Status Quo of the CC group

CC='Computational Chemistry'
(Quantum chemistry, simulations,
energy surfaces, programming …)

Members … (we are a very small group)

Michael Probst - supervisor

PhD-students

- Natcha Injan
- Chadchalerm Raksakoon

Diploma student

- Andreas Mauracher

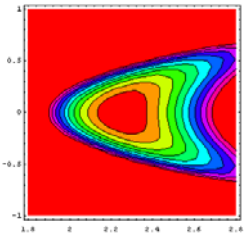
Collabrations & frequent guests:
(across Europe)

Collabrations & frequent guests:
(across the world)

Other universities in Thailand, Germany, Japan, Korea…

what we do…

- **Quantum mechanics of molecules and clusters** (quantum chemical calculations of the electronic structure)
- **Potential energy surfaces** and **Molecular Dynamics simulations**



Applied to

- Single molecules in vacuum and in media and electron-molecule reactions
- Condensed phases (liquids & solutions…zeolites)
- Electronic impact ionization cross sections

Quantum mechanics of molecules and clusters

(quantum chemical calculations of the electronic structure)

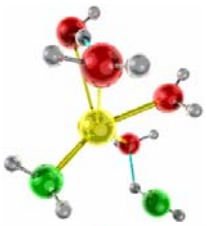
- Electron affinities and ionisation potentials
- Bond energies and energies of reactions
- Vibrational and electronic spectra
- Molecular orbitals and electron densities
- Electrostatic properties
- Providing wavefunction properties for calculation of electron-impact cross sections (Deutsch, Märk, Becker…)

Potential energy surfaces and Molecular Dynamics simulations

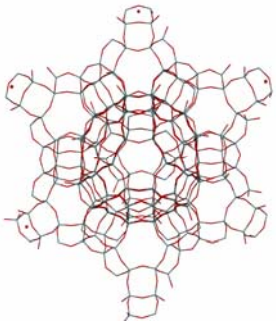
- Potential energy surfaces from quantum chemistry.
- Intermolecular interactions and forces. Inclusion of polarisation in the PES.
- Molecular Dynamics simulations – classical and Car-Parinello.
- Analysis of dynamical properties of ensembles of molecules from their trajectory: Distribution functions, reaction rates, structural data.

Condensed phases (liquids & solutions…)

- **Behaviour of liquids and solvated ions**
- Important in surface- and materials science
- Examples:
  - Ethylene Carbonate-Li+ (used in fuel cells)
  - Dimethylsulfoxid (in the chem/med/pharm industry)
  - Carbon tetrachloride
  - etc…



- **Zeolites and related materials**
- Important in materials science and catalysis
- Examples:
  - chemical reaction dynamics (formic acid …)
  - adsorbtion (Pyridine …)
  - MD simulations



future …we are (or want to be …)

- Looking to combine different methods in interesting ways
- Always interested in interesting systems
- Very interested in strong collaborations
- Expanding the repository of methods to the 'state of art'

AG Computational Chemistry

Institut für Ionenphysik und Angewandte Physik
Leopold-Franzens-Universität Innsbruck

2. Dezember 2006