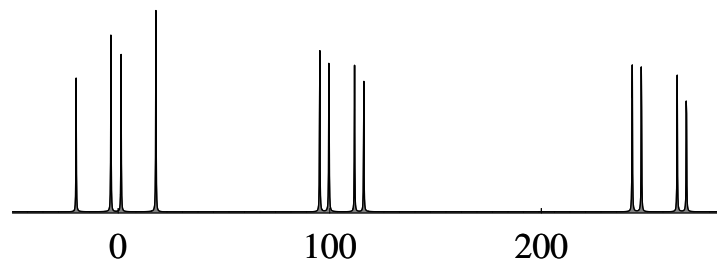
RHF



MCSCF



B3LYP

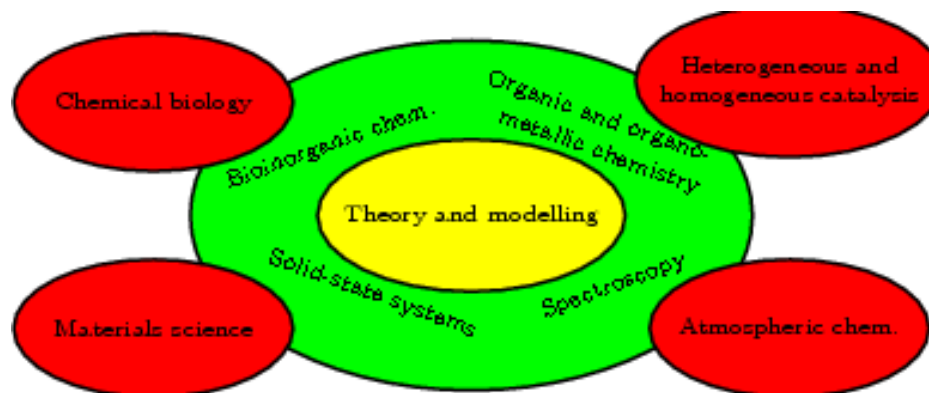


New Challenges

- Today quantum chemistry has become an integral part of modern chemistry
 - used by specialists and nonspecialists alike
 - for prediction, elucidation, explanation and confirmation
 - **Computational Science** has become an important area of modern science
- But, chemistry itself is in constant change
 - biochemistry
 - materials science
- This development provides ever new challenges to quantum chemistry
 - we must prepare ourselves for tomorrow's important problems
- Quantum chemistry is an interdisciplinary science
 - theory, experiment, computation
 - chemistry, physics, mathematics, computer technology
- The future of quantum chemistry requires knowledge of all these areas!

CTCC: Theory and Modeling

- CTCC has therefore been established as a collaborative effort



- five senior researchers and one affiliated from the University of Tromsø
- five senior researchers and two affiliated from the University of Oslo
- experimentalists and theorists from chemistry, physics, and mathematics
- two professor II, eight researches and postdocs, ten phd-students

“The vision of the CTCC is to become a leading international contributor to computational chemistry by carrying out cutting-edge research in theoretical and computational chemistry at the highest international level.”

www.ctcc.no

- Research meetings six times a year, alternating between Oslo and Tromsø
- Larger meetings twice a year, with all participants—young researchers speak!
- Weekly seminar in Oslo—well attended and lively
- Half-day seminar series initiated with other groups and centers in Oslo
- 40 papers have been published after CTCC was established
 - 9 of these involve two or more CTCC researchers
- 20 visitors first year from 13 different countries
- Two meetings coorganized in 2007
 - Coastal Voyage in Current Density Functional Theory (Tromsø–Trondheim)
 - Norwegian Theoretical Chemistry: From Molecules to Nanostructures (NTNU)
- Computational chemistry established as division of the Norwegian Chemical Society
 - first session ever held at "Landsmøtet for kjemi" in 2007 (Lillestrøm)
- Application made for National Research School
- International summer school coorganized in 2008 (70 participants)
- CTCC granted coordinating responsibility for Nordic Network of National Centres of Excellence in Computational Chemistry

