



Course Syllabus: Contemporary Topics in Materials Science - MSE 394

Division	Physical Science and Engineering Division
Course Number	MSE 394
Course Title	Contemporary Topics in Materials Science
Academic Semester	Summer
Academic Year	2017/2018
Semester Start Date	06/10/2018
Semester End Date	08/09/2018
Class Schedule (Days & Time)	10:00 AM - 01:00 PM Sun Tue

Instructor(s)

Name	Email	Phone	Office Location	Office Hours
Udo Schwingenschloegl	Udo.Schwingenschloegl@kaust.edu.sa	+966128084399 8084399	3233, 3, Ibn Sina (bldg. 3)	Sunday 4-5 pm

Teaching Assistant(s)

Name	Email
------	-------

Course Information

Comprehensive Course Description	Prerequisite: Ab-Initio Computational Methods (MSE 314). Content: Short summary of MSE 314. Properties of common density functionals. Introduction into phonon calculations. First-principles Boltzmann transport theory for electrons and phonons. Introduction into the nudged elastic band method. Application of advanced ab-initio computational methods in case studies.
Course Description from Program Guide	Lecture-based class
Goals and Objectives	<ul style="list-style-type: none"> - The student will obtain an overview of density functionals and their properties. - The student will be able to calculate and interpret phonon spectra. - The student will be able to employ first-principles Boltzmann transport theory. - The student will be able to perform nudged elastic band calculations.
Required Knowledge	MSE 314
Reference Texts	Recent articles from the literature
Method of evaluation	50.00% - Oral presentation 50.00% - Course Project(s)
Nature of the assignments	Oral presentations, Case study
Course Policies	Active participation required. No absences. No credit for late work.
Additional Information	

Tentative Course Schedule

(Time, topic/emphasis & resources)

Week	Lectures	Topic
1	Sun 06/10/2018	Revision of the contents of MSE314
1	Tue 06/12/2018	Revision of the contents of MSE314
2	Sun 06/17/2018	Eid Al-Fitr break
2	Tue 06/19/2018	Eid Al-Fitr break
3	Sun 06/24/2018	Density functionals and their properties
3	Tue 06/26/2018	Density functionals and their properties
4	Sun 07/01/2018	Calculation of phonon spectra: Theory
4	Tue 07/03/2018	Calculation of phonon spectra: Applications
5	Sun 07/08/2018	Electronic Boltzmann transport: Theory
5	Tue 07/10/2018	Electronic Boltzmann transport: Applications
6	Sun 07/15/2018	Phononic Boltzmann transport: Theory
6	Tue 07/17/2018	Phononic Boltzmann transport: Applications
7	Sun 07/22/2018	Nudged elastic band method: Theory
7	Tue 07/24/2018	Nudged elastic band method: Applications
8	Sun 07/29/2018	Case study
8	Tue 07/31/2018	Case study
9	Sun 08/05/2018	Case study
9	Tue 08/07/2018	Case study

Note

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