TECHNISCHE UNIVERSITÄT KAISERSLAUTERN

Berkeley UNIVERSITY OF CALIFORNIA

UCDAVIS UNIVERSITY OF CALIFORNIA

Kick-off Meeting
International Research Training Group 2057

Computational Molecular Engineering for Engineering Thermodynamics

Martin Horsch and Hans Hasse

TU Kaiserslautern
Engineering Thermodynamics (LTD)

Davis, California, October 8, 2014

IRTG 2057
Physical Modeling for Virtual Manufacturing Systems and Processes

Since April 2008, the Laboratory of Engineering Thermodynamics (LTD) is directed by Prof. Dr.-Ing. Hans Hasse. Our research activities cover all areas of thermodynamics:

Thermodynamic Properties

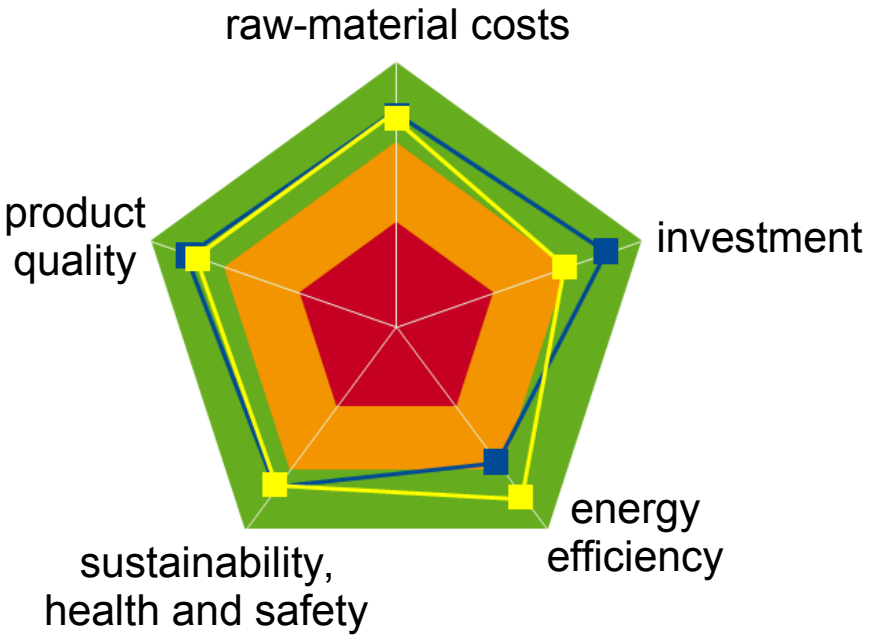
Process Thermodynamics

Biothermodynamics

Molecular Thermodynamics

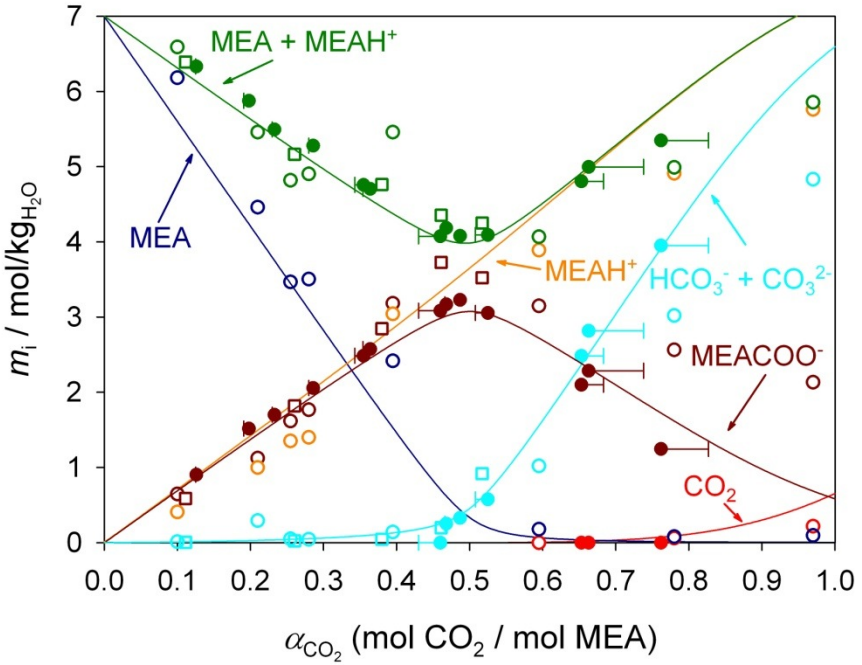
Process Design and Raw Material Change

Jun. Prof. Dr.-Ing. Jakob Burger



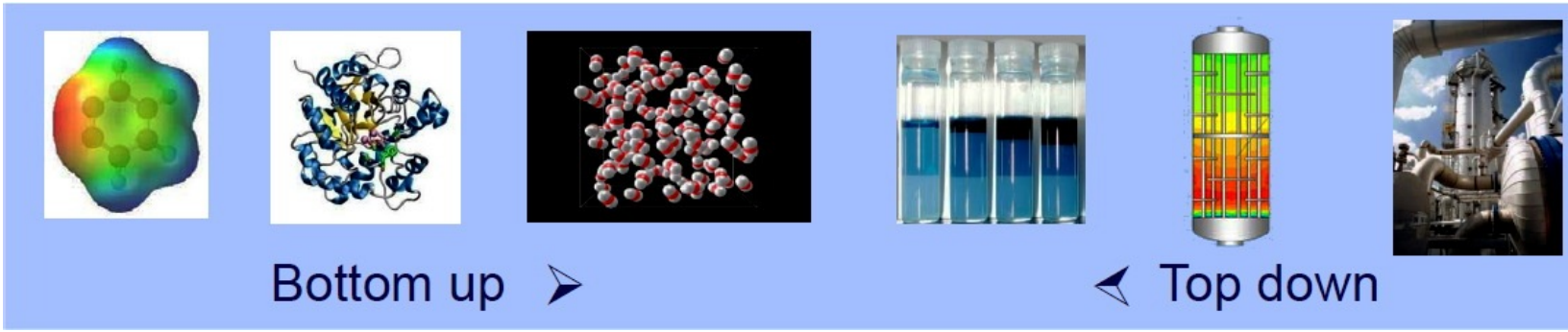
