MODULE HANDBOOK

<table>
<tr><td>Modul Name</td><td>Computational Chemistry</td></tr>
<tr><td>Module Leve</td><td>Bachelor of Chemistry</td></tr>
<tr><td>Abbreviation, if applicable</td><td>3074112061</td></tr>
<tr><td>Sub-heading, if applicable</td><td>-</td></tr>
<tr><td>Course included in the module, if applicable</td><td>-</td></tr>
<tr><td>Semester/term</td><td>5th/3rd year</td></tr>
<tr><td>Module coordinator(s)</td><td>Dr. I Gusti Made Sanjaya, M.Si.</td></tr>
<tr><td>Lecturer(s)</td><td>Dr. I Gusti Made Sanjaya, M.Si.</td></tr>
<tr><td>Language</td><td>Indonesian Language</td></tr>
<tr><td>Classification within the curriculum</td><td>Elective Course</td></tr>
<tr><td>Teaching format/class hours per week during the semester</td><td>2 hours lectures (50 min / hour)</td></tr>
<tr><td>Workload</td><td>2 x 50 minutes lectures, 2 x 60 minutes structured activity,
2 x 60 minutes individual activity, 14 weeks per semester,
79.33 total hours per semester ~ 3.18 ECTS**</td></tr>
<tr><td>Credit point</td><td>2 CU x 1.59 = 3.18 ECTS</td></tr>
<tr><td>Prerequisite course(s)</td><td>-</td></tr>
<tr><td>Learning Outcomes</td><td>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.</td></tr>
<tr><td>Content</td><td>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).</td></tr>
<tr><td>Study/exam achievements</td><td>Students are considered to complete the course and pass if they obtain at least 40% of maximum final grade. 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>
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Media	Internet, Computer, LCD, White board
Learning Methods	Lectures, discussion, problem solving, projects, and assignment
Literature	• 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 CU in learning process = three periods consist of: (a) scheduled instruction in a classroom or laboratory (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.
	**1 CU = 1.59 ECTS according to Rector Decree Of Universitas Negeri Surabaya No. 598/UN38/Hk/Ak/2019