SEMESTER LEARNING ACTIVITY PLANS
(SLAP)
SEMESTER EVEN 2022/2023

Condensed Matter Electronics Structure Computation

MFF5514 / 3 Credits

Lecturer Coordinator:

Dr. Iman Santoso, S.Si., M.Sc.

UNIVERSITAS GADJAH MADA
FACULTY OF MATHEMATICS AND NATURAL SCIENCE
2022

Universitas Gadjah Mada
Faculty of Mathematics and Natural Science
Physics Department / Study Program Master Physics
Semester Even 2022/2023

SEMESTER LEARNING ACTIVITY PLANS (SLAP)

Code	Course Name	Credits (credits)	Semester	Status	Prerequisite
MFF5514	*Condensed Matter Electronics Structure Computation*	*3*	*Even*	*Elective*	*None*

Short Description

Condensed Matter Electronics Structure Computation course is Elective course 3 credits (Theory) in the 2022 Curriculum Master Physics Study Program, Faculty of Mathematics and Natural Science UGM.

The syllabus of this course is as follows:
Theory of electronic and atomic structures, molecules and solids, factorization and iteration methods for eigenvalues problems, pseudo-potential models of field waves, integration of Brillouin zones, Self-Consistent Field, Hartree-Fock Method, Tight Binding Method, Density Functional Theory (DFT) Method, Classical molecular dynamics model, and Car-Parrinello Lagrangian.

The courses are held in class for 14 weeks, each week's session last for 3 x 50 minutes. Four weeks of course period is used for Midterm Exam and Final Exam, each held for two weeks as scheduled.

Student evaluation for course assessments is performed summative and formative. The summative evaluation is implemented as written exams, both Midterm and Final Exam, which take a maximum of 120 minutes. The formative evaluation is implemented as individual assignments for each student in the form of completing an assignment individually. Monitoring is carried out by observing student activities during the course, such as attendance, Q&A and discussion about the material presented, and student performance in completing individual assignments.

Program Learning Outcomes (PLO) Imposed on the Course

PLO 3	Mastering further knowledge of classical and modern physics theory, and its relationship with other disciplines, and has mastered an advanced field of physics specialization that allows him to keep up with the latest international research developments.
PLO 4	Mastering various mathematical disciplines related to an advanced field of physics, and able to develop physical models using various mathematical and computational tools with an inter or multidisciplinary approach to solving problems related to an advanced field of physics.
PLO 6	Able to apply knowledge to analyze, synthesize, formulate problems and solve problems comprehensively in one of advanced field of physics, through experimental or theoretical research, then be able to classify and draw conclusions about their findings for the development of science and technology.

Course Outcomes (CO)	**Upon completion of this course, students should be able to:**			
	CO1	Describe and evaluate the use of computational methods in solving the problem of the electronic structure of condensed matter.		
	CO2	Describe and discuss the completion of eigenvalues by the Numerov method, factorization, diagonalization, self-consistent field, and Hartree-Fock.		
	CO3	Describe and discuss the Tight-Binding method in solving the problem of the electronic structure of condensed matter.		
	CO4	Describe and discuss the first principle-density functional theory (DFT) method in solving the problem of the electronic structure of condensed matter.		
	CO5	Interpret and correlate between experimental data (optical spectroscopy and electron spectroscopy) and computational calculations for many-particle systems (example: for 2D materials).		
	CO6			
	CO7			
	CO8			
The Correlation of CO to Learning Materials and Methods, and Time Allocation		**Learning Materials**	**Learning Methods**	**Time Allocation**
	CO1	INTRODUCTION: Explanation and agreement of lectures. Brief review of nanoscience and nanotechnology ,A brief overview of the influence of computing on the electronic structure of incompressibles Computational methods of numerical derivatives (finite difference)	Lecture	3 x 50 minutes
	CO1	2.1 Summary of computational methods: Numerical Integration (Trapseium and Simpson 1/3 Methods) 2.2.TIME INCREDIBLE SCHRODINGER EQUATION: Numerical solution using the Numerov method	Lecture	3 x 50 minutes
	CO1	"3.1.TIMEINCREDIBLE SCHRODINGER EQUATIONS: Numerical solutions using the Numerov method 3.2 Introduction to Programming IGOR Pro"	Lecture	3 x 50 minutes
	CO2	4.1 Introduction to IGOR Pro Programming 4.2 Use of IGOR Pro Programming to complete Eq. Schrodinger didn't	Lecture	3 x 50 minutes

		hang around using the Numerov method.		
	CO2	5.1. Matrix Diagonalization Numerical Method : Similarity transformation, Householder, Jacobi rotation. 5.2.TIME INCREDIBLE SCHRODINGER EQUATION: Numerical solution using matrix diagonalization method	Lecture	3 x 50 minutes
	CO2	6.1 POWER LEVEL DIAGRAM FOR PARTICLES IN PERIODIC POTENTIALS: Bloch's theorem, numerical method for solving central equations. Brillouin zone. Application of the diagonalization method in obtaining the band structure of a 1D system 6.2. TIGHT-BINDING METHOD: Numerical method to solve band structure using tight-binding method, transfer integral, overlap integral, orbital overlap. Application of the numerical method of the diagonalization method to solve the tight-binding model	Lecture	3 x 50 minutes
	CO2	7. 1. TIGHT - BINDING METHOD: Numerical method for solving band structure using tight – binding, transfer integral, overlap integral, orbital overlap method. Application of numerical method diagonalization method to solve tight-binding model 7.2. Brillouin Zone Sampling in the momentum space	Lecture	3 x 50 minutes
	CO3	AN INTRODUCTION TO THE BORN –OPPENHEIMER AND HARTREE-APPROACH FOCK: Born-Oppenheimer approach, variation principle, Hartree-Fock approach.	Lecture	3 x 50 minutes
	CO3	INTRODUCTION TO DENSITY - FUNCTIONAL THEORY (DFT): Schrodinger's equation for the many-body problem, Hohenberg-Kohn theorem.	Lecture	3 x 50 minutes

