Theoretical Chemistry at Lund University

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Theoretical Chemistry

- Research
  - Statistical mechanics
  - Quantum chemistry
  - Experiments

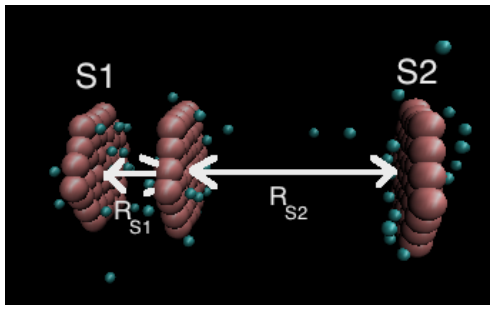
- Software development
  - FAUNUS, a molecular simulation framework
  - MOLCAS, a quantum chemistry package

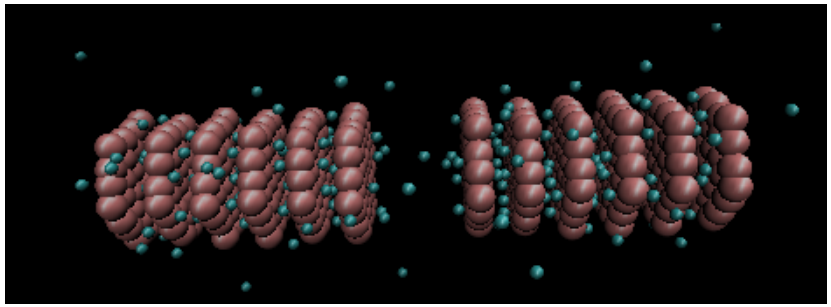
Clay and Cement

- Important technical applications
  - Clay: base in cosmetics, paper filler, drilling lubricant and sealant for long-term nuclear waste disposal
  - Cement: building material
- Charged, sheet-like particles: platelets
- Ion correlations lead to attraction between platelets
- Methods
  - Monte Carlo simulations
  - Experiments (scattering, swelling …)
- PI: Bo Jönsson, Torbjörn Åkesson, Magnus Ullner

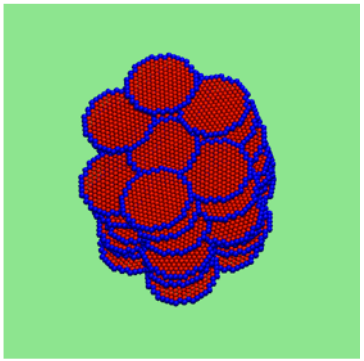
Clay

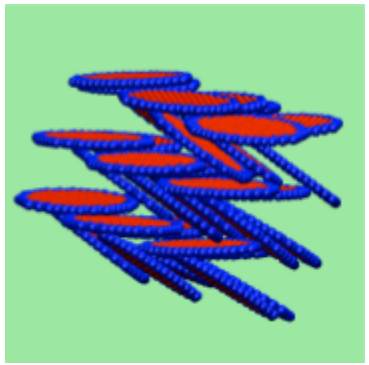
- Tactoid formation (low volume fractions)

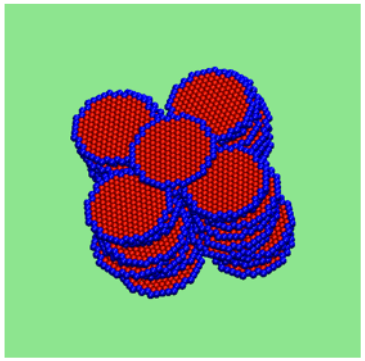




- Phases (high volume fractions, oppositely charged rim)





