

MODULE HANDBOOK

Module Name :	Computational Chemistry
Module level :	Bachelor of Chemistry
Course Code :	3074112061
Abbreviation, if applicable:	-
Courses included in the module, if applicable:	-
Semester/Term	5 th /3 rd year
Module coordinator(s)	Dr. I Gusti Made Sanjaya, M.Si.
Lecturer(s):	Dr. I Gusti Made Sanjaya, M.Si.
Language:	Indonesian
Classification within the curriculum:	Compulsory / Elective
Teaching format/class hours per week during the semester:	2 contact hours of lectures and lab activity (Indonesia credit semester or sks*)
Workload :	a. Lecture: 1 x 50 minutes lectures, 1 x 60 minutes structured activity, 1 x 60 minutes individual activity, 14 weeks per semester, 39.67 total hours of lecture per semester ~ 1.59 ECTS b. Lab activity: 1x170 minutes lab activity, 14 weeks per semester 39.67 total hours of lab activity per semester ~ 1.59 ECTS Total of lecture and lab activity= 79.33 total hours per semester ~ 3.18 ECTS**
Credit Point:	2 sks (3.18 ECTS)
Requirements:	Quantum chemistry

Learning goals/competencies:	General Competence (knowledge): Students can understand chemical programming, chemical modeling, and computation of various aspects of chemical behavior. Spesific Competence: Students can characterize the behavior of materials and chemical reactions through computational and virtualization processes.																																								
Content	The course material examines the basics of programming in chemistry, chemical modeling, and computation of various aspects of chemical behavior by applying classical mechanics through molecular mechanics methods and quantum mechanics through electronic structure methods such as ab- initio, semi-empirical, and DFT (Density Functional Theory).																																								
Attribute Soft skill:	Active communication; Disipline; Collaboration; Responsibility; and Argumentation in class and outdoor setting																																								
Study/exam achievements:	The final grade (NA) is calculated based on the following ratio: <table><tr><td>Assessment Components</td><td>Percentage of contribution</td></tr><tr><td>Participation</td><td>20%</td></tr><tr><td>Assignment</td><td>30%</td></tr><tr><td>Mid-semester test</td><td>20%</td></tr><tr><td>Final semester test</td><td>30%</td></tr></table> Grade Conversion of 0-100 scale into 0-4 scale is set as below: <table><tr><td>Letter</td><td>Number</td><td>Grade interval</td></tr><tr><td>A</td><td>4.00</td><td>$85 \leq A \leq 100$</td></tr><tr><td>A-</td><td>3.75</td><td>$80 \leq A- < 85$</td></tr><tr><td>B+</td><td>3.50</td><td>$75 \leq B+ < 80$</td></tr><tr><td>B</td><td>3.00</td><td>$70 \leq B < 75$</td></tr><tr><td>B-</td><td>2.75</td><td>$65 \leq B- < 70$</td></tr><tr><td>C+</td><td>2.50</td><td>$60 \leq C+ < 65$</td></tr><tr><td>C</td><td>2.00</td><td>$55 \leq C < 60$</td></tr><tr><td>D</td><td>1.00</td><td>$40 \leq D < 55$</td></tr><tr><td>E</td><td>0.00</td><td>$0 \leq E < 40$</td></tr></table>	Assessment Components	Percentage of contribution	Participation	20%	Assignment	30%	Mid-semester test	20%	Final semester test	30%	Letter	Number	Grade interval	A	4.00	$85 \leq A \leq 100$	A-	3.75	$80 \leq A- < 85$	B+	3.50	$75 \leq B+ < 80$	B	3.00	$70 \leq B < 75$	B-	2.75	$65 \leq B- < 70$	C+	2.50	$60 \leq C+ < 65$	C	2.00	$55 \leq C < 60$	D	1.00	$40 \leq D < 55$	E	0.00	$0 \leq E < 40$
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Learning Methods :	Lecture and laboratory activity using: Student-centered approach; project-based learning; lab activity, and discussion, presentations (structured activities), and assignment																																								
Form of Media:	Internet, Computer, LCD, White board																																								

Literature (primary references):	Mammino, L.L. 2021. Green Chemistry and Computational Chemistry: Shared Lessons in Sustainability. US: Elsevier Science Atkins, P., Paula, J.d., and Friedman, R. 2009. Quanta, Matter, and Change: A Molecular Approach to Physical Chemistry. USA:Oxford University Press. Jensen, F. 2007. Introduction to Computational Chemistry, 2nded. 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.
Notes:	*1 sks in learning process = three periods consist of: (a) scheduled instruction in a classroom (50 minutes); (b) structured activity (60 minutes); and (c) individual activity (60 minutes) according to the Regulation of Indonesia Ministry of Research, Technology, and Higher Education No. 44 Year 2015 jo. the Regulation of Indonesia Ministry of Research, Technology, and Higher Education No. 50 Year 2018. For lab activity: 1 sks in learning process = two periods consist of: (a) scheduled lab activity (100 minutes); (b) structured lab activity (70 minutes);
	**1 sks = 1.59 ECTS according to Rector Decree Of Universitas Negeri Surabaya No. 598/Un38/Hk/Ak/2019