- Multi-criteria optimization of chemical processes based on Pareto sets
- Assessment and comparison of value-added chains
- Decision support for the chemical industry

Jun. Prof. Dr.-Ing. Erik von Harbou



- Modeling and simulation of complex reacting multi-phase systems
- Model-based design of experiments and uncertainty quantification
- NMR spectroscopy for process and reaction monitoring

Computational Molecular Engineering



From Physics (qualitative accuracy)

- Physically realistic modeling of intermolecular interactions
- Separate contributions due to repulsive and dispersive as well as electrostatic interactions

To Engineering (quantitative reliability)

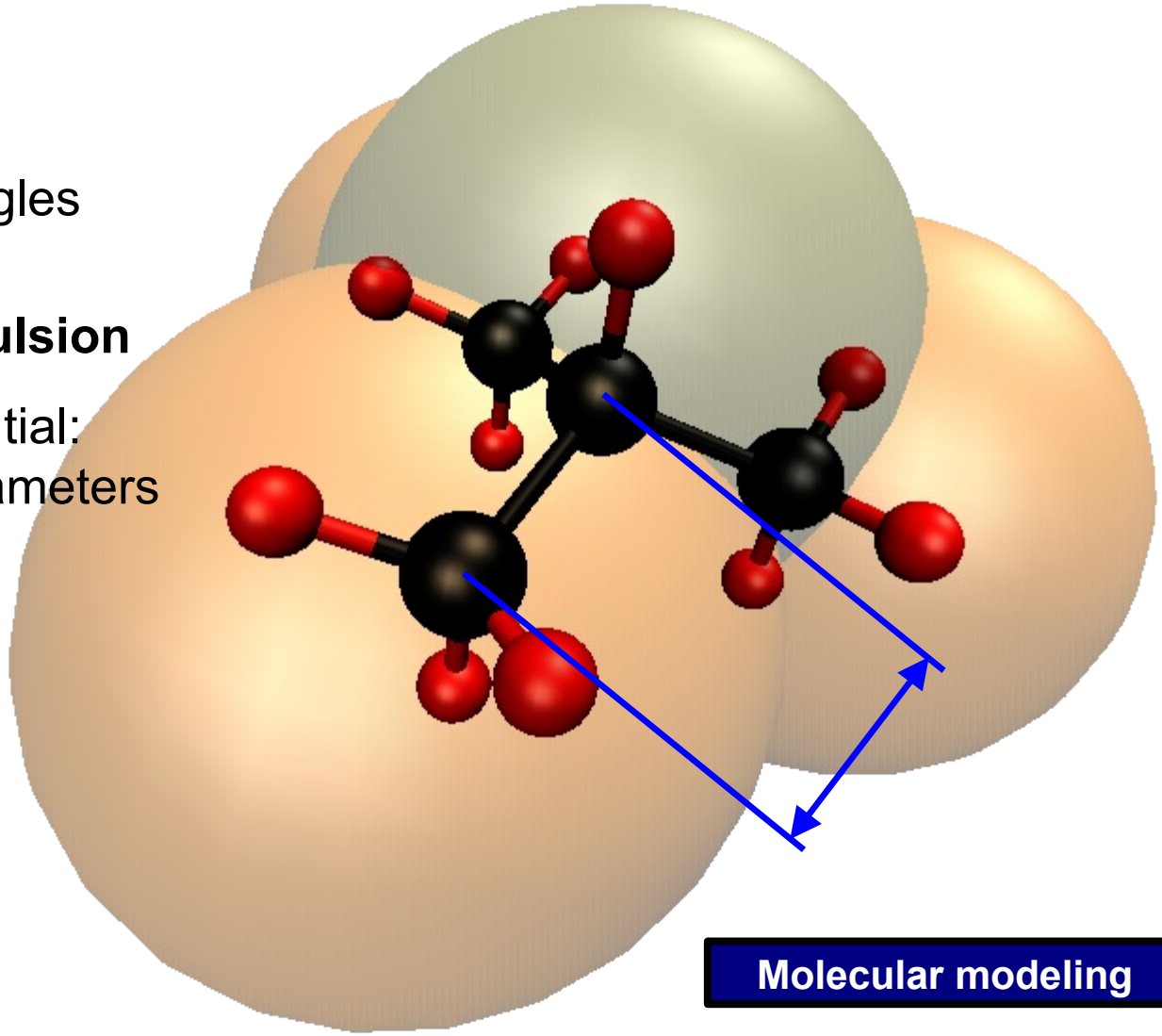
- No blind fitting, but parameters of effective pair potentials are adjusted to experimental data
- Physical realism facilitates reliable interpolation and extrapolation