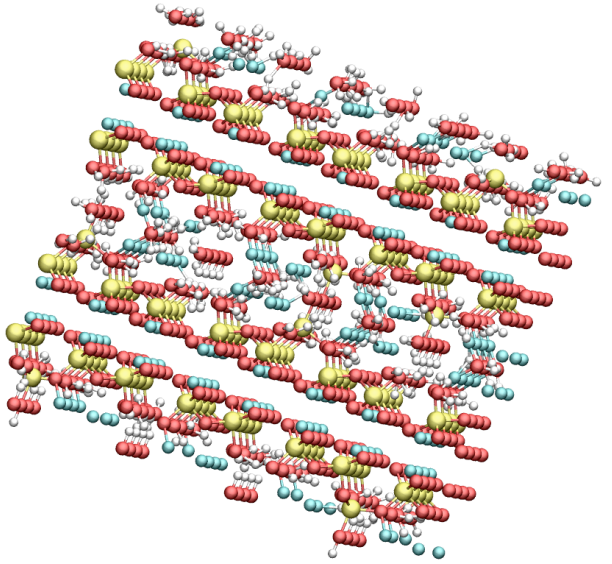


Cement: Solid-Solution Interface

- Tricalcium silicate dissolves to form calcium silicate hydrate platelets when cement is mixed with water
- Atomistic description of calcium silicate materials and the solution interface to understand the process at the interface

- Methods
  - Combination of quantum chemistry and statistical mechanics

- PI: Valera Veryazov, Bo Jönsson

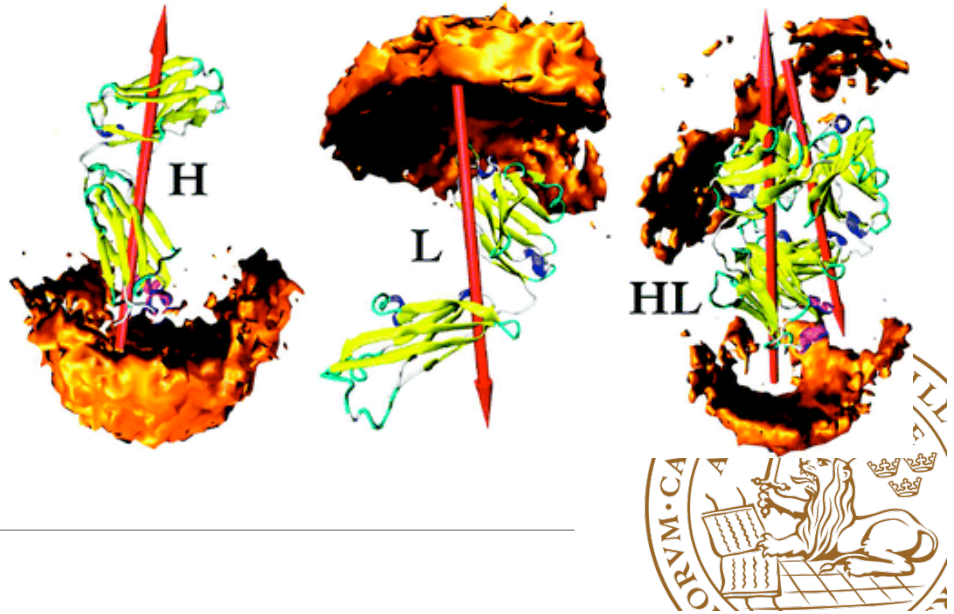


Protein-Protein Interactions

- Important in biology and industrial applications
- Proteins often have a net charge as well as dipolar properties
- Certain combinations of proteins form aggregates

