

## Enquiry for Course Details

<b>CHEM3541 Physical chemistry: Introduction to quantum chemistry (6 credits)</b>		Academic Year	2022
Offering Department	Chemistry	Quota	100
Course Co-ordinator	Prof G H Chen, Chemistry < ghc@yangtze.hku.hk >		
Teachers Involved	(Dr J Yang, Chemistry) (Prof G H Chen / (Visiting Professor) Prof. Karl Johnson, Chemistry)		
Course Objectives	The course presents fundamental principles and topics on quantum chemistry in order to provide a soiled foundation for students intending to further their studies in chemistry.		
Course Contents & Topics	Elementary quantum mechanics: Historical development, Postulates of quantum mechanics, Principles of quantum mechanics, Theory of angular momentum, Heisenberg uncertainty principle. Applications to simple systems: particle in a box, harmonic oscillator, rigid rotator; Atomic structure: Hydrogen and many electron atoms. Molecular structure and chemical bonds. Approximation methods: variational method, Hartree-Fock method, valence bond theory, and perturbation theory.		
Course Learning Outcomes	On successful completion of this course, students should be able to:		
	CLO 1	understand and use the terminology and nomenclature in quantum chemistry and topics discussed in the course	
	CLO 2	demonstrate knowledge and understanding of basic concepts in quantum mechanics, atomic and molecular structure	
	CLO 3	understand elementary numerical procedures and the basic relationships of quantum mechanics and molecular systems	
	CLO 4	hands-on experience of the application of Hartree-Fock method to molecules	
Pre-requisites (and Co-requisites and Impermissible combinations)	Pass in CHEM2541		
Course Status with Related Major/Minor /Professional Core	2022 Major in Chemistry ( Core/Compulsory ) 2022 Major in Chemistry (Intensive) ( Core/Compulsory ) 2022 Minor in Chemistry ( Disciplinary Elective ) 2021 Major in Chemistry ( Core/Compulsory ) 2021 Major in Chemistry (Intensive) ( Core/Compulsory ) 2021 Minor in Chemistry ( Disciplinary Elective ) 2020 Major in Chemistry ( Core/Compulsory ) 2020 Major in Chemistry (Intensive) ( Core/Compulsory ) 2020 Minor in Chemistry ( Disciplinary Elective ) 2019 Major in Chemistry ( Core/Compulsory ) 2019 Major in Chemistry (Intensive) ( Core/Compulsory ) 2019 Minor in Chemistry ( Disciplinary Elective ) 2018 Major in Chemistry ( Core/Compulsory ) 2018 Major in Chemistry (Intensive) ( Core/Compulsory ) 2018 Minor in Chemistry ( Disciplinary Elective )		
Course to PLO Mapping	2022 Major in Chemistry < PLO 2,4,5 > 2022 Major in Chemistry (Intensive) < PLO 2,4,5 > 2021 Major in Chemistry < PLO 2,4,5 > 2021 Major in Chemistry (Intensive) < PLO 2,4,5 > 2020 Major in Chemistry < PLO 2,4,5 > 2020 Major in Chemistry (Intensive) < PLO 2,4,5 > 2019 Major in Chemistry < PLO 2,4,5 > 2019 Major in Chemistry (Intensive) < PLO 2,4,5 > 2018 Major in Chemistry < PLO 2,4,5 > 2018 Major in Chemistry (Intensive) < PLO 2,4,5 >		
Offer in 2022 - 2023	Y	1st sem	Examination Dec
Offer in 2023 - 2024	Y		
Course Grade	A+ to F		
Grade Descriptors	A	Demonstrate thorough mastery at an advanced level of extensive knowledge and skills required for attaining all the course learning outcomes. Show strong analytical and critical abilities and logical thinking, with thorough grasp of the subject, and ability to apply knowledge to a wide range of complex, familiar and unfamiliar situations. Apply highly effective lab skills and techniques. Critical use of data and results to draw appropriate and insightful conclusions.	
	B	Demonstrate substantial command of a broad range of knowledge and skills required for attaining at least most of the course learning outcomes. Show evidence of analytical and critical abilities and logical thinking, and substantial grasp of the subject, ability to apply knowledge to familiar and some unfamiliar situations. Apply effective lab skills and techniques. Correct use of data of results to draw appropriate conclusions.	
	C	Demonstrate general but incomplete command of knowledge and skills required for attaining most of the course learning outcomes. Show evidence of some analytical and critical abilities and logical thinking, and general but incomplete grasp of the subject, ability to apply knowledge to most familiar situations. Apply moderately effective lab skills and techniques. Mostly correct but some erroneous use of data and results to draw appropriate conclusions.	
	D	Demonstrate partial but limited command of knowledge and skills required for attaining some of the course learning outcomes. Show evidence of some coherent and logical thinking, but with limited analytical and critical abilities. Show partial but limited grasp of the subject, retention of some relevant information of the subject, ability to apply knowledge to solve problems. Apply partially effective lab skills and techniques. Limited ability to use data and results to draw appropriate conclusions.	
	Fail	Demonstrate little or no evidence of command of knowledge and skills required for attaining the course learning outcomes. Lack of analytical and critical abilities, logical and coherent thinking. Show little or no grasp of the knowledge and understanding of the subject, very little or no ability to apply knowledge to solve problems. Apply minimally effective or ineffective lab skills and techniques. Misuse of data and results and/or unable to draw appropriate conclusions.	

Course Type	Lecture with laboratory component course			
Course Teaching & Learning Activities	<b>Activities</b>	<b>Details</b>	<b>No. of Hours</b>	
	Laboratory		24	
	Lectures		24	
	Tutorials		6	
	Reading / Self study		100	
Assessment Methods and Weighting	<b>Methods</b>	<b>Details</b>	<b>Weighting in final course grade (%)</b>	<b>Assessment Methods to CLO Mapping</b>
	Examination		50	CLO 1,2,3
	Laboratory reports	(experiment & lab report)	20	CLO 1,2,3,4
	Test	(test/quiz)	30	CLO 1,2,3
Required/recommended reading and online materials	D. A. McQuarrie: Quantum Chemistry (2nd Edition, 2007) I. N. Levin: Quantum Chemistry (5th Edition, 2008)			
Course Website	NIL			
Additional Course Information	Laboratory classes are mandatory. Students must complete ALL experiments and laboratory reports to pass this course.			