<table>
<tr><td>Course Code</td><td colspan="2">CHE406M3</td></tr>
<tr><td>Course Title</td><td colspan="2">Advanced topics in Thermodynamics, Surface Chemistry and Macromolecules and Aggregates</td></tr>
<tr><td>Credit Value</td><td colspan="2">03</td></tr>
<tr><td rowspan="2">Hourly Breakdown</td><td>Theory</td><td>Independent Learning</td></tr>
<tr><td>45</td><td>105</td></tr>
<tr><td>Objective/s</td><td colspan="2">• Describe a partial molar property and determination of the properties of mixtures.
• Discuss the concepts of fugacity to the Van der Waals gases
• Explain the special nature and properties of solid surfaces and their specific interaction with environment
• Provide the factors that contribute to the properties of macromolecules
• Discuss the aggregation of particles by self-assembly</td></tr>
<tr><td>Intended Learning Outcomes</td><td colspan="2">• Determine thermodynamic properties of a given system
• Solve problems related to single and multi-phase chemical systems
• Describe the surface orientations
• Discuss the electronic structure of solid surfaces
• Distinguish categories of adsorption of solid surfaces
• Describe over layer structures
• Apply the surface science techniques to characterize solid surfaces and the adsorption of molecules at surfaces
• Explain mechanisms and kinetics involved with different types of polymerization
• Identify the forces responsible for self-assembly</td></tr>
<tr><td>Course Contents</td><td colspan="2">Advanced Thermodynamics
• Brief resume of basic concepts in thermodynamic principles and laws: zeroth, first, second and third law of thermodynamics.
• Thermodynamic relationships for systems in equilibria: Gibbs-Duhem relationship, Gibbs-Helmoltz relationship, Maxwell relationship, thermodynamic equation of states, specific heat capacities and their relationship, Joule-Thomson coefficient.
• Partial molar quantities and its physical significance: partial molar free energy and its variation with temperature and pressure, Gibbs free energy and entropy of mixing of ideal gases, partial molar volumes, method of determination of partial molar volumes
• Phase transitions: phase equilibrium, phase diagrams of pure substances, thermodynamic description of phase transitions and Clapeyron-Clausius equation
• Fugacity and activity: variation with temperature and pressure, graphical method for the determination of</td></tr>
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<tr><td></td><td colspan="2">fugacity, fugacity of a real gas and Van der Waals gases, fugacity species in gas mixtures, Duhem-Margules' equation

Advanced Surface Chemistry

• Description of Solid Surfaces: Ideal single crystal surfaces, surface free energy, reconstruction of the clean surface
• Electronic Structure of Solid Surfaces: Free Electron model, work function, surface states
• Adsorption on Solid Surfaces: Physisorption, work function change induced by physisorption, chemisorption, potential energy profiles for chemisorption, work function changes induced by chemisorption, covalent bonding, lateral interactions between adsorbed species, adsorbate-induced surface reconstruction
• Crystallographic description of overlayer structure: Matrix notation, Wood's Notation
• Surface Science Techniques: Spectroscopy, microscopy and diffraction
• Heterogeneous catalysis: Trends in catalytic reactivity of metals, selectivity, catalytic promoters and poisons, geometric and electronic factors
• Kinetic models for surface reactions: Langmuir-Hinshelwood mechanism, Eley - Rideal mechanism

Macromolecules and Aggregates
• Molar mass: Types of molar mass, methods of determination of molar mass, degree of polymerization
• Polymerization: Synthesis, characterization, kinetics, structure and properties of Step growth, free radical addition, cationic, anionic and co-polymerization
• Self-assembly: Colloids, micelles and biological membranes, surface films, nanofabrication with self-assembled monolayers</td></tr>
<tr><td>Teaching learning Methods/Activities</td><td colspan="2">Lectures, tutorial discussion, small group assignment, home-work assignments, e-learning, online learning</td></tr>
<tr><td rowspan="2">Evaluation/Assessment Strategy</td><td>In-course Assessment</td><td>End-of-course Examination</td></tr>
<tr><td>30 %</td><td>70 %</td></tr>
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Recommended References	• Kapoor, K. L., A "Textbook of Physical Chemistry: Thermodynamics and Chemical Equilibrium", 6th Edition, McGraw Hill Education India, 2019. • Price, G., "Thermodynamics of Chemical Processes", 2nd Edition Oxford University Press, 2019. • Atkins, P., Paula, J. D., and Keeler, J., "Physical Chemistry", 11th Edition, Oxford University Press, 2018. • Smith, E. B., "Basic Chemical Thermodynamics", 6th Edition, Imperial College Press, 2013. • Klotz, I. M., "Chemical Thermodynamics", 7th Edition, Wiley-Inter science, 2010. • Sun, S. F., "Physical Chemistry of Macromolecules", 2nd edition, John Wiley & Sons, 2004. • Laurence, A. B., "Physical Properties of Macromolecules", 1st edition, John Wiley & Sons, 2011. • Gary Attard, and Colin Barnes, "Surfaces" 1st Edition, Oxford University Press, 1998. • Kurt W., Kolasinki, "Surface Science: Foundations of Catalysis and Nanoscience"4th Edition, Wiley, 2020.