Module Handbook

Module Name	**Computational Chemistry**
Module Level	Bachelor
Abbreviation, if applicable:	KIT 302
Sub-heading, if applicable:	-
Courses included in the module, if applicable:	-
Semester/term:	6th / third year
Module coordinator(s):	Dr. Faidur Rochman, M.S
Lecturer(s):	Drs. Imam Siswanto, M.Si
Language:	Bahasa Indonesia
Classification within the curriculum	Elective course
Teaching format / class hours per week during semester:	2 hours lectures (50 min / hour)
Workload:	2 hours lecture, 2 hours individual activities, 2 hours structured activities, 13 weeks per semester, and total 78 hours per semester ~ 2.6 ECTS *
Credit Points:	2 SCU
Requirements:	Physical Chemistry III
Learning goals/competencies:	**General competence (Knowledge):** After getting this course, students are expected to perform the calculation mechanics and quantum mechanics using the software Hyper Chem **Specific Competence:** 1. Able to understand PES, Born-Oppenheimer Approximation, computational method, 2. Able to nderstanding the molecular mechanics calculation, 3. Able to nderstand calculation semi-empirical quantum mechanics and ab initio, 4. Able to apply computational methods of quantum mechanics to the determination of Single Points on a Potential Energy Surface, Local Minima on a Potential Energy Surface, Transition Structures on a Potential Energy Surface, Molecular Dynamics on a Potential Energy Surface, UV-Visible Spectroscopy, Vibrational Analysis and IR Spectroscopy
Content:	The material is presented in the form of lectures, discussions and practice in front of the computer include: 1. Background on Computational Chemistry: Potential Energy Surfaces, The Born-Oppenheimer Approximation, Molecular Mechanics versus Quantum Mechanics, Classical Mechanics on a Potential Energy Surface Force-Energy Generators 2. Molecular Mechanics: Atom Types, Force Fields, Parameters, Periodic Boundary Conditions and Solvent, Restraints, The Default MM + Force Field 3. Quantum Mechanics, Independent Electron Methods, Self-

	Consistent Field Methods, Post Self-Consistent Field Calculations, The Neglect of Differential Overlap Approximation, characterizations of the Wave function, Mixed Quantum / Classical Model, ab initio method, Extended Hückel Theory, CNDO , INDO, Mindo / 3, MNDO, AM1 and PM3, ZINDO / 1, ZINDO 4. Computational Options: Single Points on a Surface Potential Energy, Local Minima on a Potential Energy Surface, Transition Structures on a Potential Energy Surface, Molecular Dynamics on a Potential Energy Surface, UV-Visible Spectroscopy, Vibrational Analysis and IR Spectroscopy
Attribut soft skill	Effort, Discipline
Study/exam achievements:	Students are considered pass if : 1. Attend the class more than 75% 2. Get score >= 55 Score Presentation: 20% assessment +40% UTS (mid exam) + 40% UAS (final exam) Score grade : A : 75 – 100 AB : 70 – 74.99 B : 65 – 69.99 BC : 60 – 64.99 C : 55 – 59.99 D : 40 – 54.99 E : 0 – 39.99
Forms of Media:	Projector, Whiteboard, Workstation Computer
Learning Methods	Lectures , tutorial and discussion
Literature:	1. HyperChem release 7 : Getting Started, Hypercube, Inc., 2002 2. Introduction to Computational Chemistry, 2nd edition, Frank Jensen, Wiley, 1999 3. Pengantar Kimia Komputasi, Lubuk Agung, Bandung, 2010
Notes:	*Total ECTS = {(total hours workload x 50 min) / 60 min } / 25 hours **Each ECTS is equals with 25 hours**