Diponegoro University
Faculty of Science and Mathematics
Undergraduate Program Of Chemistry

Module designation	**Supramolecular Chemistry (SM)**
Semester(s) in which the module is taught	5
Person responsible for the module	Dr. Parsaoran Siahaan, MS
Language	Indonesian
Relation to curriculum	~~Compulsory /~~ elective ~~/ specialisation~~
Teaching methods	Lecture
Workload (incl. contact hours, self-study hours)	Face to face : 1 x (2 x 50 min); Structured study: 1 x (2 x 60 min); Self study: 1 x (2 x 60 min)
Credit points	2
Required and recommended prerequisites for joining the module	KRX

Module objectives/intended learning outcomes	1. S9 Demonstrates an attitude of being responsible for work in his field of expertise independently. 2. PP1 Mastering the theoretical concepts of structure, properties, changes, kinetics, and energetics of molecules and chemical systems, identification, separation, characterization, transformation, synthesis of micromolecular chemicals, and their application. 3. PP3 Mastering the basic principles of software for analysis, synthesis, and molecular modeling in general or more specific chemical fields. 4. KU1 Able to apply logical, critical, systematic, and innovative thinking in the development or implementation of science and technology that pays attention to and uses humanities values by their field of expertise. 5. KU2 Able to demonstrate independent, quality, and measurable performance. 6. KU5 Able to make decisions regularly in the context of solving problems in their area of expertise, based on the results of analysis of information and data. 7. KK2 Able to solve science and technology problems in general and straightforward chemical fields such as identification, analysis, isolation, transformation, and synthesis of micro-molecules through the application of knowledge of structure, properties, kinetics, and energetics of molecules and chemical systems, with analysis and synthesis methods on specific chemical fields, as well as the application of relevant technologies. 8. KK4 Able to use software to determine the structure and energy of micromolecules, software to assist analysis and synthesis in general or more specific chemical fields (organic, biochemical, or inorganic), and for data processing (analytical chemistry)

Content	1. Introduction: Definition and development of supramolecular chemistry • Monomers, dimers, supermolecules, and supramolecules. • Non-covalent bonds and molecular associations. • Building-Blocks. • Bottom-Up and Top-Down Processes. 2. Electrical properties of single molecules • The charge on the atoms of a molecule. • Electric dipole moment. • Polarisability. • Relative permittivity. • Molecular structure and geometry. 3. Single-molecule computing method • Ab initio method. • Base set. Calculation of energy and electrical properties of molecules: • Molecular energy • Partial load • Dipole moment • Polarisability • Molecular geometry 4. Intermolecular Interaction • Potential energy of interaction. • Dipole-dipole interaction: Eg. H2O...H2O. • Dipole interactions – induced dipoles. • Induced dipole interaction – induced dipole: e.g. Cl2...Cl2. • Hydrogen Bonding: e.g., H2O...CH3OH. • Laws of interaction: Mie potential, van der Waals. • Intermolecular interactions of large molecules: e.g., cellulose, chitin, chitosan with vitamin C, water, metalions; zeolite with phenol derivatives. Water and metal ions. • Gibbs free energy, constant of association, constant of inhibition. 5. Computational method of intermolecular interactions • Ab initio method. • Base set. • Calculation of energy, structure, and geometry of intermolecular interactions, the potential energy of interaction (PES-Potential Energy Surface), stability of molecular associations (dimers) 6. X-ray and DSC method 7. Neutron Diffraction and IR Spectroscopy Methods 8. NMR Spectroscopy Method and Electron Microscopy (AFM – Atomic Force Microscopy)

Exams and assessment formats	Mid-Semester Exam and Final Exam
Study and examination requirements	Participatory Activities 20% Project Results 30% Task 10% Quiz 10% Mid-semester 15% Final exams 15%
Reading list	1. Lehn, J.M., 1995, “Supramolecular Chemistry: concepts and perspectives“, VCH Verlagsgesellschaft mbH, Weinheim 2. Atkins dan de Paula, 2014, Physical Chemistry, 10th ed., W. H. Freeman and Company, New York 3. Anslyn, E.V. dan Dougherty, D.A., 2006, “Modern Physical Organic Chemistry”, University Science Books." 4. Atkins, P. dan De Paula, J., 2006, “Physical Chemistry for the Life Sciences”, Oxford University Press, Oxford." 5. Van Holde, K.E., Johnson, W.C., dan Shing Ho, P., 2006, Principles of Physical Biochemistry, 2nd ed., Pearson Education, Inc. 6. Siahaan, P., 2010, “Kimia Supramolekul”, Bahan Ajar, tidak diterbitkan, Jurusan Kimia UNDIP, Semarang