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

Material Design Computational

MFF5713 / 3 Credits

Lecturer Coordinator:

Moh. Adhib Ulil Absor, S.Si., M.Sc., Ph.D.

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 Odd 2022/2023

SEMESTER LEARNING ACTIVITY PLANS (SLAP)

Code	Course Name	Credits (credits)	Semester	Status	Prerequisite
MFF5713	*Material Design Computational*	*3*	*Odd*	*Elective*	*None*

Short Description

Material Design Computational 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:
Quantum mechanics of multiple particles, variational methods, Hartree-Fock method, Functional Theory of Density, Periodic Structure and wave base plane, Molecular Dynamics Simulation, calculation of optimization of geometric structures: surface, interface, and defect system, calculation of the electronic structure of materials, calculation of magnetic properties of materials, calculation of optical properties of materials, calculation of material topology properties, Hands-on and case studies.

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	Formulate, model, and design material systems along with material characteristics (electronic, optical, magnetic, topological, etc.), also reveal essential information through specific mathematical procedures and computational algorithms.		
	CO2	Solve a problem with a structured solution (well-defined solutions) in the material system.		
	CO3	Apply various forms of visualization, graphics, or simulations through computer assistance and the use of appropriate software, programming languages, and packages or numerical tools (numerical tools) to solve problems in material systems.		
	CO4			
	CO5			
	CO6			
	CO7			
	CO8			
The Correlation of CO to Learning Materials and Methods, and Time Allocation		**Learning Materials**	**Learning Methods**	**Time Allocation**
	CO1	Introduction: Summary of basic concepts of Quantum Mechanics (II)	Lecture	3 x 50 minutes
	CO1	Introduction: Summary of the fundamental concepts of quantum mechanics (Part II).	Lecture	3 x 50 minutes
	CO1	Variational method, Hartree-Fock method, density functional theory.	Lecture	3 x 50 minutes
	CO2	Variational method, Hartree-Fock method, density functional theory.	Lecture	3 x 50 minutes
	CO2	Variational method, Hartree-Fock method, density functional theory.	Lecture	3 x 50 minutes
	CO2	Periodic structure and plane wave basis.	Lecture	3 x 50 minutes
	CO2	Molecular Dynamics Simulation.	Lecture	3 x 50 minutes
	CO3	Calculation of optimization of geometric structures: surface (surface), interface (interface), crystal defect system (defect).	Lecture	3 x 50 minutes
	CO3	Calculation of optimization of geometric structures: surface, interface, crystal defect system.	Lecture	3 x 50 minutes
	CO3	Calculation of the electronic structure of the material.	Lecture	3 x 50 minutes
	CO4	Calculation of the magnetic properties of materials.	Lecture	3 x 50 minutes
	CO4	Calculation of the optical properties of materials.	Lecture	3 x 50 minutes
	CO4	Hands on and case studies.	Lecture	3 x 50 minutes

<table>
<tr><td rowspan="2"></td><td>CO4</td><td>Hands on and case studies.</td><td>Lecture</td><td>3 x 50 minutes</td></tr>
<tr><td colspan="4">Final Exam/ Project Task Results/ Case Analysis Results</td></tr>
<tr><td>Learning Methods</td><td colspan="4">Lecture</td></tr>
<tr><td>Student Learning Experience</td><td colspan="4">Learn to analyze and review: Introduction: Summary of basic concepts of Quantum Mechanics (II), Introduction: Summary of the fundamental concepts of quantum mechanics (Part II)., Variational method, Hartree-Fock method, density functional theory., Variational method, Hartree-Fock method, density functional theory., Variational method, Hartree-Fock method, density functional theory., Periodic structure and plane wave basis., Molecular Dynamics Simulation., Calculation of optimization of geometric structures: surface (surface), interface (interface), crystal defect system (defect)., Calculation of optimization of geometric structures: surface, interface, crystal defect system., Calculation of the electronic structure of the material., Calculation of the magnetic properties of materials., Calculation of the optical properties of materials., Hands on and case studies., Hands on and case studies..</td></tr>
<tr><td>Access to Learning Media/ LMS and Offline and Online Percentage</td><td colspan="4">Sync (google meet), Asynchronous (google classroom, video)</td></tr>
<tr><td>Assessment Methods and Synchronization with CO</td><td colspan="4">
<table>
<tr><td>Assessment Methods</td><td>Assessment Percentage</td><td>Criteria/Indicators</td><td>CO1</td><td>CO2</td><td>CO3</td><td>CO4</td></tr>
<tr><td>Participatory Activity*</td><td></td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>Project Results/ Case Study Results/ PBL Results*</td><td></td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td colspan="7">Cognitive</td></tr>
<tr><td>Assignment</td><td>30%</td><td></td><td>7,5%</td><td>7,5%</td><td>7,5%</td><td>7,5%</td></tr>
<tr><td>Quiz</td><td></td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>Midterm Exam</td><td>35%</td><td></td><td>17,5%</td><td>17,5%</td><td></td><td></td></tr>
<tr><td>Final Exam</td><td>35%</td><td></td><td></td><td></td><td>17,5%</td><td>17,5%</td></tr>
<tr><td colspan="7">*) 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%.</td></tr>
</table>
</td></tr>
<tr><td>References</td><td colspan="4">Main references:
1. David Sholl and Janice A. Steckel, 2011, Density Functional Theory: A Practical Introduction, John Wiley & Sons, USA.
2. F. Giustino et.al., 2014, Materials modelling using density functional theory : properties and predictions, Oxford University Press, , Oxford, UK.
3. Richard LeSar, 2013, Introduction to Computational Materials Science, Fundamentals to Applications, Cambridge University Press, Cambridge, UK.</td></tr>
<tr><td>Lecturers (Team Teaching)</td><td colspan="4">1. Moh. Adhib Ulil Absor, S.Si., M.Sc., Ph.D.
2. Sholihun, S.Si., M.Sc., Ph.D.Sc.
3.
4.</td></tr>
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Authorization	**Date of Drafting**	**Lecturer Coordinator**	**Head of Curriculum Committee**	**Head of Study Program**
		Moh. Adhib Ulil Absor, S.Si., M.Sc., Ph.D.	Dr.Ing. Ari Setiawan	Mirza Satriawan, M.Si., Ph.D