Geometry

Bond lengths and angles

Dispersion and repulsion

Lennard-Jones potential:
Size and energy parameters



Molecular modeling

Molecular models of real fluids

Geometry

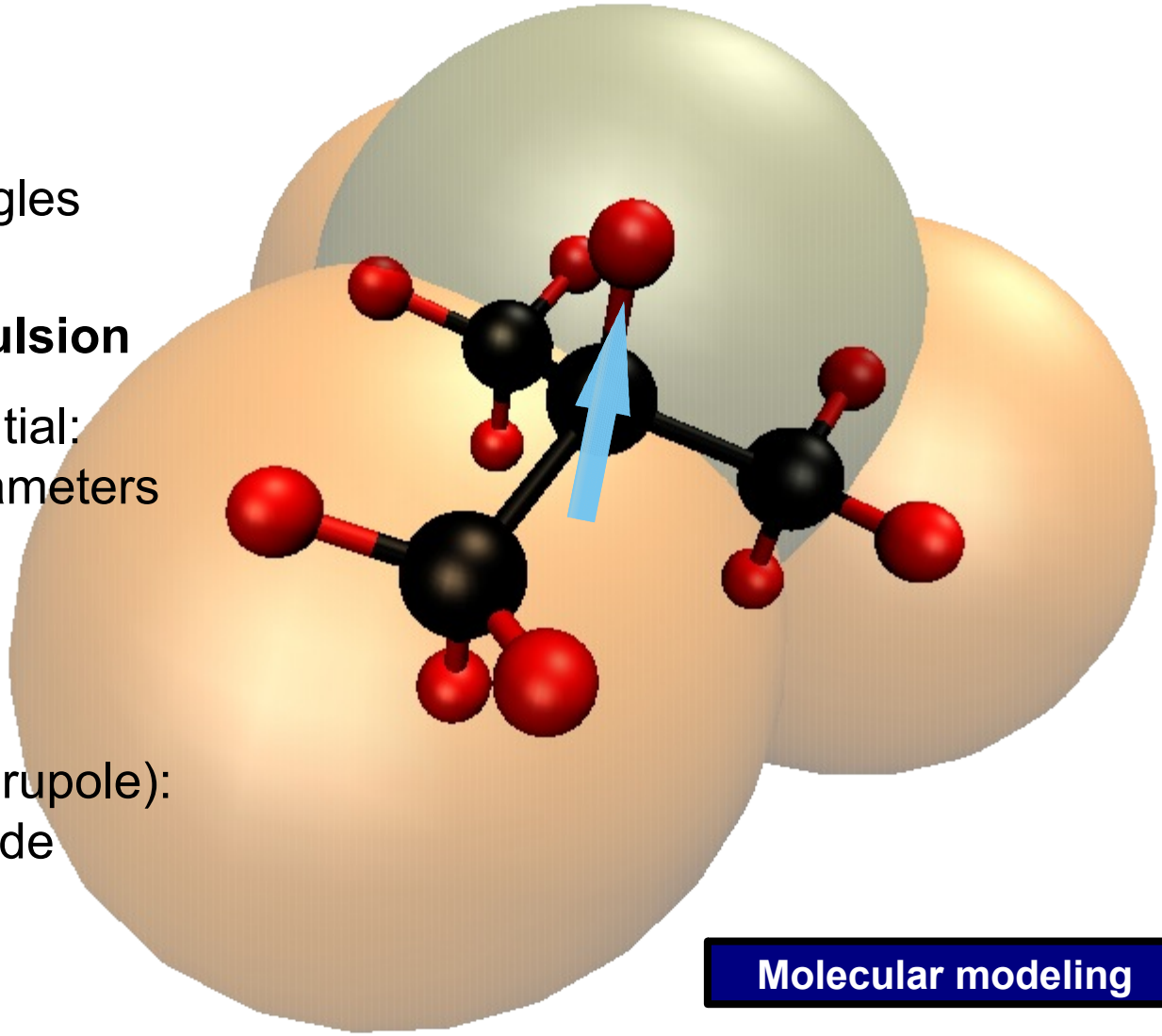
Bond lengths and angles

Dispersion and repulsion

Lennard-Jones potential:
Size and energy parameters

Electrostatics

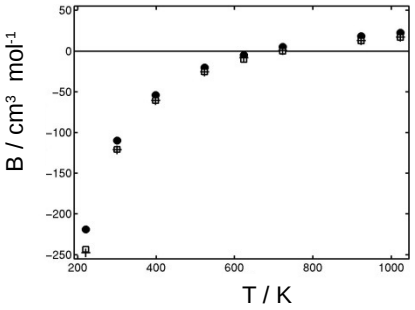
Point polarities
(charge, dipole, quadrupole):
Position and magnitude