- Methods
  - Monte Carlo simulations
  - Molecular Dynamics

- PI: Mikael Lund

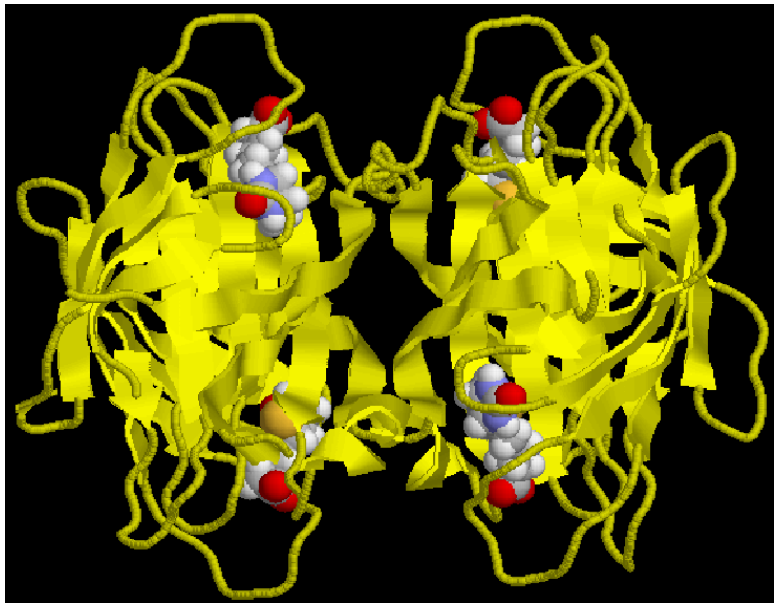


Ligand Affinity

- Interactions between a protein and a small molecule
- Important in drug development
- Test and improvement of computational methods

- Methods
  - MM/PBSA

- PI: Ulf Ryde

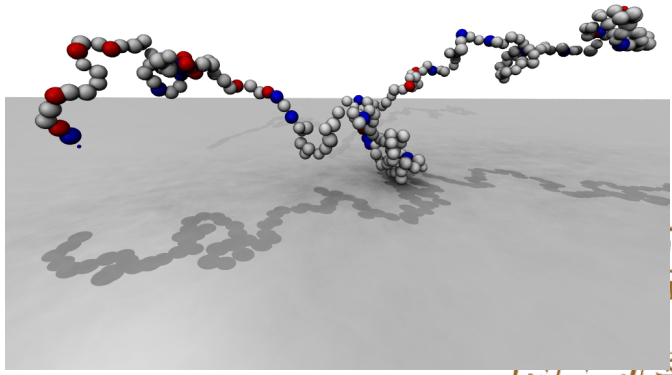


Flexible Proteins

- Found in saliva and milk products
- Both saliva and fermented milk tend to stick to surfaces, which has implications for oral health and packaging materials (prevent food waste), respectively
- Studied in bulk and at surfaces

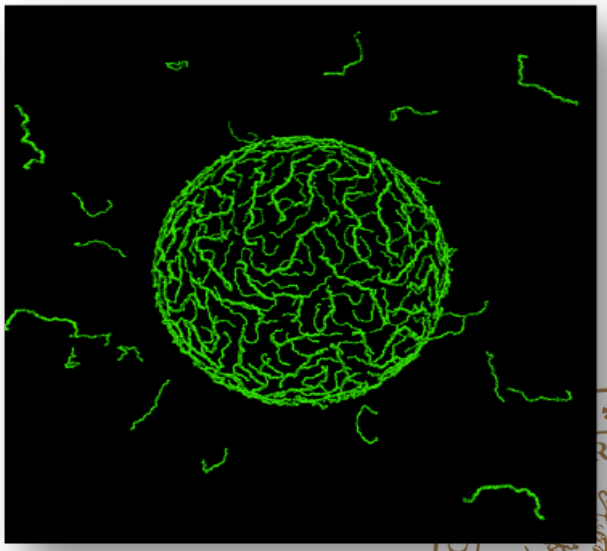
- Methods
  - Monte Carlo simulations
  - Molecular Dynamics
  - Experiments

