WP8 – Molecular Dynamics of Time-Dependent Phenomena

10.07.2026

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Clausius-Institute for Physical and Theoretical Chemistry

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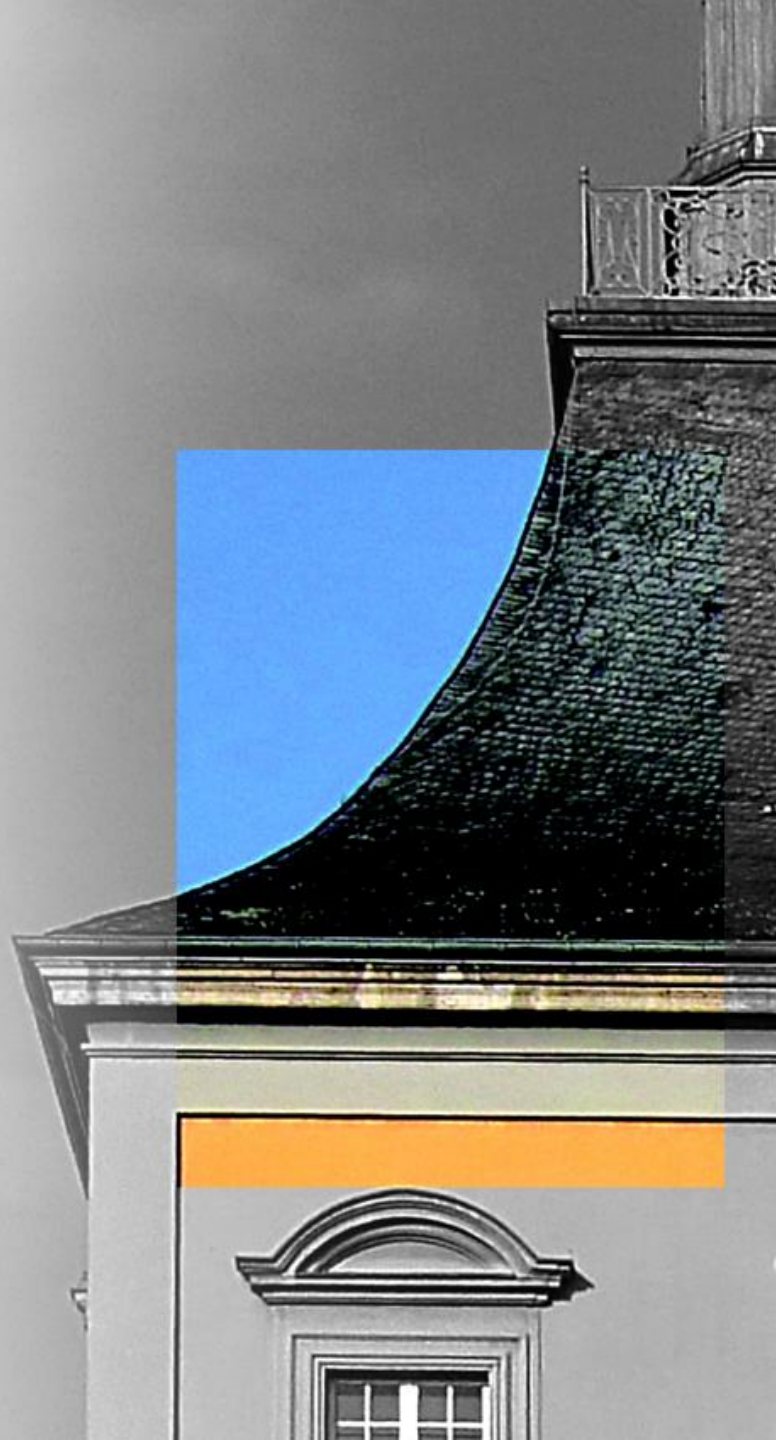
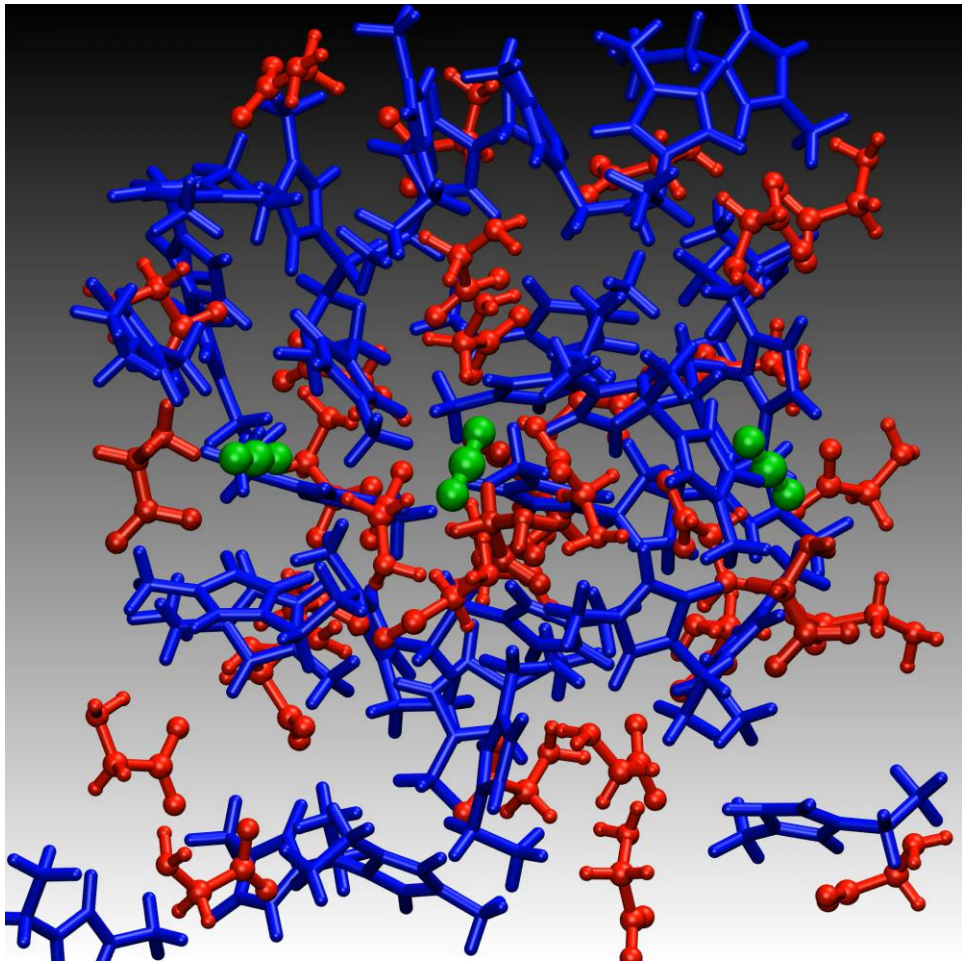


