PKU Globex Julmester

Fundamentals and Applications of Molecular Simulations (3 Credits)

分子模拟基础与应用

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Synopsis	This course will provide the students with an introductory level understanding of the concepts and techniques for the modeling and simulations of materials on atomistic and molecular scales. Both fundamentals and applications of the most popular molecular simulation methods including Monte Carlo (MC) simulations, Molecular Dynamics (MD) methods and Density Functional Theory (DFT) will be discussed, through examples distilled from the frontier of computational materials and soft matter research.	
Audience	Students taking this course should have some general knowledge of college physics and a background in and working knowledge of a computer programming language (C/ C++/ FORTRAN/ MATLAB).	
Classroom		
Schedule	Class: , M-F, July 1 -19, 2024	Total Contact Hours: 45
Topics	1. Essence of statistical mechanics and C/C++ programming 2. Fundamentals of Monte-Carlo simulation 3. Monte-Carlo simulations in different ensembles 4. Case study: Phase transitions in colloids 5. Optimization via simulated annealing 6. Fundamentals of molecular dynamics 7. Case study: Self-diffusion in liquid Argon 8. Many-body Schrödinger equation 9. Fundamentals of density functional theory 10. Equilibrium structure of materials: calculations vs. Experiment 11. Elastic properties of materials 12. Vibrations of molecules and solids 13. Phonons, vibrational spectroscopy, and thermodynamics 14. Band structures and photoelectron spectroscopy 15. Dielectric function and optical spectra	
Grading	Class Project Assignments (2 class projects) 70% Final Project 30% Total 100%	