

Universitas Negeri Surabaya Faculty of Mathematics and Natural Sciences Undergraduate Chemistry Study Program

Document Code

			SEM	ESTER LE	ARNI	NG	PLAN						
Courses		CODE	Cou	Course Family		Credit Weight	SEMESTER	Compilation Date					
Computational Chemistry		4720102104				T=2 P=0 ECTS=3.18	8 4	July 17, 2024					
AUTHORIZATION		SP Develop	SP Developer		Course Cluster Coordinator		Study Program Coordinator						
			Dr. I Gusti M	lade Saanjaya, M.S	i.	Prof. [Dr. Suyono, M.Pd.	Dr. Ama	ıria, M.Si.				
Learning model	I	Project Based L	earning										
Program Learning Outcomes		PLO study program that is charged to the course											
		Program Objec	tives (PO)										
(PLO)		PLO-PO Matrix											
		P.O											
		PO Matrix at th	e end of each lea	rning stage (Sub	-PO)								
			P.O Week 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16										
Short Course Description		Study of the basics of programming in chemistry, chemical modeling, and computing on various aspects of chemical behavior studied with classical mechanics using molecular mechanics methods or with quantum mechanics using electronic structure methods such as ab-initio, semi-empirical, and density functional theory or DFT (Density Functional Theory) through study, practicum and simple engineering.											
References		Main :											
		 Atkins, P., Paula, J.d., and Friedman, R. 2009. Quanta, Matter, and Change: A Molecular Approach toPhysical Chemistry. USA: Oxford University Press. Jensen, F. 2007. Introduction to Computational Chemistry, 2nd ed. New York: John Wiley & Sons, Ltd. Commitee on RCACIBCSTDELS, 2006, Visualizing Chemistry, USA: National Academy of Scienc. Hinchliffe, A. 2008. Molecular Modelling For Beginners, 2nd ed. United Kingdom: : John Wiley & Sons, Ltd. 											
		Supporters:											
		1. Computational Chemistry Highlight											
Support lecturer	ing Dr. I Gusti Made Sanjaya, M.Si. Dr. Moh. Muʻalliful Ilmi, S.Si, M.Si.												
Week-	Final abilities of each learning stage (Sub-PO)		Eval	Evaluation		H Lea Stude	elp Learning, rning methods, ent Assignments, estimated time]	Learning materials	Assessment Weight (%)				
			Indicator	Criteria & Form	Offli offli	ine(ne)	Online (<i>online</i>)]					
(1)		(2)	(3)	(4)	(!	5)	(6)	(7)	(8)				
1 Ur dii de co ch		nderstand the ection of velopment of mputational emistry	Explain the benefits of computational chemistry for the development of chemical science	Criteria: Participation assessment	Preser and discuss 2 X 50				0%				

2	Understand the principles of chemical modeling	Designing chemical models	Criteria: Participation Assessment and assignments	performance, presentation and discussion 2 X 50			0%
3	Understanding the Hartree-Focks approach in computational chemistry	Describes the Hartree-Fock approach to materials computing	Criteria: participation assessment	Presentation and discussion 2 X 50	resentation nd liscussion 2 X 50		0%
4	Understanding Roothaan's approach to computational chemistry	Explains improvements in material computing using the Roothaan approach	Criteria: Participation assessment	Presentation and discussion 2 X 50			0%
5	Understanding Basis Sets	Analyze the types of basis sets according to their basis functions used in chemical computing	Criteria: Assignment assessment	performance 2 X 50			0%
6	Understand computational approaches using ab initio methods	Computationally engineering chemicals with an ab-initio approach	Criteria: Assignment Assessment	performance, presentation and discussion 1 X 1			0%
7	Understand computational approaches with semi-empirical methods	Designing chemical computations using semi- empirical methods	Criteria: Assignment of assignments	performance, presentation and discussion 2 X 50			0%
8				2 X 50			0%
9	Understand computational approaches with density functional theory or DFT (density functional theory)	Analyzing the use of approaches to the DFT method in computational chemistry	Criteria: Participation Assessment	Presentation and discussion 2 X 50			0%
10	Understand computational approaches with density functional theory or DFT (density functional theory)	Designing chemical computations using the DFT method	Criteria: Assignment of assignments	performance, presentation and discussion 2 X 50			0%
11	Analyzing the precision of computational results	Comparing chemical computational results with experimental results	Criteria: Participation Assessment and assignments	Presentation and discussion 2 X 50			0%
12	Understanding computational chemistry for large molecules	Designing computations for large molecules	Criteria: Participation Assessment and assignments	performance, presentation and discussion 2 X 50			0%
13	Understanding computational chemistry for nanoparticles	Designing computations for nano-sized molecules	Criteria: Participation Assessment and assignments	performance, presentation and discussion 2 X 50			0%
14	Understanding computational chemistry for drug development	Designing computational chemistry with QSAR methods for drug development	Criteria: Participation Assessment and assignments	performance, presentation and discussion 2 X 50			0%
15	Understanding the performance of new medicinal substances through the docking process	Designing the docking of new medicinal materials in the disease healing process	Criteria: Participation Assessment and assignments	performance, presentation and discussion 2 X 50			0%
16				2 X 50			0%

Notes

- 1. Learning Outcomes of Study Program Graduates (PLO Study Program) are the abilities possessed by each Study Program graduate which are the internalization of attitudes, mastery of knowledge and skills according to the level of their study program obtained through the learning process.
- 2. The PLO imposed on courses are several learning outcomes of study program graduates (CPL-Study Program) which are used for the formation/development of a course consisting of aspects of attitude, general skills, special skills and knowledge.
- 3. **Program Objectives (PO)** are abilities that are specifically described from the PLO assigned to a course, and are specific to the study material or learning materials for that course.
- 4. **Subject Sub-PO (Sub-PO)** is a capability that is specifically described from the PO that can be measured or observed and is the final ability that is planned at each learning stage, and is specific to the learning material of the course.
- 5. **Indicators for assessing** abilities in the process and student learning outcomes are specific and measurable statements that identify the abilities or performance of student learning outcomes accompanied by evidence.
- 6. Assessment Criteria are benchmarks used as a measure or measure of learning achievement in assessments based on predetermined indicators. Assessment criteria are guidelines for assessors so that assessments are consistent and unbiased. Criteria can be quantitative or qualitative.
- 7. Forms of assessment: test and non-test.

0%

- 8. Forms of learning: Lecture, Response, Tutorial, Seminar or equivalent, Practicum, Studio Practice, Workshop Practice, Field Practice, Research, Community Service and/or other equivalent forms of learning.
- Learning Methods: Small Group Discussion, Role-Play & Simulation, Discovery Learning, Self-Directed Learning, Cooperative Learning, Collaborative Learning, Contextual Learning, Project Based Learning, and other equivalent methods.
- 10. Learning materials are details or descriptions of study materials which can be presented in the form of several main points and sub-topics.
- 11. The assessment weight is the percentage of assessment of each sub-PO achievement whose size is proportional to the level of difficulty of achieving that sub-PO, and the total is 100%.
- 12. TM=Face to face, PT=Structured assignments, BM=Independent study.