Module MCh WP 12
Theoretical Methods for Condensed Matter

Stefan Grimme, Barbara Kirchner, Thomas Bredow

Mulliken Center for Theoretical Chemistry
Institut für Physikalische und Theoretische Chemie

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Aims I

- **Theoretical background of non-covalent interactions and application to molecular crystals (Grimme)**

- Physical background of non-covalent interactions

- Effect of non-covalent interactions on chemical bonding

- Methods for the calculation of non-covalent interactions

- Applications of current chemical interest (supramolecular chemistry, molecular crystals)
Aims II

- Concepts and methods for the description of liquids (Kirchner)

- Characterization and structure determination of liquids

- Sustainable chemistry: more efficient and less toxic processes

- Improvement of solvents: tailored electrolytes, switchable solvents, phase-transfer catalysts
Aims III

- Quantum-chemical treatment of crystalline solids and their surfaces (Bredow)
  - Prediction of new materials
  - Optical properties: photovoltaics
  - Ion conductivity: battery materials
  - Adsorption: heterogeneous catalysis
**Registration**
- Max. no. of participants: 24
- Until **30.09.** via Email: bredow@thch.uni-bonn.de
- Requirements:
  - passed Module MCh 1.4
- First meeting on **Monday October 7 at 16:00**
  - seminar room 0.005, Beringstr.4
- Website: https://www.chemie.uni-bonn.de/pctc/mulliken-center/teaching/wp12/

**Examination**
- Prerequisite:
  - passed practical part (protocols until February 1)
- Oral examination (100 %)
  - Mid February / Mid March
Lectures from 09/10–11/12/2019, 3 parts

Wednesday 12:15 – 13:45

Thursday 10:15 – 11:45

Part 1 (Kirchner):
- Relation between structure and dynamics of liquids
- Classical and ab initio-molecular dynamics, continuum models
- Nanostructures and hydrogen bond network
- Locality and (hydrogen bond) dynamics
- Transport properties
- Applications (ionic liquids, associated liquids, solvent effects)
Part 2 (Grimme):
- Classification of non-covalent interactions:
  - Decomposition of contributions
- Intermolecular force fields
- Supermolecular QC-treatment:
  - MPn- and CC-methods (basis sets and BSSE)
  - DFT and dispersion corrections
- Applications (large complexes, molecular crystals)

Part 3 (Bredow):
- Solid-state theory: periodic boundary conditions, band structure, density of states, phonons
- Point defects
- Surface models
- Adsorption
- Applications (solid-state reactions, phase diagrams)
Practical course: 3 parts within 09/10/2019 and 01/02/2020

- CIP pools of MCTC (2.008 and 3.007), Beringstr.4
- Opened: Mo–Fr from 09:00-17:00
- Flexible supervision by group members
Computer experiments:

Part 1:
- Continuum models
- Explicit solvation
- Effect of force-field parameters on the simulation
- Reactions in solvent

Part 2:
- SAPT calculations for small systems
- Supermolecular calculations with correlated methods (MP2, CCSD(T))
- DFT-D3- and DFT-NL calculations of molecules in solution
- Calculation of molecular crystals

Part 3:
- Structure optimization of simple solids
- Calculation of phase stabilities
- Calculation of surface energies
- Adsorption of small molecules