What is „Molecular Dynamics“?

- Kinetics of chemical reactions during Bachelor curriculum:
  PC III: *„Kinetics and Statistical Thermodynamics“*

- Molecular Dynamics is research on (and teaching of) the **motions of molecules**
- Time dependence of dynamical phenomena originates from molecular motions
- In WP8 both, **theory and experiment** are covered



Virtual Molecular Dynamics Lab (Kirchner)

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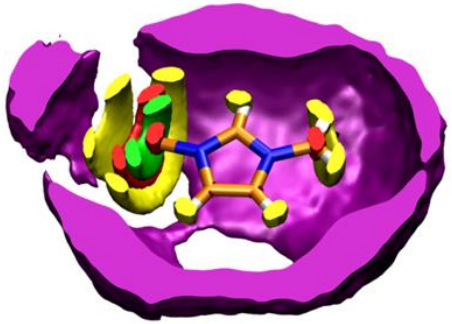
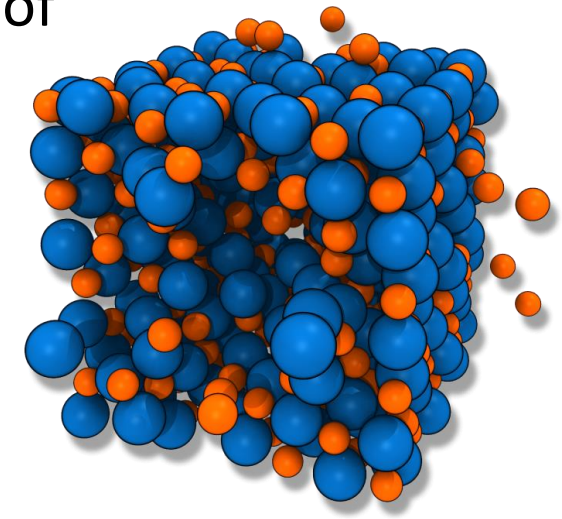
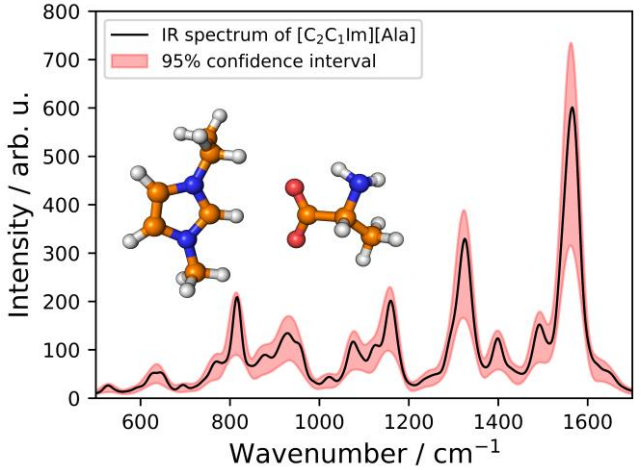
Lectures