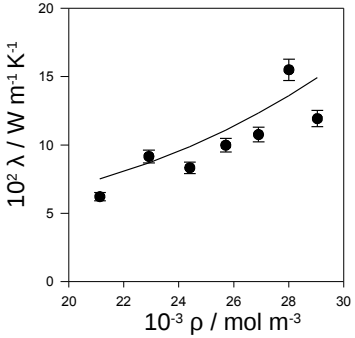
Molecular modeling

Simulation of bulk fluid properties with the *ms2* program

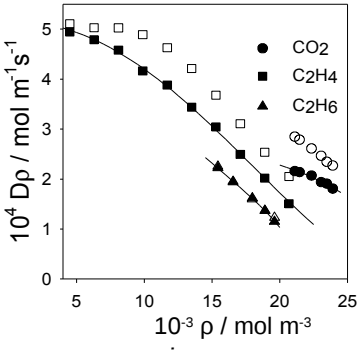
Second virial coefficient



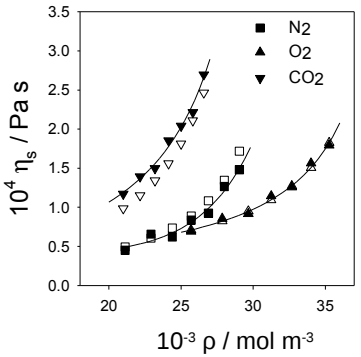
Thermal conductivity



Self-diffusion coefficient

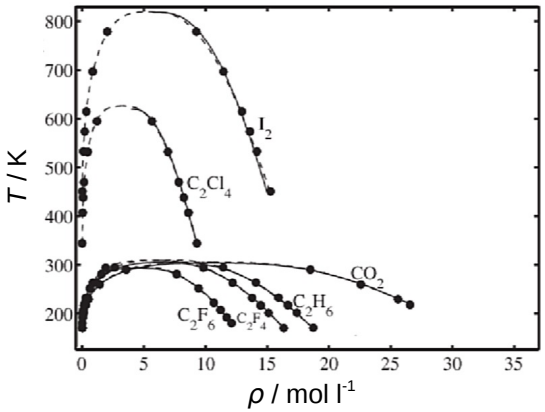


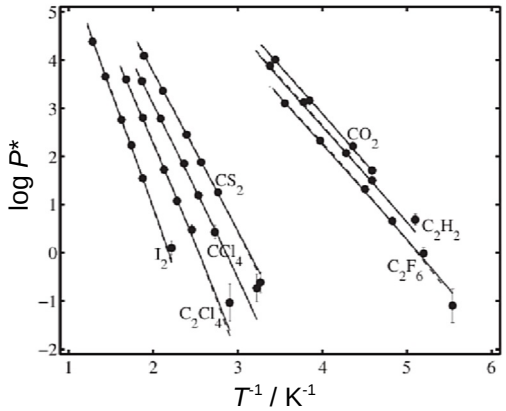
Shear viscosity



ms2 is freely available for academic use – register at http://www.ms-2.de/

