

WHAT IS QUANTUM CHEMISTRY GOOD FOR?

(... just some examples from my imagination, including from this department; not at all exhaustive ... *Disclaimer: this is my very personal interpretation, not necessarily the complete truth :-)*)

IN CHEMISTRY IN GENERAL

- Interpretation of *any kind* of spectroscopy
- The concept of orbitals
- A full understanding of the concept of a *chemical bond*
(*Although I fully admit that we theoreticians still struggle with that ...*)
- Computational chemistry as a separate but an integral part of modern chemistry

IN INDUSTRY

- Modeling of catalysis (*such as for polymerization*)
- Drug design
- Development of computational chemistry software

WITHIN THIS DEPARTMENT

Dr. Bieringer

- Magnetic interactions in solids
- Interaction between crystal lattices and photons (X-ray crystallography)

Dr. Budzelaar

- Quantum-chemical modeling of organometallic complexes and their reactions

Dr. Cullen

- Development of novel quantum-chemical methods and their implementation in computer codes

Dr. Freund

- Interpretation of various spectra (such as UV-vis or IR)

Dr. Gough

- Interpretation and modeling of vibrational spectra, ranging from small molecules to fungi

Dr. Hultin

- Quantum-chemical modeling of organic molecules, their bonding and reactions

Dr. Kroeker

- Interpretation of NMR spin systems (NMR pulse sequences, etc.)
- Quantum-chemical modeling of inorganic solids such as glasses

Dr. O'Neil

- Interpretation of NMR spin systems

Dr. Schweizer

- Quantum-chemical modeling of proline derivatives: cis-trans isomer ratios

Dr. Schreckenbach

- Quantum-chemical modeling of molecules across the periodic table
- Development of new quantum-chemical methods

Dr. Stetefeld

- Interpretation of X-ray diffraction patterns
- Modelling of protein-metal interactions

Dr. Wang

- Interpretation of various spectra
- Modelling of chemical compounds involved in the mercury-selenium antagonism

Dr. van Wijngarden

- Microwave spectra (rotational/vibrational spectra) and IR spectra of small molecules