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

Physics Undergraduate Study Program

Physics Department

Computational Material Physics

MFF 3820/ 3 Credits

Lecturer Coordinator:

Dr. Iman Santoso
Dr. Sholihun

UNIVERSITAS GADJAH MADA
FACULTY OF MATHEMATICS AND NATURAL SCIENCE
2022

<table>
<tr><td></td><td colspan="4">Universitas Gadjah Mada
Faculty of Mathematics and Natural Science
Physics Department / Physics Undergraduate Study Program
Semester EVEN 2022/2023</td><td>Document Number :
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<tr><td colspan="6">SEMESTER LEARNING ACTIVITY PLANS (SLAP)</td></tr>
<tr><th>Code</th><th>Course Name</th><th>Credits (Credits)</th><th>Semester</th><th>Status</th><th>Prerequisite</th></tr>
<tr><td>MFF 3820</td><td>Computational Material Physics</td><td>T: 3 | P: …</td><td>EVEN</td><td>Elective</td><td>Computational Physics (MFF 2027), Solid state Physics I (MFF 2601)</td></tr>
<tr><td>Short Description</td><td colspan="5">Computational Material Physics Courses are elective courses in the 2016 Curriculum of the Physics Undergraduate Study Program, Faculty of Mathematics and Natural Sciences UGM. This course is intended to provide basic to intermediate-level knowledge regarding the latest development systems in nanoscience and nanotechnology that underlie advances in science and technology with a computational approach. This course is closely related to the two main branches of physics, namely theoretical and computational knowledge. As is known, physicists describe and research nature through Experiments, Analytical Theories, and computational methods. In terms of the object of study, the courses are related to the field of study of Material Physics, namely the interaction of light with materials, introduction to the electronic structure of materials, and optimization of the geometry of a material.</td></tr>
<tr><td rowspan="2">Program Learning Outcomes (PLO) Imposed on the Course</td><td>PLO 2</td><td colspan="4">Knowledge. Able to explain theoretical concepts and principles of classical and modern physics and able to apply basic concepts of physics and related mathematical methods in finding solutions to physical problems.</td></tr>
<tr><td>PLO 5</td><td colspan="4">Long Life Learning. Able to analyze various alternative solutions to physical problems and conclude them for appropriate decision-making, both in familiar and new problems.</td></tr>
<tr><td rowspan="5">Course Outcomes (CO)</td><td colspan="5">After completing this course, students are expected to be able to:</td></tr>
<tr><td>CO1</td><td colspan="4">Students can apply computational methods of numerical derivatives, numerical integration, and root search in extracting dielectric constant values from reflections and equilibrium positions of diatomic molecules.</td></tr>
<tr><td>CO2</td><td colspan="4">Students can apply computational methods of numerical derivatives, numerical integration, Discrete Fourier Transform, and Fast Fourier Transform in calculating linear response functions (e.g., optical constant, dielectric constant) of a material as well as the Kramers-Kronig relation that connects the real and imaginary parts of the linear response function.</td></tr>
<tr><td>CO3</td><td colspan="4">Students can apply computational methods of numerical derivatives, numerical integration, Numerov methods, factorization, iteration, and matrix diagonalization (similarity transformation, Householder, and Jacobi Rotation) in solving the time-independent Schrodinger equation, which will produce band diagrams of 1D material systems and 2d.</td></tr>
<tr><td>CO4</td><td colspan="4">Students can apply computational optimization methods like Gauss-Newton, Gradient descent, Levenberg-Marquardt, and BFGS (Broyden–Fletcher–Goldfarb–Shanno) to optimize the geometry of a material.</td></tr>
<tr><td rowspan="2">The Correlation of CO to Learning Materials and</td><td></td><th colspan="2">Learning Materials</th><th>Learning Methods</th><th>Time Allocation</th></tr>
<tr><td>CO 1, CO 2, CO 3, CO 4</td><td colspan="2">INTRODUCTION: the role of computing in explaining fundamental and applied</td><td>TCL-SCL mixed</td><td>3X50 minutes</td></tr>
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Methods, and Time Allocation		problems in material physics, namely linear response functions, optical constants, dielectric constants, Kramers-Kronig relations), band diagrams of 1D and 2D systems, equilibrium positions, and optimization of the geometry of materials.		
	CO 2	SUMMARY OF NUMERIC METHODS: Numerical derivative (finite difference method), numerical integration (trapezium and Simpson1/3), Discrete Fourier Transform, and Fast Fourier Transform	TCL-SCL mixed	***3X50 minutes***
	CO 2	TIME DEPENDENT SCHRODINGER EQUATION: Numerical solution using the second-order Numerov method	TCL-SCL mixed	***3X50 minutes***
	CO 2	Timeless SCHRODINGER EQUATION: Numerical solution using matrix diagonalization method (similarity transformation, Householder transformation, Jacobi rotation)	TCL-SCL mixed	***3X50 minutes***
	CO 2, CO 3	POWER LEVEL DIAGRAM FOR 1D and 2D SYSTEM PARTICLES: Bloch's Theorem, Application of the diagonalization method in obtaining the band structure of 1D and 2D systems	TCL-SCL mixed	***3X50 minutes***
	CO 3	Introduction to the tight-binding method: Numerical methods for solving band structures use tight-binding, integral transfer, integral overlap, and orbital overlap methods.	TCL-SCL mixed	***3X50 minutes***
	CO 3	Geometry Optimization	TCL-SCL mixed	***3X50 minutes***
	Midterm exam/Project Task Results/Case Analysis Results			
	CO 4	Geometry Optimization	TCL-SCL mixed	***6X50 minutes***
	CO 4	Geometry Optimization	TCL-SCL mixed	***6X50 minutes***
	CO 4	DFT	TCL-SCL mixed	***9X50 minutes***
	Final exams/ Project Task Results/Case Analysis Results			
Learning Methods	**SCL (Student Centered Learning): Project-based learning (Team-based Project)/Case-based learning/PBL/other SCL methods**			
Student Learning Experience	**Learn to examine and study computational methods on materials**			

