AYDIN ADNAN MENDERES UNIVERSITY
COURSE INFORMATION FORM

Course Title	Quantum Chemistry of Solid								
Course Code	FZK610		Couse Level		Third Cycle (Doctorate Degree)				
ECTS Credit	7	Workload	170 *(Hours)*	Theory	3	Practice	0	Laboratory	0
Objectives of the Course	The lecture deals with the basic concepts of the theory and calculations of electronic structure of solids.								
Course Content	Crystal structure, discrete and continuous groups, Basic concepts of quantum physics and chemistry, Principles of methods for electronic structure calculations, Electronic structure calculations for surfaces and interfaces.								
Work Placement	N/A								
Planned Learning Activities and Teaching Methods	Explanation (Presentation), Discussion, Individual Study, Problem Solving								
Name of Lecturer(s)									

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	Introduction to the quantum chemistry of solids,C. M. Quinn
2	Physical Chemistry, P. Atkins and J. De Paul
3	The physics and chemistry of solids, S. Elliott, S. R. Elliott

Week	Weekly Detailed Course Contents	
1	Theoretical	Basic concepts of quantum physics and chemistry
2	Theoretical	Symmetry of Periodic Solids
3	Theoretical	LCAO Hartree-Fock and Density Functional Methods
4	Theoretical	Space groups and crystal structure
5	Theoretical	Irreducible representations of space groups
6	Theoretical	Representations of point and space groups
7	Theoretical	Use of the space symmetry groups in LCAO methods
8	Intermediate Exam	Midterm
9	Theoretical	Hartree-Fock-Roothaan LCAO method for periodic solid
10	Theoretical	DFT LCAO methods for periodic solids
11	Theoretical	Band structure, optical properties and density of states in bulk crystals
12	Theoretical	Crystal structure optimization in LCAO method
13	Theoretical	Chemical bonding in periodic solids
14	Theoretical	Point defects in ionic solids
15	Theoretical	The electronic properties of Graphene and Silicene
16	Final Exam	Final Exam

Workload Calculation				
Activity	Quantity	Preparation	Duration	Total Workload
Lecture - Theory	14	2	3	70
Assignment	12	4	1	60
Midterm Examination	1	10	2	12

Final Examination	1	25	3	28
			Total Workload (Hours)	170
			[Total Workload (Hours) / 25*] = **ECTS**	7
**25 hour workload is accepted as 1 ECTS*				

Learning Outcomes	
1	After completion of the course student will be able to understand the connections between the electronic structure and technologically important properties of solids
2	To perform electronic calculations for simpler systems structure
3	To use the results of such calculations to analyze the connection between structure and properties of solids (structure-property relations).
4	To be able to calculate the ground states of simple lattices by using strong bound approximation.
5	To be able to explain how the chemical bounds occur and the causes of variations.
6	To be able to write the ground state configurations of elements by using the Hund rule.

Programme Outcomes *(Physics Doctorate)*	
1	
2	
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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
P1	4	3	5	4	5	4
P2	5	4	4	3	4	5
P3	4	3	4	4	5	4
P4	3	4	4	4	3	3
P5	3	5	3	3	4	4
P6	4	4	4	4	3	3
P7	2	3	3	3	4	3
P8	3	4	4	3	4	3