	CO3	DENSITY - FUNCTIONAL THEORY: Hohenberg-Kohn theorem, Self-Consistent Kohn - Kohn -Sham equation.	Lecture	3 x 50 minutes
	CO4	EXCHANGE AND CORRELATION FUNCTIONAL: Local density approximation (LDA), Generalized gradient approximation (GGA).	Lecture	3 x 50 minutes
	CO4	BASE SET OF WAVE FUNCTIONS AND PSEUDOPOTENTIAL TIAL: Plane wave and linear combination of atomic orbitals, norm-conserving and ultrasoft pseudopotential.	Lecture	3 x 50 minutes
	CO4	COMPUTING DENSITY FUNCTIONAL THEORY: self-consistent field for optimization of geometry, density of states, band structure.	Lecture	3 x 50 minutes
	CO4	DENSITY FUNCTIONAL THEORY APPLICATIONS: Optimization of lattice constants, calculation of supercell systems, molecular systems.	Lecture	3 x 50 minutes
	Final Exam/ Project Task Results/ Case Analysis Results			
Learning Methods	Lecture			
Student Learning Experience	Learn to analyze and review: INTRODUCTION: Explanation and agreement of lectures. Brief review of nanoscience and nanotechnology ,A brief overview of the influence of computing on the electronic structure of incompressibles Computational methods of numerical derivatives (finite difference), 2.1 Summary of computational methods: Numerical Integration (Trapseium and Simpson 1/3 Methods) 2.2.TIME INCREDIBLE SCHRODINGER EQUATION: Numerical solution using the Numerov method, "3.1.TIMEINCREDIBLE SCHRODINGER EQUATIONS: Numerical solutions using the Numerov method 3.2 Introduction to Programming IGOR Pro", 4.1 Introduction to IGOR Pro Programming 4.2 Use of IGOR Pro Programming to complete Eq. Schrodinger didn't hang around using the Numerov method., 5.1. Matrix Diagonalization Numerical Method : Similarity transformation, Householder, Jacobi rotation. 5.2.TIME INCREDIBLE SCHRODINGER EQUATION: Numerical solution using matrix diagonalization method, 6.1 POWER LEVEL DIAGRAM FOR PARTICLES IN PERIODIC POTENTIALS: Bloch's theorem, numerical method for solving central equations. Brillouin zone. Application of the diagonalization method in obtaining the band structure of a 1D system 6.2. TIGHT-BINDING METHOD: Numerical method to solve band structure using tight-binding method, transfer integral, overlap integral, orbital overlap. Application of the numerical method of the diagonalization method to solve the tight-binding model, 7. 1. TIGHT - BINDING METHOD: Numerical method for solving band structure using tight – binding, transfer integral, overlap integral, orbital overlap method. Application of numerical method diagonalization method to solve tight-binding model 7.2. Brillouin Zone Sampling in the momentum space, AN INTRODUCTION TO THE BORN – OPPENHEIMER AND HARTREE-APPROACH FOCK: Born-Oppenheimer approach, variation principle, Hartree-Fock approach. , INTRODUCTION TO DENSITY - FUNCTIONAL THEORY (DFT): Schrodinger's equation for the			

	many-body problem, Hohenberg-Kohn theorem., DENSITY - FUNCTIONAL THEORY: Hohenberg-Kohn theorem, Self-Consistent Kohn - Kohn -Sham equation., EXCHANGE AND CORRELATION FUNCTIONAL: Local density approximation (LDA), Generalized gradient approximation (GGA)., BASE SET OF WAVE FUNCTIONS AND PSEUDOPOTENTIAL TIAL: Plane wave and linear combination of atomic orbitals, norm-conserving and ultrasoft pseudopotential., COMPUTING DENSITY FUNCTIONAL THEORY: self-consistent field for optimization of geometry, density of states, band structure., DENSITY FUNCTIONAL THEORY APPLICATIONS: Optimization of lattice constants, calculation of supercell systems, molecular systems..
Access to Learning Media/ LMS and Offline and Online Percentage	In-focus and whiteboard, video synchronous and asynchronous
Assessment Methods and Synchronization with CO	

Assessment Methods	**Assessment Percentage**	**Criteria/Indicators**	**CO1**	**CO2**	**CO3**	**CO4**
Participatory Activity*						
Project Results/ Case Study Results/ PBL Results*						
Cognitive						
Assignment	30%		7,5%	7,5%	7,5%	7,5%
Quiz						
Midterm Exam	35%		17,5%	17,5%		
Final Exam	35%				17,5%	17,5%

*) can also be obtained from the Midterm or Final Exam as the result of participatory activities or project/ case study results. According to IKU 7, the percentage of project results/ case study/ PBL results is at least 50%.

References	**Main references:** 1. Richard Martins, 2004, Electronic Structure, Cambridge University Press. 2. J.M., Thijssen, 1999, Computational Physics, Cambridge University Press. 3. Haile, J.M., 1992, Molecular Dynamics Simulation, John-Wiley & Sons, Inc.
Lecturers (*Team Teaching*)	1. Dr. Iman Santoso, S.Si., M.Sc. 2. Sholihun, S.Si., M.Sc., Ph.D.Sc. 3. 4.

Authorization	**Date of Drafting**	**Lecturer Coordinator**	**Head of Curriculum Committee**	**Head of Study Program**
		Dr. Iman Santoso, S.Si., M.Sc.	Dr.Ing. Ari Setiawan	Mirza Satriawan, M.Si., Ph.D