Vapor-liquid equilibria: Saturated densities and vapor pressures

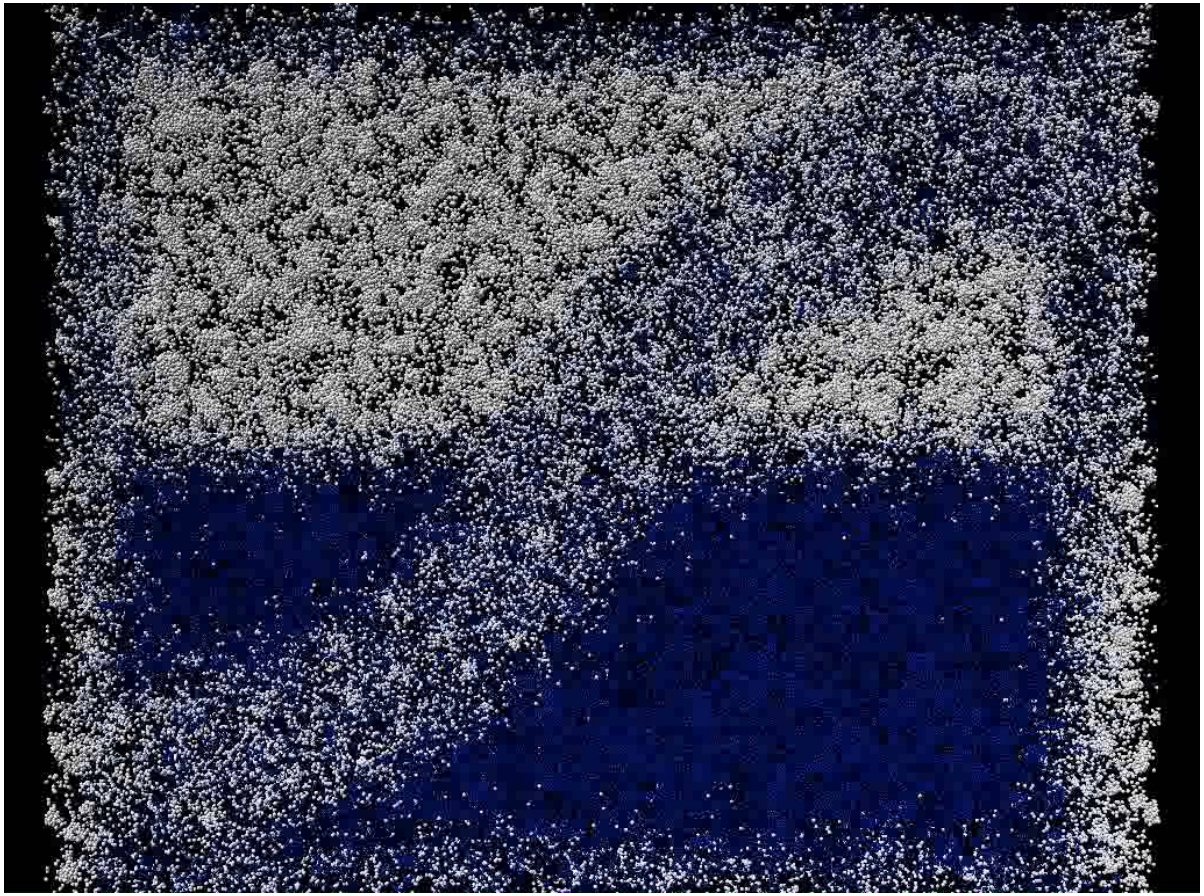


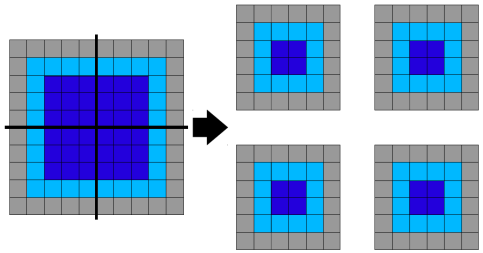


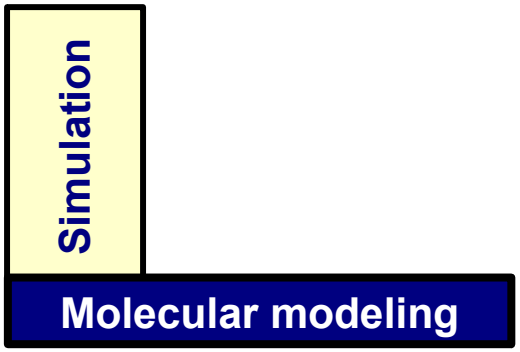
Simulation

Molecular modeling

Large-scale MD simulation with the *ls1 mardyn* program

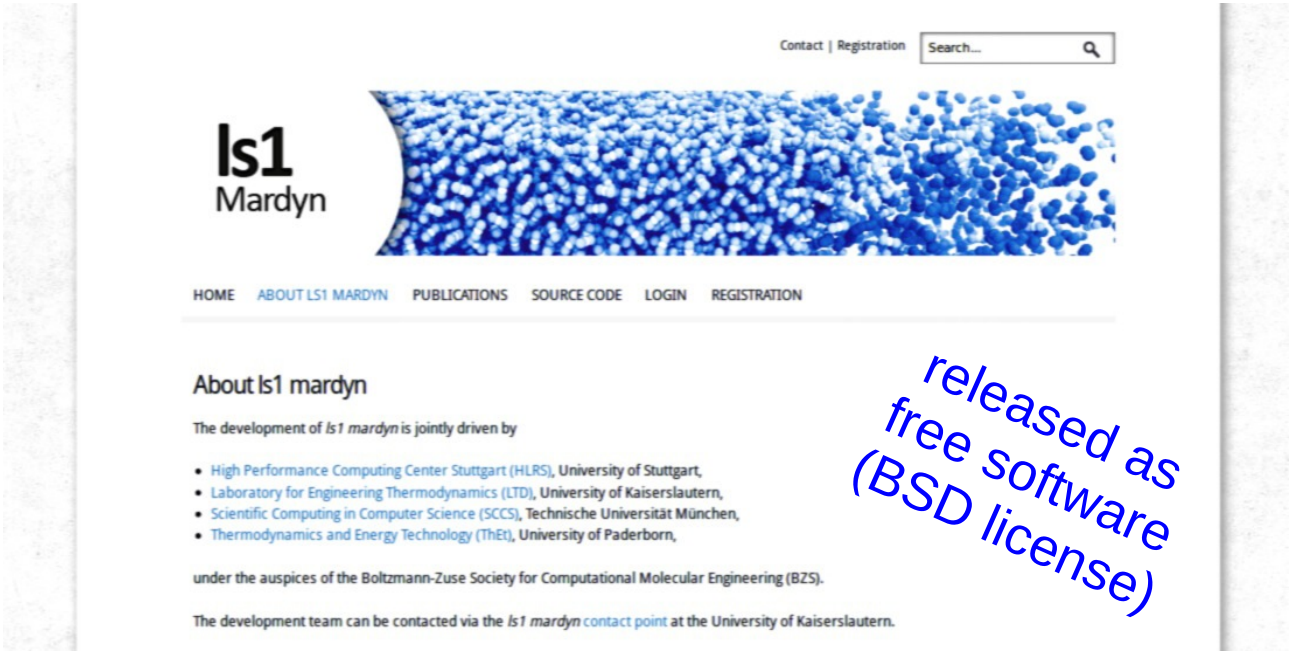




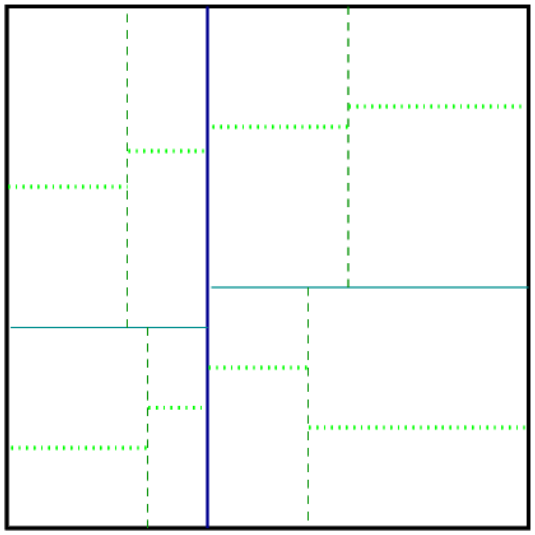


large systems 1: molecular dynamics

