



T.C.
FIRAT UNIVERSITY
Course Syllabus Form

Document No	EGTM - 0001
Publication Date	13.09.2021
Revision Date	-
Revision No	0

Code and Name:

FİZ5480 MOLECULAR MODELING AND ALGORITHMS

Unit:

Graduate School of Natural and Applied Sciences

Detail:

Period: 2023-2024

Status: Optional

Class: 1

Credits: 3-0-0-3

ECTS: 6

Language: Turkish

INSTRUCTOR

Title, Name and Surname: -

Phone: -

Email: -

Social Account: -

Student Day and Time: -

COURSE ASSISTANT

Title, Name and Surname:

Phone:

Email:

Social Account:

Student Day and Time:

Lessons Weekly Program:

Monday

Tuesday

Wednesday

Thursday

Friday

Saturday

-

Rendering Place:

Face-to-face lessons per week 3 It will be done on an hourly basis.

YY: -

UE: -

Purpose:

In the field of molecular physics, it is aimed to catch up with the era and go beyond the relevant field by using the developing technology and the highest methods together with the relevant modeling and algorithms.

Material:

G. Herzberg, Diatomic Molecules; G.W. King, Spectroscopy and Molecular Structure, Holt-Rinehard and Winston INC, NY

Student Responsibility :

Preparing before and after class

Weekly Lesson Plan	Week	Topic	Method		
	1	Basic Molecular Modeling Concepts , Bağ Teorisi ve Bağ Uzunlukları	YY		
	2	Wave Function and quantum mechanical interpretation and analysis	YY		
	3	Electronic Structure Calculations , MP2, M062x	YY		
	4	Base sets and their meaning	YY		
	5	Molecular Optimization Algorithms ,	YY		
	6	Genetic Algorithms	YY		
	7	Hartree-Fock and Condensed Calculations	YY		
	8	Condensed Matter and Circulation Calculations	YY		
	9	MIDTERM EXAM	YY		
	10	Molecular Recognition and Interactions	YY		
	11	Integration of Artificial Intelligence and Molecular Modeling	YY		
	12	Machine Learning and Molecular Design	YY		
	13	Drug Design and Development	YY		
	14	Applications of Materials Science and biological systems analysis	YY		
Assessment and Evaluation	Method		umbe	Weight	
	Break Exam	Exam	Face	1	% 50
		Quiz	-	-	
		Homework	-		
		Project	-	-	-
General Exam	Face		1	% 50	
Course Outcomes:	1	Molecular modeling and algorithms are learned.			
	2	Learns molecular optimization.			
	3	Have knowledge in artificial intelligence and deep learning in molecular modeling .			
	4	Have knowledge about drug design and development methods.			
	5	Experience is gained for materials science and biological system arguments and analyses.			

Course-Specific Explanations:

UE: Distance Education; YY: Face-to-Face Education



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