<table>
<tr><td>Course Code</td><td colspan="2">CHE405M2</td></tr>
<tr><td>Course Title</td><td colspan="2">Advanced topics in Quantum Chemistry and Reaction Dynamics</td></tr>
<tr><td>Credit Value</td><td colspan="2">02</td></tr>
<tr><td rowspan="2">Hourly Breakdown</td><td>Theory</td><td>Independent Learning</td></tr>
<tr><td>30</td><td>70</td></tr>
<tr><td>Objective/s</td><td colspan="2">• Explain derivation of the Schrödinger equation for a particle in a box
• Discuss the phenomena to quantum tunnel over a classically forbidden barrier
• Explain the Hückel theory approximation for complex molecules
• Provide conditions related to explosion of chemical reactions
• Explain different technologies used in fast reactions
• Describe the reaction path using potential energy surfaces</td></tr>
<tr><td>Intended Learning Outcomes</td><td colspan="2">• Apply the Heisenberg Uncertainty Principle
• Analyze electron properties from quantum mechanical calculations
• Illustrate the wavefunction of the hydrogen atom, poly-electronic atoms and bonding
• Apply steady state conditions for chemical reactions
• Develop methods to study fast reactions
• Construct potential energy surfaces for chemical reactions</td></tr>
<tr><td>Course Contents</td><td colspan="2">Advanced Quantum Chemistry
• The Schrödinger equation: quantum postulates, derivation of the uncertainty principle, the time-dependent and time-independent Schrödinger equation.
• Particle in a box: eigenvalue problems of a free particle, particle in one-, two- and three-dimensional boxes, particle with potential barrier, quantum mechanical tunneling, many particles in a 3-D box.
• The harmonic oscillator: power series solution of differential equations, the 1-D harmonic oscillator, vibration of diatomic molecules.
• Angular momentum: vectors, angular momentum of one particle system, the ladder operator method for angular momentum.
• Rotational motion: particle on a ring and sphere, classical and quantum mechanical treatment of rotation motion, rotation in three dimensions, rotation of diatomic molecules.
• The Hydrogen like atom: formulation of the Schrödinger equation, the Rydberg formula, the radial wave function.
• Structure and spectra of many electron systems: variation and perturbation theory with application to helium atom, coulomb and exchange integrals,</td></tr>
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	molecular orbital theory and Hückel theory for complex molecules **Advanced Reaction Dynamics** • Multistep reactions: steady state approximation, explosions and their limits • Fast reaction kinetics: flow methods, field jump methods, pulse methods, lifetime methods • Oscillations, activated complex theory, potential energy surfaces. • Reactions in solution: nature of liquids, effects of solvent polarity on rates, solvation and its effects of rates, effects of ionic strength, diffusion-controlled reactions	
Teaching learning Methods/Activities	Lectures, tutorial discussion, small group assignment, home-work assignments, e-learning, online learning	
Evaluation/Assessment Strategy	In-course Assessment	End-of-course Examination
	30 %	70 %
Recommended References	• Atkins, P., Paula, J. D., and Keeler, J., “Physical Chemistry”, 11th Edition, Oxford University Press, 2018. • Levine, Ira N., “Physical Chemistry,” 6th Edition, Mr Graw Hill Education, 2008. • Atkins, P., and Friedman, R., “Molecular Quantum Mechanics”, 5th Edition, Oxford University Press, 2010. • Atkins, P., Paula, J. D., and Friedman, R., “Quanta Matter and Change A molecular Approach to Physical Chemistry”, 2nd Edition, Oxford University Press, 2013. • Hayward, D. O., “Quantum Mechanics for Chemists”, 1st Edition, Royal Society of Chemistry, 2002. • James, E. H., “Principles of Chemical Kinetics”, 2nd Edition, Elsevier, 2007.	