- Fundamentals/modern methods of molecular dynamics simulations
- Algorithms and implementation
- Data analysis, computation of observables
- Vibrational spectroscopy



Talks





- Each participant is assigned a recent paper
- Talk in the Kirchner group seminar

Virtual Molecular Dynamics Lab (Kirchner)

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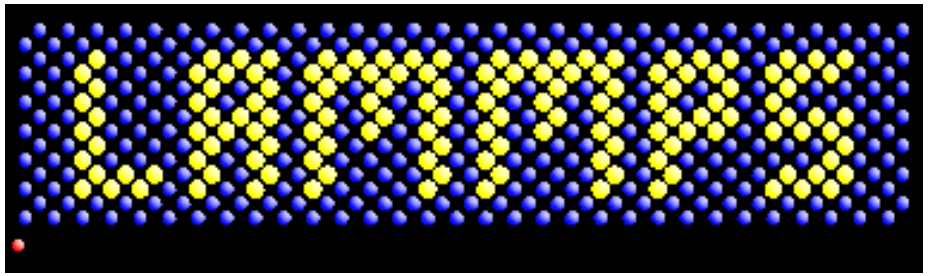
Coding your own MD software

- Implementing an MD algorithm, generate your own “molecular movies”
- No prior coding experience required, but **interest in math / problem solving**



Applying existing MD software

- Using state-of-the-art MD analysis codes
- Extract properties from simulations
- Calculate vibrational spectra

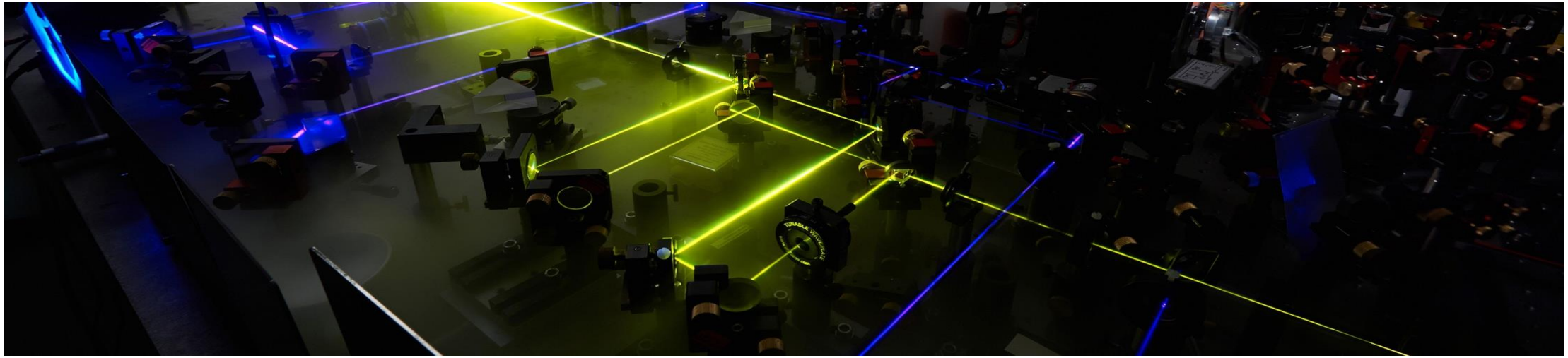
CP2K

TRAVIS
TRAJECTORY ANALYZER AND VISUALIZER

Organization

- The practical can be done in the Mulliken Center (CIP pool 3rd floor) or remotely
- 10 weeks time (until Christmas break)

