جامعة الملك عبدالله للعلوم والتقنية
King Abdullah University of Science and Technology

Course Syllabus: Ab-Initio Computational Methods - MSE 314

Division	Physical Science and Engineering Division
Course Number	MSE 314
Course Title	Ab-Initio Computational Methods
Academic Semester	Fall
Academic Year	2018/2019
Semester Start Date	08/26/2018
Semester End Date	12/11/2018
Class Schedule (Days & Time)	02:30 PM - 04:00 PM | Sun Wed

Instructor(s)

Name	Email	Phone	Office Location	Office Hours
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Teaching Assistant(s)

Name	Email

Course Information

Comprehensive Course Description	This course provides an overview of modern computer simulation methods, such as molecular dynamics and Monte Carlo techniques, free energy methods, advanced force fields, long-range interactions, coarse-graining, markov state models, machine learning, and density functional theory. The topics are designed to be accessible for graduate students, who are familiar with the basic concepts of statistical physics and quantum mechanics. Knowledge of a programming language is useful but not mandatory. Note: This course will be taught by Visiting Associate Professor Dr Denys Andriyenko from the Max Planck Institute for Polymer Research Mainz, Germany.
Course Description from Program Guide	Prerequisite: Applied Quantum Mechanics (MSE 304). Band structure approaches for crystalline solids. Fundamentals and advanced applications of density functional theory. Introduction into classical and quantum molecular dynamics. Application and use of commercial and freeware computer packages.
Goals and Objectives	At the end of the course the attendees will: - understand molecular dynamics and monte carlo simulation techniques - understand first principles methods: (post) hartree-fock, density functional theory - be able to write code in python - have an overview of available commercial/free simulation packages
Required Knowledge	Previous exposure to quantum mechanics and physical chemistry.
Reference Texts	1.) Course Script and Lecture Slides. 2.) Further reference texts will be provided during the lectures.
Method of evaluation	**50.00**% - Final exam **50.00**% - Course Project(s)
Nature of the assignments	Group projects (2 students per project) Presentation
Course Policies	Attendance is mandatory. Absences need to be fully justified.

Additional Information	This course will be taught by Visiting Associate Professor Dr Denys Andriyenko from the Max Planck Institute for Polymer Research Mainz, Germany.

Tentative Course Schedule

(Time, topic/emphasis & resources)

Week	Lectures	Topic
1	Sun 08/26/2018	Recap of statistical physics
1	Wed 08/29/2018	Recap of quantum mechanics
2	Sun 09/02/2018	Introduction to python and jupyter editor
2	Wed 09/05/2018	Error estimates of correlated data
3	Sun 09/09/2018	Molecular dynamics
3	Wed 09/12/2018	Integration algorithms. Accuracy, time-reversibility
4	Sun 09/16/2018	Thermostats
4	Wed 09/19/2018	Barostats
5	Sun 09/23/2018	Long-range interactions. Ewald summation
5	Wed 09/26/2018	Force-fields
6	Sun 09/30/2018	Advanced force-fields: distributed multipoles
6	Wed 10/03/2018	Polarizable force-fields: Thole model
7	Sun 10/07/2018	van der Waals interactions
7	Wed 10/10/2018	Hands-on: GROMACS
8	Sun 10/14/2018	Free energy methods: thermodynamic integration
8	Wed 10/17/2018	Histogram re-weighting and Bennet's acceptance ratio
9	Sun 10/21/2018	Replica Exchange MD. Weighted histogram analysis
9	Wed 10/24/2018	Umbrella sampling. Principal component analysis
10	Sun 10/28/2018	Metadynamics
10	Wed 10/31/2018	Markov state models
11	Sun 11/04/2018	Coarse-graining
11	Wed 11/07/2018	Monte Carlo: integration, importance sampling
12	Sun 11/11/2018	Metropolis Monte Carlo, Ensembles
12	Wed 11/14/2018	Master equation and Kinetic Monte Carlo
13	Sun 11/18/2018	Machine learning
13	Wed 11/21/2018	Born-Oppenheimer approximation, electronic charge density
14	Sun 11/25/2018	Hartree-Fock approximation
14	Wed 11/28/2018	Density functional theory. Kohn-Sham DFT
15	Sun 12/02/2018	Exchange-correlation functionals
15	Wed 12/05/2018	Hands-on: GAUSSIAN
16	Sun 12/09/2018	Final Exam

Note

The instructor reserves the right to make changes to this syllabus as necessary.