Large-scale MD simulation with the *ls1 mardyn* program



released as free software (BSD license)



Download *ls1 mardyn* at www.ls1-mardyn.de

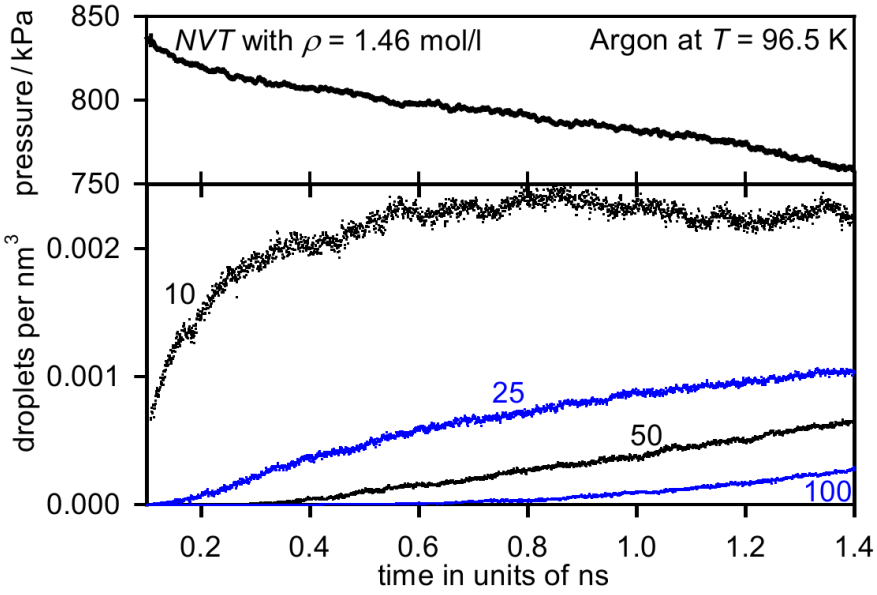
Simulation

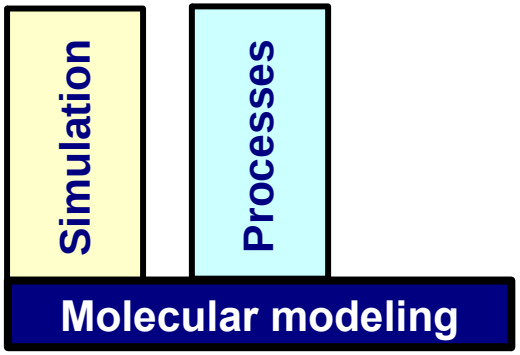
Molecular modeling

Molecular dynamics simulation of nucleation processes

Yasuoka-Matsumoto method:

- Canonical MD simulation
- Limited time interval for nucleation
- Conditions change over time





