WP8 – Molecular Dynamics of Time-Dependent Phenomena

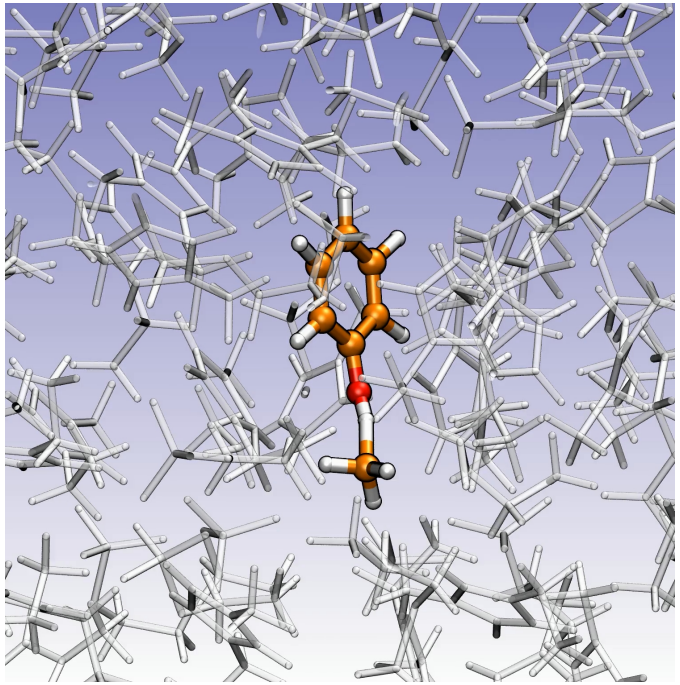
(Kirchner, Vöhringer)

Kinetics of chemical reactions during Bachelor- and Master curricula:
Phys. Chem. III:„Kinetics and Statistical Thermodynamics“

Phenomenological treatment of dynamical phenomena
Reaction rate = time derivative of concentration (dc/dt), rate coefficients

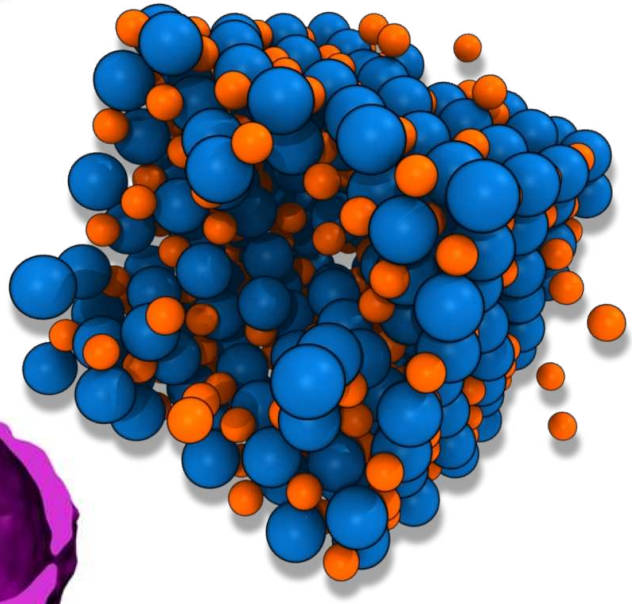
Quantum statistical treatment of dynamical phenomena
ab initio rate coefficients from theory, e.g. transition state theory

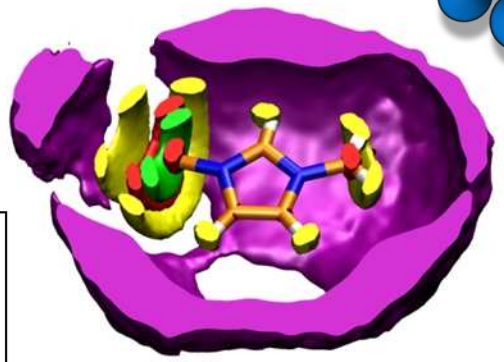
- **Molecular Dynamics** is research on (and teaching of) the motions of molecules
- Time dependence of dynamical phenomena originates from molecular motions
- In WP8 both, **theory and experiment** are covered



