UNIVERSITY of MISKOLC
Faculty of Materials and Chemical Engineering

Antal Kerpely Doctoral School of Materials Science & Technology

Computational Chemistry of Interfaces and Functional Materials

Prof. Dr. Babak MINOFAR

COURSE DESCRIPTION

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Author: Dr. Babak MINOFAR

Computational Chemistry of Interfaces and Functional Materials

Prof. Dr. Babak MINOFAR

Lecturer

Babak Minofar, Research Professor, Institute of Higher Education and Industrial Cooperation.
room: Building A2, Room B3.
e-mail: babak.minofar@uni-miskolc.hu
phone: +36 46 565-111/1141
www: https://ki.uni-miskolc.hu/munkatarsak/michael-owen/

Recommendation

The lecture is proposed for all students of the Kerpely Doctoral School, with a special focus on students interested in chemistry and computer simulations.

Language

English.

Scope

The main goal of the course is to provide students with an overview of modern molecular dynamics (MD) simulation tools and apply them to nano-materials, condensed phases, and interfaces.

Methodology

The course is conducted through in-person lectures and practical sessions. The main goal of the course is to provide students with a comprehensive overview of modern atomistic simulation methods, with particular emphasis on molecular dynamics simulations and their applications to interfaces and functional materials. The course introduces the theoretical foundations of molecular simulations and demonstrates how atomistic modeling can be used to investigate structural, dynamical, and thermodynamic properties of complex molecular systems. Special attention is given to solid–liquid and air–water interfaces, carbon-based materials such as graphene and graphene oxide, and environmentally relevant systems, including adsorption and removal of contaminants and pharmaceuticals from water. Through practical examples, students will learn how atomistic simulations can help understand molecular mechanisms governing interfacial processes, materials performance, and environmental remediation. Students are trained to apply these methods to use software packages such as AMBER and GROMACS, enabling them to apply their knowledge practically to systems of interest. Through guided exercises and case studies, students will apply simulation techniques to interfacial systems, adsorption processes, and functional materials, enabling them to connect theoretical knowledge with practical applications.

Topics

1. Introduction to atomistic simulations and molecular dynamics

2. Force field parametrization, simulation setup, and analysis using AMBER and GROMACS

3. Atomistic simulations of interfaces.

4. Molecular simulations of functional materials

5. Adsorption and environmental applications.

References

1. Leach, A. R. Molecular Modelling: Principles and Applications. 2nd ed.; Prentice Hall: Harlow, 2001.
2. Frenkel, D. and Smit, B. (2002) Understanding Molecular Simulations. 2nd Edition, Academic Press, San Diego.
3. Rapaport, D. C. The Art of Molecular Dynamics Simulation. 2nd ed.; Cambridge University Press: Cambridge, 2004.
4. Allen, M. P.; Tildesley, D. J. Computer Simulation of Liquids. 2nd ed.; Oxford University Press: Oxford, 2017.

Exam

Project work.

Complex exam questions

1. Explain what a simulation box is and describe the main requirements for defining it in molecular dynamics simulations. What are periodic boundary conditions (PBC)? Discuss their purpose and the key considerations when applying PBC to molecular systems.

2. Describe the main types of intermolecular interactions considered in molecular dynamics simulations. Explain how van der Waals and electrostatic interactions are treated and discuss the role of cutoff distances in their calculation.

3. What is a force field in molecular dynamics simulations? Describe the main components of a typical force field (bonded and non-bonded interactions) and explain how these parameters influence the accuracy of simulations.

4. Explain how temperature and pressure are controlled in molecular dynamics simulations. Discuss the role of thermostats and barostats and provide examples of commonly used algorithms.

5. Explain why long-range electrostatic interactions are important in molecular simulations. Describe the Particle Mesh Ewald (PME) method and discuss why it is commonly used in MD simulations.

6. Discuss the importance of the integration time step in molecular dynamics simulations. What factors determine the appropriate time step, and what are the consequences of choosing a time step that is too large?

7. Explain the purpose of energy minimization and equilibration steps in molecular dynamics simulations. Why are these steps necessary before starting production simulations?

8. Describe the role of solvent in molecular simulations. Compare explicit and implicit solvent models and discuss their advantages and limitations.

9. Describe several methods used to analyze molecular dynamics trajectories. Explain how properties such as diffusion coefficients, hydrogen bonding, and structural stability can be extracted from simulation data.