Real Molecular Dynamics Lab (Vöhringer)



Lecture

- Operating principles of lasers
- Generation of ultrashort light pulses / handling such pulses in the real lab
- Interaction of molecules with ultrashort light pulses
- How do we develop the spectroscopic „movies“ of chemical reactions?

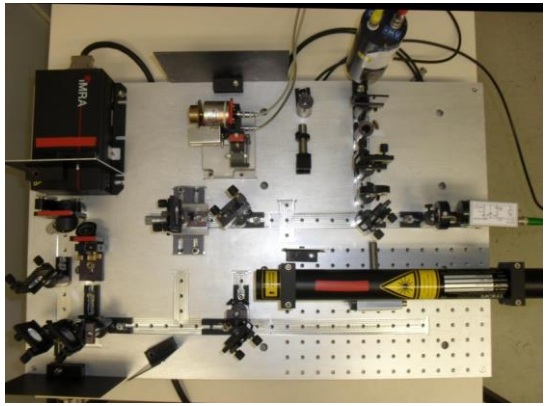
Real Molecular Dynamics Lab (Vöhringer)

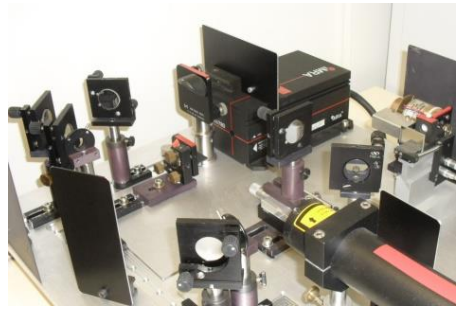
Laser Lab Internship

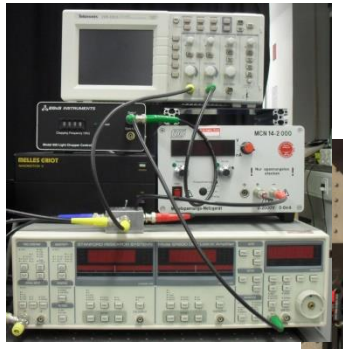
- Operation of fs-lasers
- Nonlinear-optical frequency conversion
- Determination of pulse durations
- Measurement of group velocity and GV-dispersion

Two experiments:

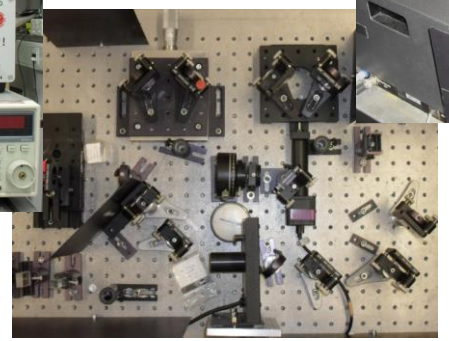
“Interferometric Autocorrelation” or “Characterization of Laser Pulses”



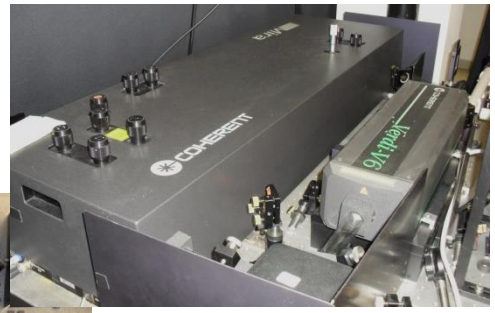




Electronics



Delay line



fs-Laser

Organization

Lectures

- Wed 10-12
- Thu 13-15

Practical courses

- Kirchner: Flexible in MCTC CIP-Pool
- Vöhringer: 30.11.-11.12.2026

  (In group of 2-3 students) approx. 12 spots

Requirements

- Passed Module MCh 20 1.3

Virtual vs. Real Molecular Dynamics Lab