CTCC: a joint project

- University of Tromsø
 - Centre leader: prof. Kenneth Ruud
 - * higher-order molecular properties
 - * solvation and vibrational effects
 - * vibronic effects
 - * multiwavelets
 - Head of office: Stig Eide
- University of Oslo
 - Node leader: prof. Trygve Helgaker
 - * electronic-structure methods
 - * molecular properties
 - * molecular dynamics
 - * calibration of QC methods
 - Office manager: John McNicol

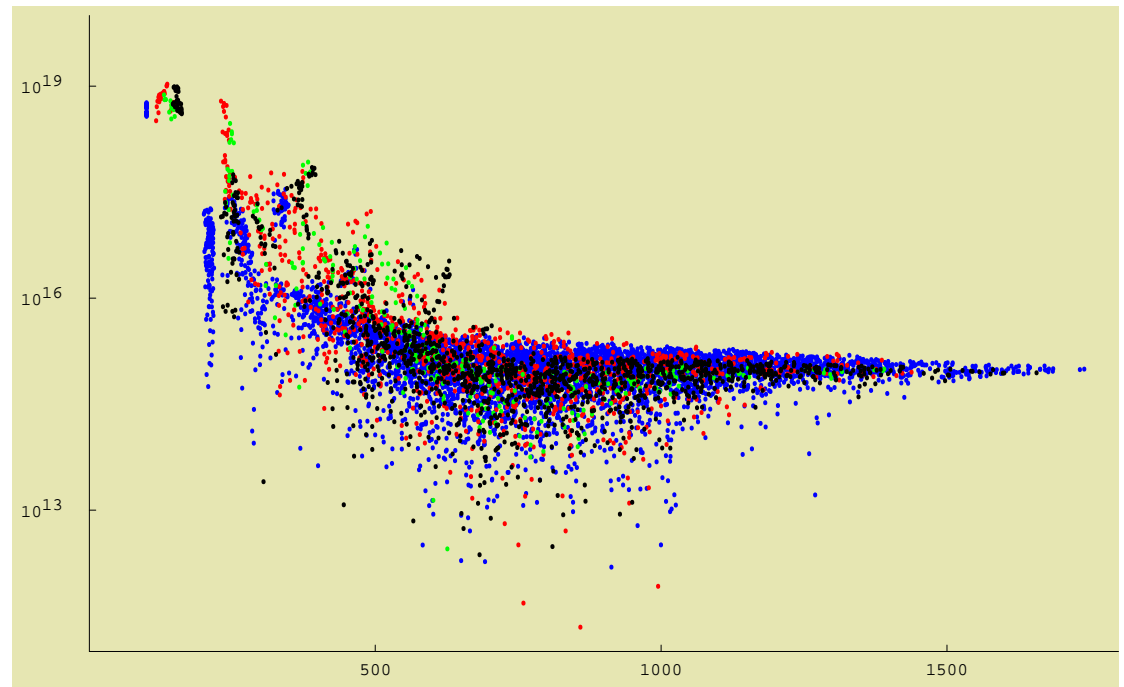
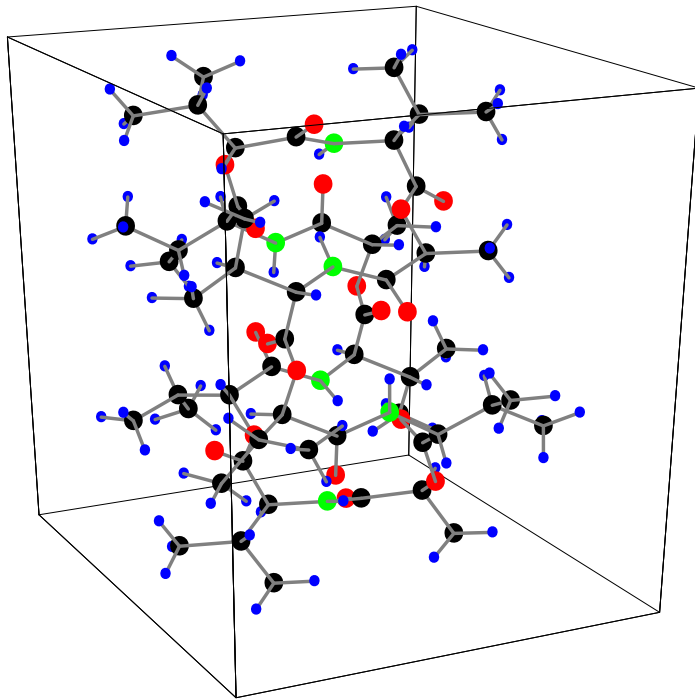


