Module MCh WP 12

Theoretical Methods for Condensed Matter

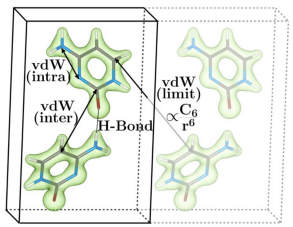
Thomas Bredow, Stefan Grimme, Andreas Hansen, Johannes Ingenmey, Barbara Kirchner

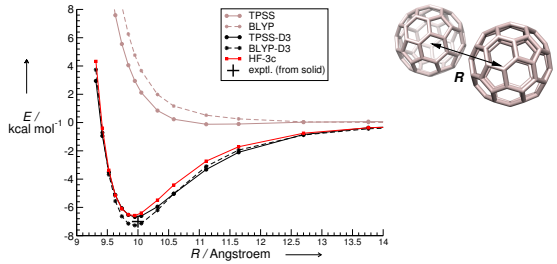
Mulliken Center for Theoretical Chemistry
Institut für Physikalische und Theoretische Chemie

18/07/2025

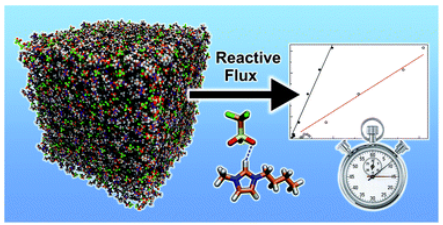
Topics

- Part I: Theoretical background of non-covalent interactions and application to molecular crystals (Grimme/Hansen)

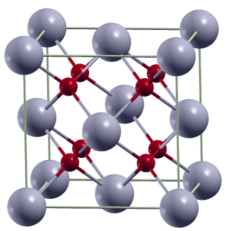


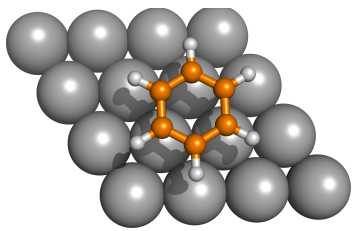


- Part II: Concepts and methods for the description of liquids (Kirchner/Ingenmey)



- Part III: Quantum-chemical treatment of crystalline solids and their surfaces (Bredow)





Part I (Grimme/Hansen)

Lectures:

- 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

Computer experiments:

- Energy decomposition: SAPT for small systems
- Supermolecular calculations with correlated methods
- DFT-D3-calculations of molecules in solution
- Molecular crystals

Part II (Kirchner/Ingenmey)

Lectures:

- Classical and ab initio molecular dynamics
- Nanostructures and hydrogen bond network
- Transport properties

Computer experiments:

- Continuum models
- Explicit solvation
- Effect of force-field parameters
- Reactions in solvents

Part III (Bredow)

Lectures:

- Introduction to CRYSTAL23
- Applications
- Solid-state theory

Computer experiments:

- Phase stabilities
- Surface energies
- Adsorption of small molecules
- Activation barriers for surface migration

Organization I

- Lectures from 15/10–17/12/2025 in 3 parts

  Wednesday 12:15 – 13:45

  Thursday 10:15 – 11:45

- Practical course: 3 parts between 15/10 and 18/12/2025
  - CIP pools of MCTC (2.008 and 3.007), Beringstr.4
  - Opening hours: Mo-Fr 09:00–17:00
  - Flexible supervision by group members

Organization II

- Requirements
  - Max. no. of participants: 20
  - Requirements: **passed Module MCh 1.4**
  - Kickoff meeting on **Monday October 13 at 16:00, seminar room 0.005 Beringstr. 4**
  - Ecampus: **https://ecampus.uni-bonn.de/goto_ecampus_crs_2348897.html**
  - Basic knowledge of Linux
- Examination
  - Prerequisite:
    passed practical part (accepted protocols until **end of January 2026**)

Organization III

- Oral examination (100 %)
  February / March 2026