UNIVERSITY OF PANNONIA

SUBJECT DATASHEET

Semester:	2010/11/1
Subject:	Molecular Simulations
Code:	VEMKFKV112S
Responsible department:	Department of Physical Chemistry
Responsible department code:	MKFK
Responsible lecturer:	dr. Tamás Kristóf

Educational objectives:

Acquaint the students with the basic knowledge and potential applications of molecular simulation via lectures and source code examples.

Detailed content of the subject:

Introduction. Purpose, conception, area of application, and history of molecular simulations. Physical properties in molecular simulations. Configurational properties. Microscopic vs. macroscopic properties. Particle interactions. Born-Oppenheimer approximation. Holonomic constraints. Intermolecular potential functions. System size in molecular simulations (periodic boundary conditions, minimum image convention). Statistical mechanics. Statistical ensemble, partition function, ergodic system. Ensemble and time averages. Fluctuations. Monte Carlo simulations. Monte Carlo integration. Quasi-random numbers. Importance sampling. Metropolis method (canonical ensemble). Markov-chain. Criterion of microscopic reversibility. Basic Monte Carlo moves and their algorithms. Monte Carlo simulations in natural ensembles (isothermal-isobaric, grand canonical, microcanonical). Molecular dynamics (MD). Equations of motion. Thermodynamic boundary conditions. Newtonian, Lagrangian and Hamiltonian formulation. Numerical integration schemes. Verlet and other algorithms. Canonical and isothermal-isobaric MD. Calculation of transport properties. Nonequilibrium MD. Ab initio MD. Running simulations: initial configuration (velocity distribution), equilibration. Convergence. Simple biasing techniques. Efficient calculation of force, potential energy and pressure. Saving computational time: neighbour-list, potential cut-off. Code structure. Input-output file handling. Main routines and algorithms. Object orientation. Long-range corrections. Reaction field method. Ewald summation. Estimation of errors in molecular simulations. Calculation of correlation functions and structural properties. Calculation of free energy in molecular simulations. Determination of phase equilibria. Special biasing techniques. Adaptive methods. Use of rigid and flexible molecular models. Complex models. Simulation in special geometries. Pores and other confined geometries. Molecular simulation of surfaces. Industrial application of molecular simulation. MC and MD algorithms for parallel computers. Summary.

Requirements:

Nincs.

Required and suggested references:

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Required and suggested references:

D. Frenkel - B. Smit: Understanding Molecular Simulation: From Algorithms to Applications. Academic Press, San Diego, 1996. M. P. Allen - D. J. Tildesley: Computer Simulation of Liquids. Clarendon Press, Oxford, 1987.