Module Description
MPKP 308 Computational Chemistry

Module Name	**Computational Chemistry**
Module level, if applicable	Undergraduate Program
Code, if applicable	MPKP 308
Subtitle, if applicable	-
Course, if applicable	-
Semester(s) in which the module is taught	6th Semester
Module coordinator(s):	Berlian Sitorus, S.Si, M.Si, M.Sc, Ph.D
Lecturer	Berlian Sitorus, S.Si, M.Si, M.Sc, Ph.D Ferdinand Hidayat, S.Si, M.Si
Language	Bahasa Indonesia
Relation to curriculum	Elective Courses for the undergraduate programme in Chemistry
Type of teaching, contact hours	Decide teaching/training components for each course outcome ● Theory /Face-to-face lecture (for understanding): 4 lecture meetings ● Practical: 6 ● Seminar (for communication skills) : 1 ● Assignments: 2 ● Project: 1
Workload	*(Estimated)* *Total workload: 2 x 2,83 hours = 5,67 hours per week.* *Contact hours (lecture): 2 x 0,83 hours = 1,66 hours per week* *Private study including examination preparation, specified in hours: 2 x 2 hours = 4 hours per week* *2 x 50 minutes lectures,* *2 x 60 minutes practical,* *2 x 60 minutes individual activity,* *14 weeks per semester,* *80 total hours*
Credit points	2 (3.34 ECTS)
Requirements according to	Registered in this course

<table>
<tr><td>the examination regulations</td><td>Minimum 75% attendance in this course</td></tr>
<tr><td>Learning goals/competencies:</td><td>Intended Learning Outcomes (ILO)
After taking this course, students will be able to:
1. LO-1
2. LO-2
3. LO-3
4. LO-6</td></tr>
<tr><td>Module objectives</td><td>1. Students are able to describe basic concepts and calculation methods in computational chemistry
2. Students are able to explain an appropriate computational chemistry method in predicting the physical and chemical properties of substances.
3. Students are able to explain an appropriate computational chemistry method for molecular modelling</td></tr>
<tr><td>Content:</td><td>1. Introduction of computational chemistry
2. Calculation method in computational Chemistry
3. Molecular mechanics method
4. Ab initio method
5. Semiempirical method
6. Electron Correlation method
7. DFT method
8. Geometry optimization
9. Introduction of hyperchem and gaussian
10. Quantitative correlation between structure and chemical activity</td></tr>
<tr><td>Attribute Soft skill:</td><td>Discipline, collaboration, responsibility, and argumentation in the natural classroom setting</td></tr>
<tr><td>Recommended prerequisites</td><td>-</td></tr>
<tr><td>Study and examination requirements and forms of examination</td><td>Students are considered to be competent and pass if they get at least 50% of the maximum final grade. The final grade (NA) is calculated based on the following :

<table><tr><th>Assessment Components</th><th>Percentage Contribution</th></tr><tr><td>Participation</td><td>10%</td></tr></table></td></tr>
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	<table><tr><td>Assignment</td><td>20%</td></tr><tr><td>Mid-semester test</td><td>35 %</td></tr><tr><td>Final semester test</td><td>35%</td></tr><tr><td>Total</td><td>100%</td></tr></table> **Mid and final semester tests are carried out asa project exam.**
Learning Methods	Case-based teaching method Project-based learning
Media employed	white board; power point presentation; and e-learning system
Reading list	1. McQuarrie, D. A., 1983, Quantum Chemistry, University Science Books. California, USA 2. Engel, T., 2019, Quantum Chemistry and Spectroscopy, Pearson. Washington, USA 3. Cramer, C.J., 2004, Essentials of Computational Chemistry, 2nd edition, Wiley, England.