A video course on

„Computational Materials Science“

-November 2019-

This annual course is part of the Materials Science specialization within the Master program ‚Computer Simulation in Science‘. Students enrolled in the Physics Master may take this course in partial fulfillment of their ‚Fachliche Spezialisierung‘, where it is worth up to 6LP. Please be sure to consult with your prospective thesis advisor about your intention prior to taking the course.

Week 1	Lec 1	Introduction: introduction and basic concepts (simulation boxes, boundary conditions, error analysis)	
W1	Lec 2	Monte Carlo Simulation: Monte Carlo - sampling configuration space using the Metropolis criterium	
W2	Lec 3	changing ensembles – example (gas-liquid phase coexistence)	
W3	Lec 4	changing ensembles – more examples (adsorption and osmosis)	
W3	Lec 5	MC for small rigid and large flexible molecules	
W4	Lec 6	bias-MC and non-Boltzmann sampling – spec. example: Rosenbluth & umbrella sampling	
W5	Lec 7	Molecular Dynamics Simulation: Molecular Dynamics - general ideas and program structure; H-theorem	
W5	Lec 8	MD temperature control – example (thermal conductivity via Green-Kubo)	
W6	Lec 9	MD pressure control; forcefields	
W7	Lec 10	forcefield parameterization	
W7	Lec 11	long-range forces	
W8	Lec 12	accelerating the calculation of energies and forces	
W9	Lec 13	coarse-grained methods (Langevin dynamics and force-equilibrium)	
W9	Lec 14	Molecular Conformation and configuration at T=0 Molecular Mechanics - local and global minimization methods	
W10	Lec 15	Finite Element Method FEM - basic ideas	
W11	Lec 16	FEM in one dimension	
W11	Lec 17	FEM applied to a problem in the theory of elasticity	
W12	Lec 18	concepts in the theory of elasticity	
W13	Lec 19	Elastic constants from displacement fluctuations	
W13	Lec 20	an industry project – understanding and improving tire tread rubber using computational material science	

(Supplementary) literature:

General Overview:
D. Raabe (1998) *Computational Materials Science*. Wiley-VCH

Basic Principles of Mechanics, Thermodynamics and Statistical Mechanics:
R. Hentschke (2017) *Classical Mechanics*. Springer
R. Hentschke (2014) *Thermodynamics*. Springer
D.A. McQuarrie (2015) Statistical Mechanics. Viva Books; R. Hentschke (2004) *Statistische Mechanik*. Wiley-VCH

General Introduction to Computer Simulation of Molecular Systems:
M.P. Allen, D.J. Tildesley (1990) *Computer Simulation of Liquids*. Oxford University Press
D. Frenkel, B. Smit (1996) *Understanding Molecular Simulation*. Academic Press
D.C. Rapaport (1995) *The Art of Molecular Dynamics Simulation*. Cambridge University Press

Special Topics:
M. Kotelyanskii, D.N. Theodorou (2004) *Simulation Methods for Polymers*. Marcel Dekker
M. Meyer, V. Pontikis (1991) *Computer Simulation in Materials Science*. Kluwer Academic Press

FEM:
T.R. Chandrupatla, A.D. Belegundu (2007) Introduction to Finite Elements in Engineering

Note: Most of these references have been around for many years. Despite of this, these are good sources of information for beginners.