



Code and Name:

FİZ5400 QUANTUM MECHANICAL REACTION DYNAMICS

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:

Analysis of Atomic and Molecular Reactions by Quantum Methods

Material:

R. D. Levine; Molecular Reaction Dynamics, 2005, Cambridge, United Kingdom; P. W. Atkins, Physical Chemistry, 1998, Oxford Melbourne Tokyo

Student Responsibility :

Conducting preparation and research before and after the lecture.

Weekly Lesson Plan

Week	Topic	Method
1	Introduction to quantum mechanical methods for reaction dynamics	YY
2	Time-Independent Quantum Method; Closed Pairing-Dual State Approach	YY
3	Time-Dependent Quantum Method	YY
4	Solution of the Time-Dependent Schrödinger Equation for Chemical Reactions	YY
5	Elastic, Inelastic and Reactive Scattering of Atoms and Molecules	YY
6	Photodecomposition phenomenon	YY
7	Equations of Motion for Three-Dimensional Scattering Reactions	YY
8	B Hang Defining the Wave Function and Solving it in Schrödinger's Equation	YY
9	MIDTERM EXAM	YY
10	Fourier Grid Transform Technique of the Time-Dependent Schrödinger Equation Extraction	YY
11	Conversion of Wavepackets into Reaction Channels	YY
12	Calculating Reaction Costs	YY
13	Calculation of Reaction Impact Cross-Sections	YY
14	Calculation of Reaction Rate Constants	YY

Assessment and Evaluation

Method		Number	Weight
Break Exam	Exam	Face	1 % 50
	Quiz	-	-
	Homework	-	-
	Project	-	-
General Exam	Face	1	% 50

Course Outcomes:

1	Have general knowledge about molecular systems.
2	Molecular Hamilton and Understands en terms in detail.
3	To analyze the electronic structures of a molecular system by theoretical methods
4	Describe wave functions representing a molecular system undergoing a chemical reaction and can perform theoretically analyzes throughout the reaction.
5	

Course-Specific Explanations:

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



T.C.
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Course Syllabus Form

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