Virtual Molecular Dynamics Lab

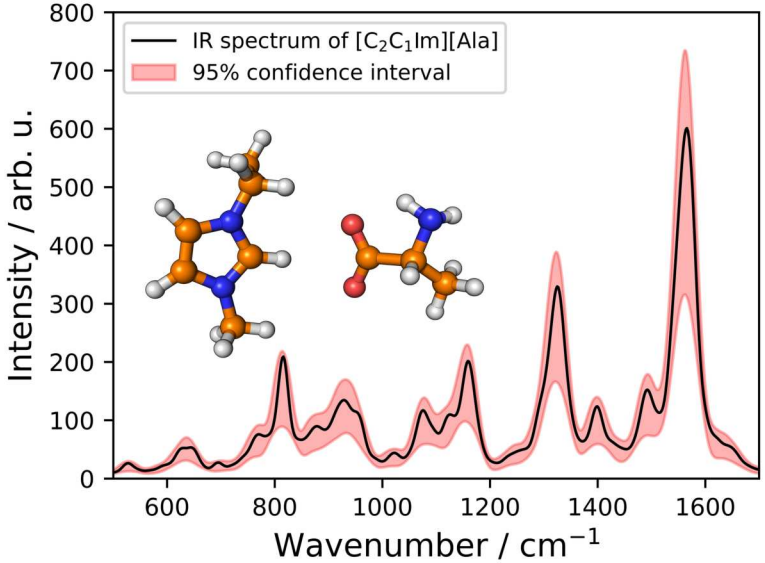
Mulliken-Center – Kirchner Group





Lecture content

- Methodology of simulations
- Need for simulations
- Algorithms and implementation
- Data analysis, calculation of observables
- Vibrational spectroscopy
- Modern developments in the field



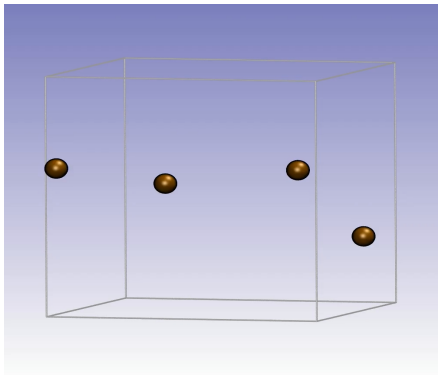
Seminar presentation

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

Computer lab internship

Programming your own MD code

- Implementing an MD algorithm (Fortran)
- No prior coding experience required
- Understanding challenges and limitations in MD simulations
- Generate your own “molecular movies”



Applying existing MD software

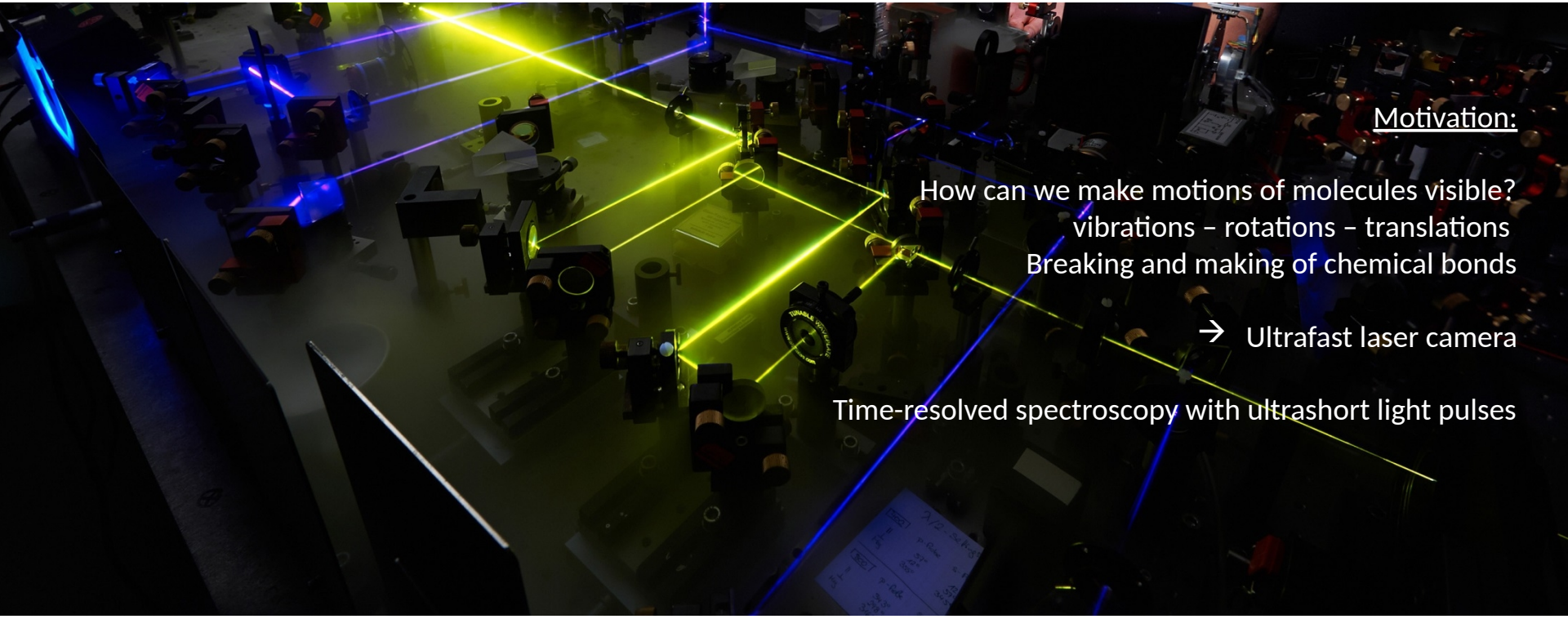
- Using state-of-the-art MD analysis codes
- Extract properties from simulations
- Calculate vibrational spectra

