AYDIN ADNAN MENDERES UNIVERSITY
COURSE INFORMATION FORM

Course Title	Density Functional Theory								
Course Code	FZK530		Couse Level	Second Cycle (Master's Degree)					
ECTS Credit	6	Workload	150 *(Hours)*	Theory	3	Practice	0	Laboratory	0
Objectives of the Course	Students acquire advanced knowledge on the basis of density-functional theory and the basics of solid state physics.								
Course Content	Fundamentals of DFT, Summary of basic quantum mechanics, historic origin of DFT, Further plane wave-based DFT methods								
Work Placement									
Planned Learning Activities and Teaching Methods	Explanation (Presentation), Discussion, Individual Study, Problem Solving								
Name of Lecturer(s)	Prof. Ethem AKTÜRK								

Assessment Methods and Criteria		
Method	Quantity	Percentage (%)
Midterm Examination	1	20
Final Examination	1	30
Quiz	2	8
Attending Lectures	14	28
Assignment	14	14

Recommended or Required Reading	
1	Electronic Structure : Basic Theory and Practical Methods, Richard Martin
2	Methods of Electronic Structure Calculations Micheal Springborg

Week	Weekly Detailed Course Contents	
1	Theoretical	Preliminary topics : variational principle, solid state concepts, the many-body Hamiltonian, Born-Oppenheimer approximation
	Preparation Work	Micheal Springborg, 2000. Methods of Electronic Structure Calculations.West Sussex: John Wiley & Sons Ltd. (p1-66)
2	Theoretical	The Hartree-Fock approach
	Preparation Work	Micheal Springborg, 2000. Methods of Electronic Structure Calculations.West Sussex: John Wiley & Sons Ltd. (p82-109)
3	Theoretical	Hamiltonian in terms of density, Hohenberg-Kohn theorems, Kohn-Sham formalism
	Preparation Work	Micheal Springborg, 2000. Methods of Electronic Structure Calculations.West Sussex: John Wiley & Sons Ltd. (p123-144)
4	Theoretical	Exchange and correlations : LDA and GGA approximations
	Preparation Work	Richard M. Martin, 2004. Electronic Structure : Basic Theory and Practical Methods. Cambridge: Cambridge University Press (p152-170)
5	Theoretical	Pseudopotentials
	Preparation Work	Richard M. Martin, 2004. Electronic Structure : Basic Theory and Practical Methods. Cambridge: Cambridge University Press (p152-170)
6	Theoretical	Plane-wave formalism
	Preparation Work	Richard M. Martin, 2004. Electronic Structure : Basic Theory and Practical Methods. Cambridge: Cambridge University Press(p236-241)
7	Theoretical	Tricks for self-consistent solution of the Kohn-Sham system
	Preparation Work	Richard M. Martin, 2004. Electronic Structure : Basic Theory and Practical Methods. Cambridge: Cambridge University Press(p119-150)
8	Intermediate Exam	Midterm Exam
9	Theoretical	Forces, stress and the Hellman-Feynman theorem
	Preparation Work	Micheal Springborg, 2000. Methods of Electronic Structure Calculations.West Sussex: John Wiley & Sons Ltd. (p298-309)
10	Theoretical	How to deal with the ions : Ewald sum
	Preparation Work	Micheal Springborg, 2000. Methods of Electronic Structure Calculations.West Sussex: John Wiley & Sons Ltd. (p434-450)

11	Theoretical	Application of DFT with examples, PWSCF
	Preparation Work	Richard M. Martin, 2004. Electronic Structure : Basic Theory and Practical Methods. Cambridge: Cambridge University Press(p365-380)
12	Theoretical	Speacialized topic
	Preparation Work	Richard M. Martin, 2004. Electronic Structure : Basic Theory and Practical Methods. Cambridge: Cambridge University Press(p380-420)
13	Theoretical	Exchange-correlation functionals
	Preparation Work	Richard M. Martin, 2004. Electronic Structure : Basic Theory and Practical Methods. Cambridge: Cambridge University Press(p186-200)
14	Theoretical	Density functional, perturbation theory
	Preparation Work	Richard M. Martin, 2004. Electronic Structure : Basic Theory and Practical Methods. Cambridge: Cambridge University Press(p186-200)
15	Theoretical	Phonon spectrum
	Preparation Work	Micheal Springborg, 2000. Methods of Electronic Structure Calculations.West Sussex: John Wiley & Sons Ltd. (p387-400)
16	Final Exam	Final Exam

Workload Calculation

Activity	Quantity	Preparation	Duration	Total Workload
Lecture - Theory	14	2	3	70
Assignment	14	2	0.5	35
Quiz	2	3	1	8
Midterm Examination	1	12	3	15
Final Examination	1	19	3	22
			Total Workload (Hours)	150
			[Total Workload (Hours) / 25*] = **ECTS**	6

**25 hour workload is accepted as 1 ECTS*

Learning Outcomes

1	To be able to understand to role of symmetry in physics and chemistry and how to use group tables;
2	To be able to learn how to compute molecular structure, molecular orbitals, energy levels and spectra;
3	To be able to understand vibrational and electronic spectra in terms of symmetry and to connect real spectra with the computations they have performed
4	To be able to write the Hamiltonian of a system in terms of the density and know the meaning of each energy term.
5	To be able to calculate the ground state energy by means of the variation method.
6	To be able to know the advantages and disadvantages of the solutions which are obtained by using the plane wave.
7	To be able to know the usage of force, pressure and Hellman-Feynman theorem in density functional.

Programme Outcomes *(Physics Master)*

1	The student should conceive the concepts in physics and may apply them on her/his own
2	The student should be able to conceive the relationship between the different physics laws and integrity of them and apply them in solving different physics problems
3	The student should know the basic principles of classical, quantum and relativistic physics and use them in the solutions of problems
4	The student should be able to do research in a specific area of physics
5	The student should be able to prepare reports on papers on the subject of her/his research and present her/his research subject in scientific conferences
6	The student should be able to explain the relationship between complicated problems and basic physics laws.
7	The student should be able to use computers for solving complicated physics problems
8	The student should be able to interrelate between the theory and the experiment. If she/he is experimentalist he/she has to explain the theory behind her/his work. If she /he is a theorist she/he should has to know the experiments in her/his subject.

Contribution of Learning Outcomes to Programme Outcomes *1:Very Low, 2:Low, 3:Medium, 4:High, 5:Very High*

	L1	L2	L3	L4	L5	L6	L7
P1	3	3	3	4	3	3	3
P2	4	3	4	4	3	4	3
P3	3	3	3	3	4	4	5

P4	2	2	2	2	3	3	4
P5	2	2	2	2	2	2	3
P6	3	3	2	3	3	1	3
P7	1	1	1	3	1	3	3
P8	2	2	2	2	3	3	2