- PI: Marie Skepö



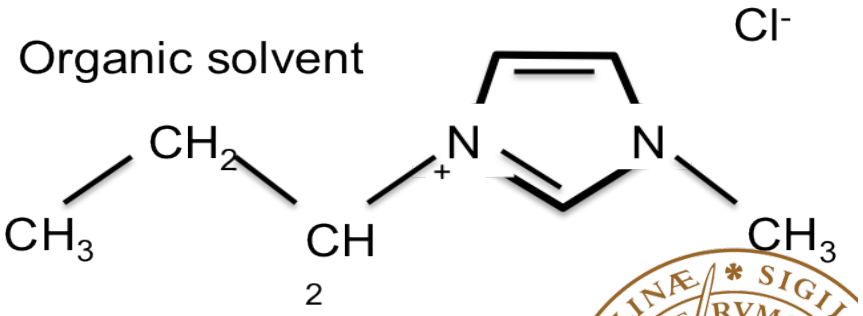
Polyelectrolyte Adsorption

- Charged polymers can adsorb on oppositely charged surfaces
- Important in biological and technological processes, such as, drug delivery, water treatment, and paper production
- Methods
  - Monte Carlo simulations
  - Density functional theory
  - Experiments (ellipsometry)
- PI: Jan Forsman



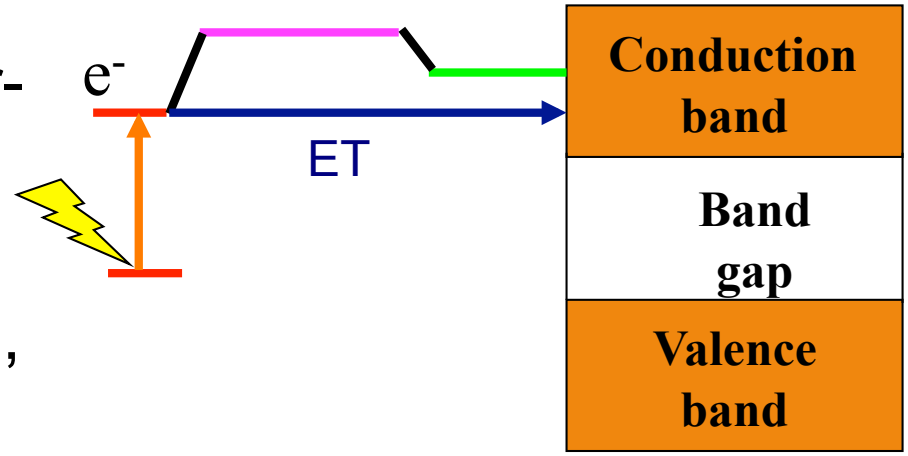
Ionic Liquids

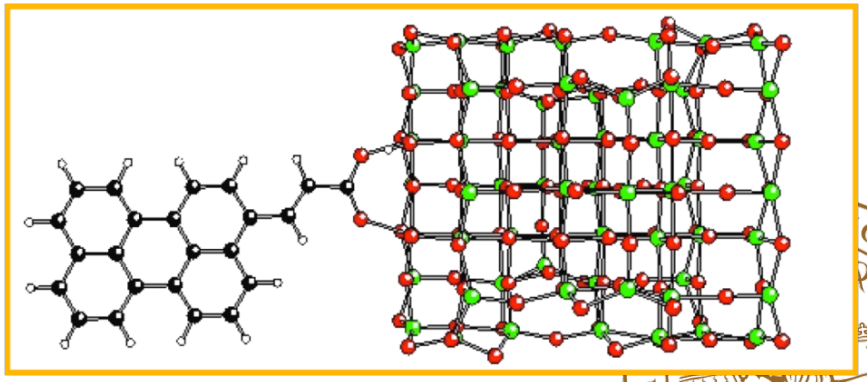
- Typically large organic positive ion with small negative ion
- The bulkiness of the organic ion prevents crystallisation and the ion pair is a liquid at room temperature
- Useful as a specialised solvent and as the electrolyte in “supercapacitors” for high-density energy storage
- Modified properties when mixing with an organic solvent
- Methods
  - Monte Carlo simulations
  - Density functional theory
- PI: Jan Forsman



