Topics for the Final Examination

“Computational Methods in Materials Science”

Prof. Dr. U. Herr:

- Definition of possible ensembles (NpT, NpE, NVE, …)
- Microcanonical/canonical ensembles
- Time scales and applications
- Interatomic potentials: types, limitations, advantages/disadvantages
- Boundary conditions, minimum image convention
- Neighbor lists, cell subdivision method
- Derivation of the equation of motion from potentials (Lagrange formalism)
- Realization of ensembles in MD simulation: T, p-control
- Integration of the equation of motion (Verlet algorithm, higher order algorithms)

- Computer lab experiment:

  interpretation of heating and cooling curves, extraction of CTE, comparison with “real” cooling experiments, formation of nanocrystalline materials in computer simulation, structure factor in comparison to ideal crystal, grain boundary energy determination and comparison with “real” values

- Monte Carlo method: Monte Carlo integration, Metropolis algorithm, Ising model, Kinetic Monte Carlo (Bortz-Lebowitz)