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

Clausius-Institute – Vöhringer Group

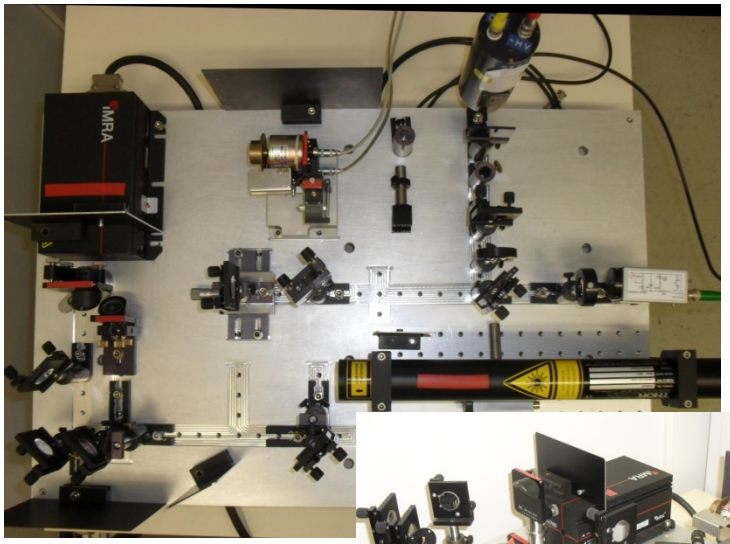


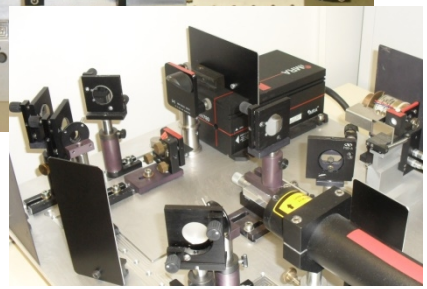
Lecture contents:

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

Laser lab internship

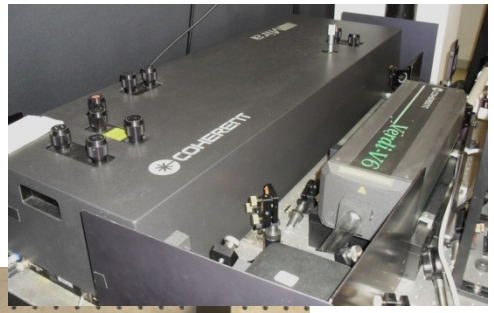
Interferometric autocorrelation

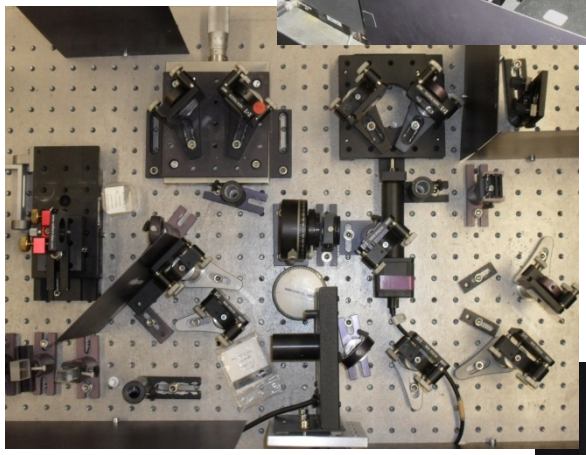




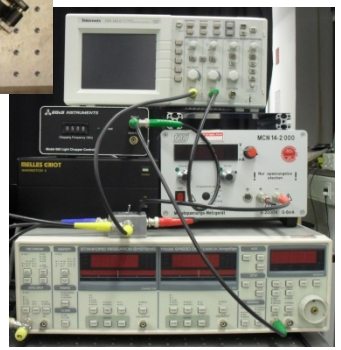
Characterization of ultrashort laser pulses

fs-Laser





Delay-line



Electronics

Contents:

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

Mandatory: Safety instructions „Working with lasers“!

Organization

Classroom teaching: Wednesdays, 10 – 12 and Thursdays, 13 – 15

Lab internships: Kirchner: by prior arrangement

Vöhringer: **17.11.-28.11.2025**,
~12 participants, in the lab
(groups of 2 - 3)

Virtual molecular dynamics lab

Real molecular dynamics lab

Requirement: Passed module Mch 20 1.3 (Advanced Physical Chemistry)