Work Packages

- WP1: Large periodic and nonperiodic systems (T. Helgaker)
- WP2: Fragment approach for large systems (I. Røggen)
- WP3: Multiscale methods with wavelets (T. Flå)
- WP4: Properties and Spectroscopy (L. Frediani)
- WP5: Dynamics and time development (E. Uggerud)
- WP6: Bioinorganic chemistry (A. Ghosh)
- WP7: Catalysis and organometallic chemistry (M. Tilset)
- WP8: Gas-phase reactions and photochemistry (C. J. Nielsen)
- WP9: Clusters, surfaces and solids (K. Fægri jr.)

WP1: Large periodic and nonperiodic systems

- Large systems demand new computational methods
 - steep increase in cost with increasing system size
 - goal: linear scaling of cost for large systems



- Example: indirect nuclear spin–spin coupling in large systems

WP2: Fragment approach for large systems

- Large molecular systems constructed from accurately calculated subsystems
 - Perturbed Atoms in Molecules and Solids (PATMOS)
- Prof. Inge Røeggen,
Department of Physics, University of Tromsø



- electron correlation
- intramolecular interactions
- computational chemistry
- chemical bonding

WP3: Multiscale methods with wavelets

- Different regions of space treated at different resolutions and accuracies
 - use of scaling and detail (wavelet) functions
- Prof. Tor Flå,
Department of Mathematics, University of Tromsø



- density-functional theory
- wavelets
- bioinformatics

WP4: Properties and spectroscopy

- Modeling of spectroscopic techniques by computation
 - linear and nonlinear optics, effects of solvation
- Ass. Prof. Luca Frediani,
Department of Chemistry, University of Tromsø



- linear and nonlinear
molecular properties
- solvation
- multiwavelets

WP5: Dynamics and time development

- The modeling of chemical reactions by on-the-fly dynamics
 - application to metal clusters, water clusters and organic reactions
- Prof. Einar Uggerud,
Department of Chemistry, University of Oslo



- mass spectroscopy
- computational chemistry
- reaction mechanisms
- molecular clusters

WP6: Bioinorganic chemistry

- Applications of quantum chemistry to problems in metallobiochemistry
 - in conjunction with experimental work in synthesis, spectroscopy and electrochemistry
- Prof. Abhik Ghosh,
Department of Chemistry, University of Tromsø



- computational chemistry
- bioinorganic chemistry
- porphyrin chemistry
- metal complexes

WP7: Catalysis and organometallic chemistry

- Organo- and organometallic catalysis
 - application of methods for large systems and dynamics
- Prof. Mats Tilset,
Department of Chemistry, University of Oslo



- organometallic chemistry
- reaction mechanisms
- homogeneous catalysis
- C-H activation
- electron transfer

WP8: Gas-phase reactions and photochemistry

- The study of complex gas-phase reactions
 - chemical processes of atmospheric relevance
- Prof. Claus Jørgen Nielsen,
Department of Chemistry, University of Oslo



- atmospheric chemistry
- spectroscopy
- gas-phase chemistry
- aerosols

WP9: Clusters, surfaces and solids

- Properties of catalytically important metals in diverse environments
 - metal clusters, molecular complexes
- Prof. Knut Fægri,
Department of Chemistry, University of Oslo



- relativistic quantum chemistry
- large molecular systems

Challenges

- Dramatic lack of master students
 - it becomes necessary to import PhD students
 - low level of mathematics and physics knowledge of chemistry students
- A shared center carries a certain overhead
 - coordination of efforts
 - duplication of efforts
 - creates also dynamism
- Added bureaucracy can be time consuming
 - new centers create many relations
 - division between the haves and have-nots
- To the department and the faculty: thanks for all your help!