UNIVERSITAS NEGERI YOGYAKARTA
FACULTY OF MATHEMATICS AND NATURAL SCIENCES
DEPARTMENT OF CHEMISTRY
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Bachelor of Science in Chemistry **MODULE HANDBOOK**

Module name:	Molecular Dynamics
Module level, if applicable:	Undergraduate
Code:	KIM 6406
Sub-heading, if applicable:	-
Classes, if applicable:	2
Semester:	4^{th}
Module coordinator:	Jaslin Ikhsan, Ph.D
Lecturer(s):	1. Jaslin Ikhsan, Ph.D 2. Dr. Eli Rohaeti 3. Dr. Crys Fajar Partana
Language:	Bahasa Indonesia and English
Classification within the curriculum:	Compulsory Subject
Teaching format / class hours per week during the semester:	• Lectures: 150 minutes lectures, 180 structured activities and 180 individual study per week • Laboratory work: 170 minutes includes the laboratory work and it's reporting per week
Workload:	Total workload of the activity is 181,33 hours per semester which consists of 150 minutes lectures, 180 structured activities and 180 individual study and also 170 minutes laboratory work with it's reporting per week for 16 weeks
Credit points:	4 SKS (7 ECTS) with the details of 3 SKS (5 ECTS) lectures and 1 SKS (2 ECTS)
Prerequisites course(s):	Chemical Equilibrium
Course Outcomes	After taking this course, the students are expected to be able to: CO1: Conduct molecular dynamics experiments to complete chemical debate and research CO2: Apply transitions to support life skills CO3: Integrate mathematical concepts into solving mathematical chemical problems
Content:	This course studies about the molecular dynamics, which include the theory of gas kinetics, moving molecules (including gases and solutions), the rate of chemical reactions (including: empirical chemical kinetics and explanation of the law of speed), and complicated reaction kinetics. This course also learn about the theory and practicum in the laboratory. Learning Materials: 1. The Gas Kinetics Theory 2. Reaction Rate 3. Moving Molecules 4. Conductance and Conductivity 5. Ostwald dilution law

<table>
<tr><td></td><td>6. pKa relationship with the results of conductivity measurements
7. IPN Mobility
8. Transport numbers
9. Measurement of transport numbers
10. Relationship of ion conductivity and transport numbers
11. Calculating thermodynamic forces
12. Infusion and Einstein's relationship
13. Diffusion and Nerst-Einstein equations
14. Stokes-Einstein's diffusions and equations</td></tr>
<tr><td>Study / exam achievements:</td><td>Attitude assessment is carried out at each meeting by observation and/or self-assessment techniques using the assumption that basically every student has a good attitude. The student is marked very good or not good attitude if they show it significantly compared to other students in general. The result of attitude assessment is not taken into account in the final grades, but as one of the requirements to pass the course. Students will pass from this course if at least have a good attitude. The final mark will be weight as follow:
<table>
<tr><th>No</th><th>CO</th><th>Assessment Object</th><th>Assessment Technique</th><th>Weight</th></tr>
<tr><td>1</td><td>CO1,
CO2,
CO3,</td><td>a. Assignments
b. Activity
c. Final Exam
d. Laboratory Activities</td><td>Presentation / written test</td><td>20%
20%
30%
30%</td></tr>
<tr><td colspan="4">Total</td><td>100%</td></tr>
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<tr><td>Forms of media:</td><td>Handout, Board, LCD Projector, Laptop/Computer, Module, Laboratory Work equipment</td></tr>
<tr><td>References:</td><td>1. Snehanshu Pal and Bankim Chandra Ray, 2020, Molecular Dynamics Simulation of Nanostructured Materials: An Understanding of Mechanical Behavior, 1st Ed., CRC Press
2. Dominik Marx, 2012, Ab Initio Molecular Dynamics: Basic Theory and Advanced Methods, Cambridge University Press
3. Zhang, YX., Wang, N., Li, QF. et al., 2020, Progress of quantum molecular dynamics model and its applications in heavy ion collisions. Front. Phys. 15, 54301
4. Hunday Govindasamy, Sivanandam Magudeeswaran & Kumaradhas Poomani, 2020, Identification of novel flavonoid inhibitor of Catechol-O-Methyltransferase enzyme by molecular screening, quantum mechanics/molecular mechanics and molecular dynamics simulations, J. Biomol. Struct. Dyn., 38:18, 5307-5319
5. Boyd, R. J. (2007). The development of computational chemistry in Canada. Reviews in Computational Chemistry, 15, 213–299</td></tr>
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	6. P.W. Atkins, Physical Chemistry, Oxford University Press. 7. P.W. Atkins, Kimia Fisika Jilid 2 (terjemahan), Erlangga Jakarta. 8. Ira N. Levine, Physical Chemistry, McGraw-Hill. 9. Keith J. Laider, Chemical Kinetics, HarperCollins Publisher.

PLO and CO mapping

	PLO									
	Attitude	General Skill		Knowledge				Specific Skill		
	PLO1	PLO2	PLO3	PLO4	PLO5	PLO6	PLO7	PLO8	PLO9	PLO10
CO1					√					
CO2							√			
CO3									√	