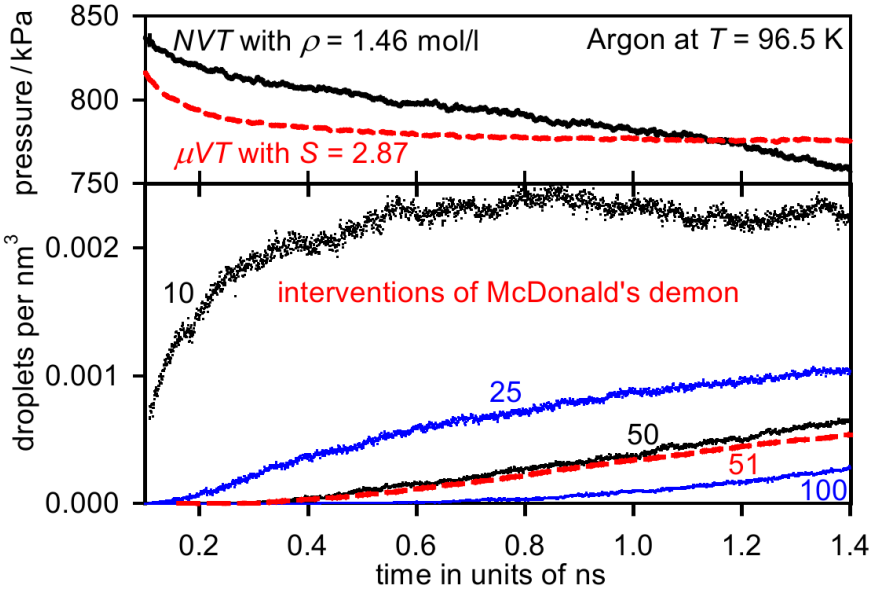
Non-equilibrium MD simulation of nucleation processes

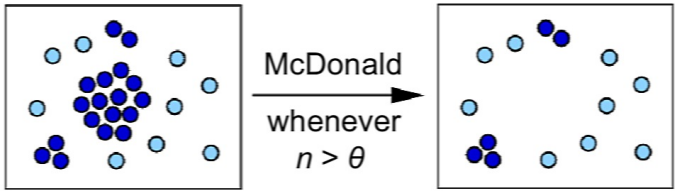
Yasuoka-Matsumoto method:

- Canonical MD simulation
- Limited time interval for nucleation
- Conditions change over time

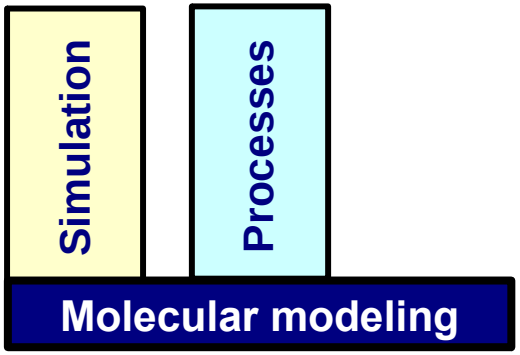
Alternative approach:

- Grand-canonical MD simulation





Constant conditions of the supersaturated vapor



Non-equilibrium MD simulation of nucleation processes

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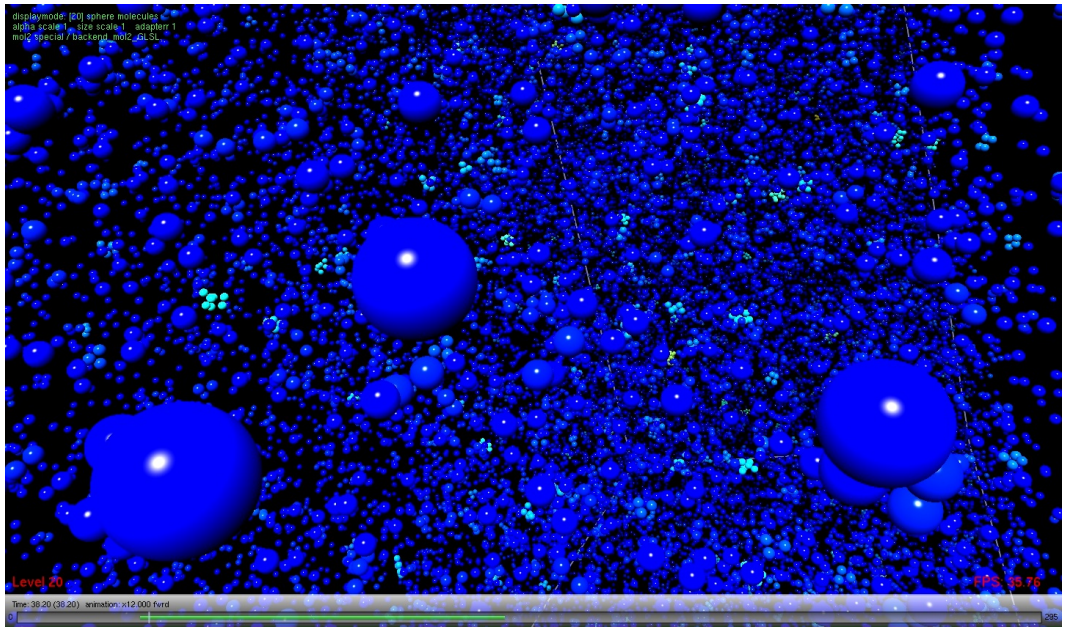