Nanostructured Solar Cells

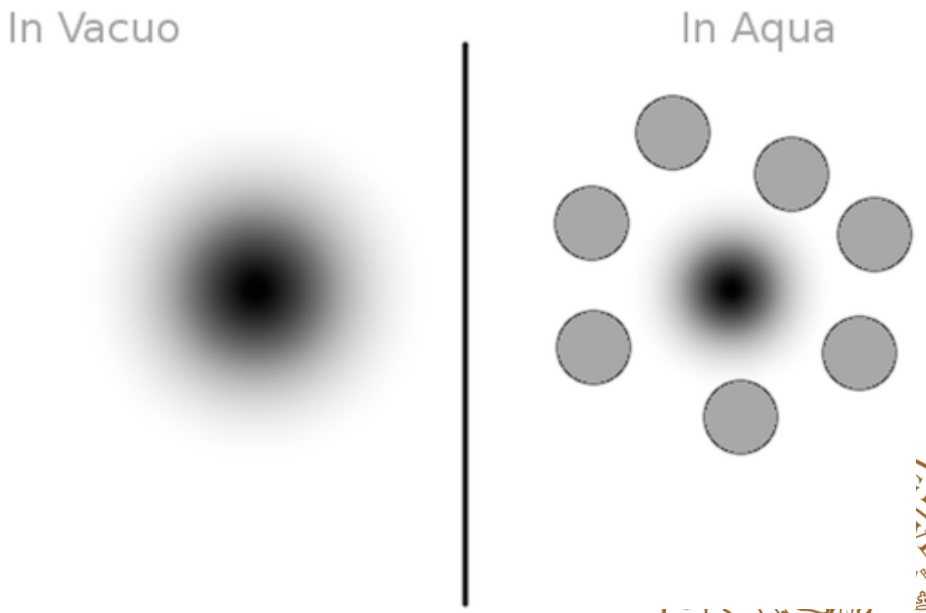
- Solar-energy conversion by dye-sensitised and polymer-based solar cells
- Sun light hitting a dye or polymer excites an electron, which is transferred to an inorganic or organic semiconductor
- Methods
  - DFT
- PI: Petter Persson





Properties of Ions in Water

- Ion-specific properties, such as polarisability
- Simulations with a quantum mechanical part surrounded by classical solvent (water) molecules surrounded by a dieelectric continuum

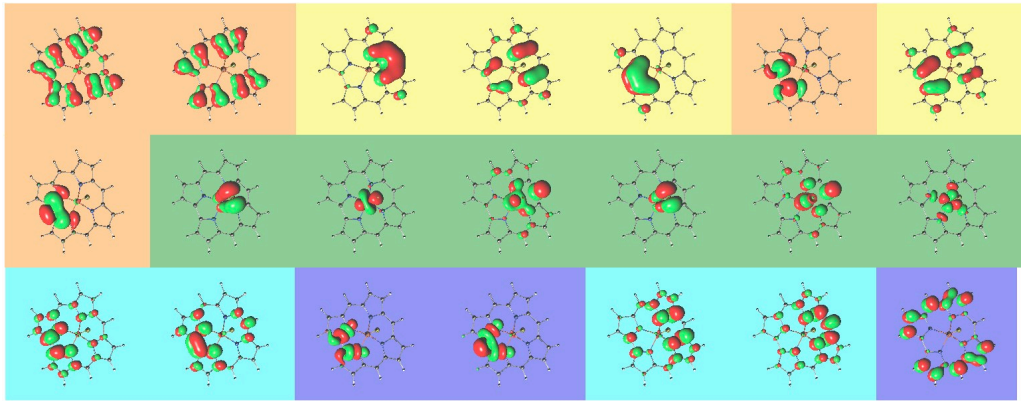


- Methods
  - QMSTAT
  - NEMO potential

- PI: Gunnar Karlström

Multiconfigurational Quantum Chemistry

- Multiconfigurational methods are essential for a precise description of the electronic structure of molecules
- Studies of excited states, electronic spectra and chemical reactions
- Software and method development
- Methods
  - CASSCF
  - RASSCF
  - CASPT2



- PI: Valera Veryazov, Per-Åke Malmqvist, Per-Olof Widmark