ABDULLAH GÜL UNIVERSITY
GRADUATE SCHOOL OF ENGINEERING & SCIENCE
MATERIALS SCIENCE AND MECHANICAL ENGINEERING PROGRAM
COURSE DESCRIPTION AND SYLLABUS

Course Title	Code	Semester	T+L Hours	Credit	ECTS
Computational Materials Science	AMN 574	FALL-SPRING	3 + 2	3	10

Prerequisite Courses	Knowledge of lunix/unix operation system

Type	Elective
Language	English
Coordinator	Murat Durandurdu
Instructor	Murat Durandurdu
Adjunt	none
Aim	To learn the theory, methods, and applications of quantum mechanical software SIESTA for computational study of materials.
Learning Outcomes	Student will have practical experiences in calculating electronic and mechanical properties of materials, modeling amorphous materials and studying temperature/pressure induced phase transformations using a density functional code SIESTA
Course Content	Applications of Density Functional Calculations on crystals, disordered materials and nanomaterials and calculations of their physical properties

WEEKLY TOPICS AND PRELIMINARY STUDY

Week	Topic	Preliminary Study
1	Introduction to materials modeling and simulation	The relevant articles from the literature
2	Brief review of unix/lunix, parallel computers and batch systems.	The relevant articles from the literature
3	Density functional theory	The relevant articles from the literature
4	Density functional theory	The relevant articles from the literature
5	Introduction to SIESTA code	The relevant articles from the literature
6	Crystal structure relaxation and lattice parameters	The relevant articles from the literature
7	Calculation of electronic and mechanical properties of crystals	The relevant articles from the literature
8	Solid-liquid phase transformation using SIESTA	The relevant articles from the literature
9	Pressure-induced solidification of liquids	The relevant articles from the literature
10	Modeling amorphous materials.	The relevant articles from the literature
11	Analyses of disordered systems (amorphous and liquids)	The relevant articles from the literature
12	Pressure-induced phase transformations	The relevant articles from the literature
13	Modeling nanomaterials	The relevant articles from the literature
14	Project Reports	
15	Project Reports	
16	Project Reports	

SOURCES	
Lecture Notes	Lecture notes and presentations
Other Sources	D. J. Barrett, *Linux Pocket Guide* (O'Reilly, 2004). D. Sholl, *Density Functional Theory: A Practical Introduction* (Wiley, 2009). R. Martin, *Electronic structure: Basic theory and practical methods* (Cambridge, 2004). E. Kaxiras, *Atomic and Electronic Structure of Solids* (Cambridge, 2003). J. G. Lee, *Computational Materials Science: An Introduction* (CRC Press, 2011). F. Jensen, *Introduction to Computational Chemistry* (Wiley, 2006).

COURSE MATERIALS SHARING	
Documents	Lectures notes are shared on the internet
Homeworks	Students will be given one homework each week
Exams	Project Report

EVALUATION SYSTEM		
SEMESTER STUDY	**NUMBER**	**CONTRIBUTION**
Homework	13	50
Final Project	1	50
Quiz		
SUB-TOTAL	14	100
Contribution of Semester Study		
Contribution of Final Exam		
TOTAL	14	100

Course Category	
Sciences and Mathematics	50%
Engineering	50%
Social Sciences	0%

RELATIONSHIPS BETWEEN LEARNING OUTCOMES AND PROGRAM QUALIFICATIONS						
No	Program Qualifications	Contribution Level				
		1	2	3	4	5
1	Accessing knowledge, evaluating and interpreting information by doing scientific research in the field of Materials Science and Mechanical Engineering					x
2	Ability to use science and engineering knowledge for development of new methods in Materials Science and Mechanical Engineering					x
3	To be able to understand and analyze materials by using basic knowledge on Materials Science and Mechanical Engineering					x
4	Design and implement analytical, modeling and experimental research					x
5	Solve and interpret the problems encountered in experimental research			x		
6	Considering scientific and ethical values during the collection and interpretation of data	x				
7	Integrating knowledge of different disciplines with the help of scientific methods, and completion and implementation of scientific knowledge using data				x	
8	To gain leadership ability and responsibility in disciplinary and interdisciplinary team works				x	
9	To be able to contribute to the solution of social, scientific and ethical problems encountered in the field of Materials Science and Mechanical Engineering		x			
10	To be able to define, interpret and create new information about the interactions					x

	between various discipline of Materials Science and Mechanical Engineering					

*Increasing from 1 to 5.

ECTS / WORK LOAD TABLE			
Activities	Number	Duration (Hours)	Total Work Load
Course Length (includes exam weeks: 16x total course hours)	16 weeks	5	80
Out-of-class Study Time (Pre-study, practice)	16 weeks	5	80
Internet search, library work, literature search	16 weeks	3	48
Presentation	3 weeks	5	15
Homework	13 weeks	5	65
Midterm			
Final Exam			
Total Work Load			288
Total Work Load / 30		23	288/23
Course ECTS Credit			10