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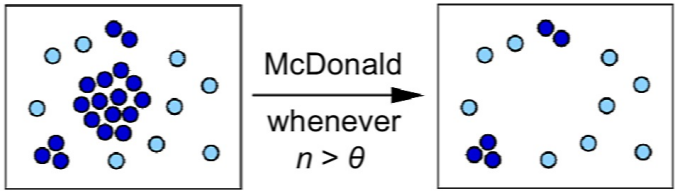

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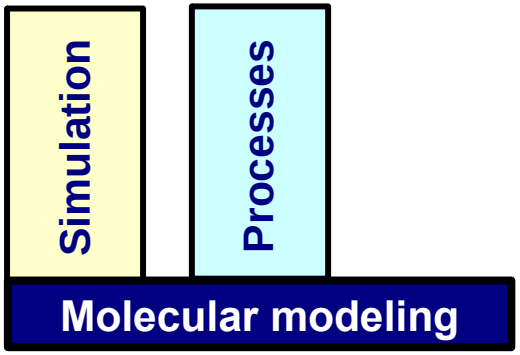
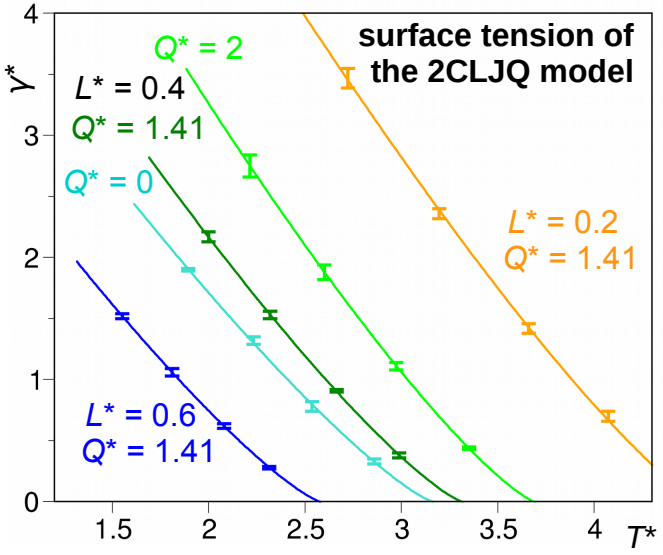
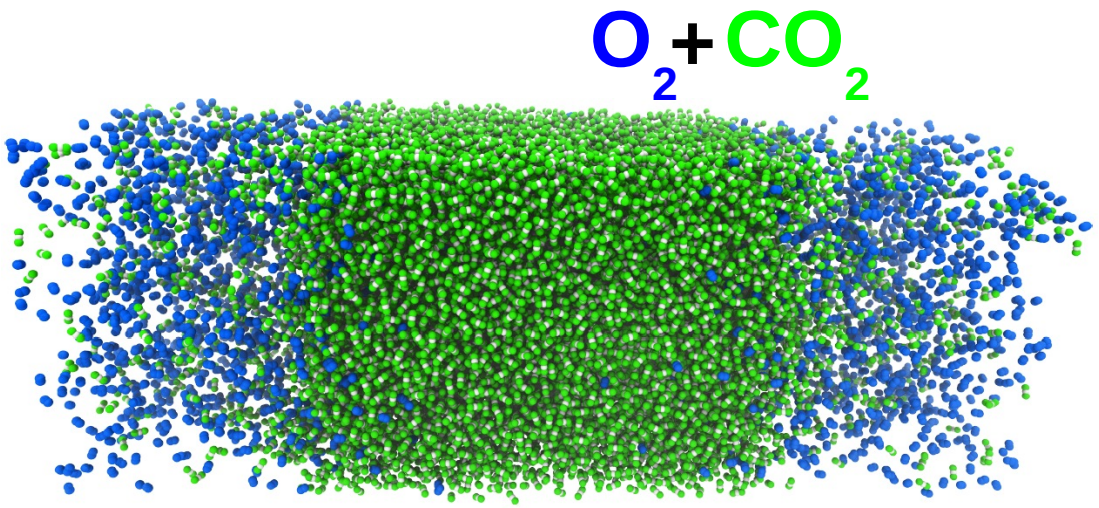
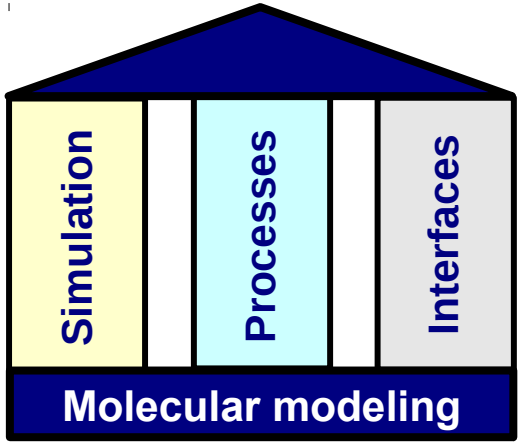


Molecular simulation of fluids at interfaces

- Adsorption (fluid-fluid and fluid-solid)
- Vapor-liquid surface tension
- Curved vapor-liquid interfaces
- Contact angle and contact line pinning
- Nucleation in supersaturated vapors







Thermodynamics and Computational Molecular Engineering