<table>
<tr><td>Access to Learning Media/ LMS and Offline and Online Percentage</td><td colspan="8">Offline (LCD, PPT Slide, Whiteboard, Laptop) and Online (Zoom Meeting, Google Meet, Google Classroom)</td></tr>
<tr><td rowspan="9">Assessment Methods and Synchronization with CO</td><td>Assessment Methods</td><td>Assessment Percentage</td><td>Criteria/ Indicators</td><td>CO1</td><td>CO2</td><td>CO3</td><td colspan="2">CO4</td></tr>
<tr><td>Participatory Activity*</td><td></td><td></td><td></td><td></td><td></td><td colspan="2"></td></tr>
<tr><td>Project Results/ Case Study Results/ PBL Results*</td><td></td><td></td><td></td><td></td><td></td><td colspan="2"></td></tr>
<tr><td colspan="8">Cognitive</td></tr>
<tr><td>Assignment</td><td>20</td><td></td><td>√</td><td>√</td><td>√</td><td colspan="2">√</td></tr>
<tr><td>Midterm Exam</td><td>40</td><td></td><td>√</td><td>√</td><td>√</td><td colspan="2"></td></tr>
<tr><td>Final Exam</td><td>40</td><td></td><td></td><td></td><td></td><td colspan="2">√</td></tr>
<tr><td>Total</td><td>100</td><td></td><td></td><td></td><td></td><td colspan="2"></td></tr>
<tr><td colspan="8">*) 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>
<tr><td>References</td><td colspan="8">Main References;
1. Richard Martins, 2004, Electronic Structure, Cambridge University Press.
2. J.M., Thijssen, 1999, Computational Physics, Cambridge University Press.
3. Tao Pang, An introduction to computational physics, Cambridge press (2006).</td></tr>
<tr><td>Lecturers (Team Teaching)</td><td colspan="8">1. Dr. Iman Santoso
2. Dr. Sholihun</td></tr>
<tr><td rowspan="2">Authorization</td><td>Date of Drafting</td><td colspan="3">Lecturer Coordinator</td><td colspan="2">Head of Curriculum Committee</td><td colspan="2">Head of Study Program</td></tr>
<tr><td></td><td colspan="3">Dr. Iman Santoso</td><td colspan="2"></td><td colspan="2">Dr. Eng. Ahmad Kusumaatmaja, S.Si., M.Sc.</td></tr>
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