Enquiry for Course Details

CHEM4542 Computational chemistry (6 credits)		Academic Year	2020
Offering Department	Chemistry	Quota	60
Course Co-ordinator	Prof G H Chen, Chemistry < ghc@yangtze.hku.hk >		
Teachers Involved	(Dr J Yang,Chemistry) (Prof G H Chen,Chemistry)		
Course Objectives	This course covers topics in computational chemistry including first-principles methods and molecular dynamics methods. It is offered to undergraduate and postgraduate students interested in computational chemistry, computational physics and computational biology.		
Course Contents & Topics	Hartree-Fock molecular orbital method, density-functional theory, time-dependent methods, Basis sets, Force Fields, QM/MM method, free energy calculation, and computer-aided drug design.		
Course Learning Outcomes	On successful completion of this course, students should be able to: CLO 1: understand the basic concepts of density-functional theory CLO 2: understand the basic numerical techniques of molecular mechanics method and quantum mechanics/molecular mechanics method CLO 3: employ the existing computational software to calculate the chemical, physical properties of various molecular systems include organic molecules, inorganic materials and biomolecules		
Pre-requisites (and Co-requisites and Impermissible combinations)	Pass in CHEM3541 or PHYS3351		
Course Status with Related Major/Minor /Professional Core	2020 Major in Chemistry (Disciplinary Elective) 2020 Major in Chemistry (Intensive) (Disciplinary Elective) 2020 Minor in Chemistry (Disciplinary Elective) 2019 Major in Chemistry (Disciplinary Elective) 2019 Major in Chemistry (Intensive) (Disciplinary Elective) 2019 Minor in Chemistry (Disciplinary Elective) 2018 Major in Chemistry (Disciplinary Elective) 2018 Major in Chemistry (Intensive) (Disciplinary Elective) 2018 Minor in Chemistry (Disciplinary Elective) 2017 Major in Chemistry (Disciplinary Elective) 2017 Major in Chemistry (Intensive) (Disciplinary Elective) 2017 Minor in Chemistry (Disciplinary Elective) 2016 Major in Chemistry (Disciplinary Elective) 2016 Major in Chemistry (Intensive) (Disciplinary Elective) 2016 Minor in Chemistry (Disciplinary Elective)		
Course to PLO Mapping	2020 Major in Chemistry < PLO 1,2,3,5 > 2020 Major in Chemistry (Intensive) < PLO 1,2,3,5 > 2019 Major in Chemistry < PLO 1,2,3,5 > 2019 Major in Chemistry (Intensive) < PLO 1,2,3,5 > 2018 Major in Chemistry < PLO 1,2,3,5 > 2018 Major in Chemistry (Intensive) < PLO 1,2,3,5 > 2017 Major in Chemistry < PLO 1,2,3,5 > 2017 Major in Chemistry (Intensive) < PLO 1,2,3,5 > 2016 Major in Chemistry < PLO 1,2,3,5 > 2016 Major in Chemistry (Intensive) < PLO 1,2,3,5 >		
Offer in 2020 - 2021	Y 2nd sem	Examination	May
Offer in 2021 - 2022	N		
Course Grade	A+ to F		

Grade Descriptors	

A	Mastery of advanced knowledge on following topics: density-functional theory, Kohn-Sham equation, time-dependent density-functional theory, open system, molecular dynamics, force field, and quantum mechanics/molecular mechanics. Strong analytical and critical abilities and logical thinking, with strong ability to apply knowledge to practical problems in physical chemistry.
B	Substantial command of a broad range of knowledge on following topics: density-functional theory, Kohn-Sham equation, time-dependent density-functional theory, open system, molecular dynamics, force field, and quantum mechanics/molecular mechanics. Evidence of analytical and critical abilities and logical thinking, with ability to apply knowledge to practical problems in physical chemistry.
C	Command of knowledge on following topics: density-functional theory, Kohn-Sham equation, time-dependent density-functional theory, open system, molecular dynamics, force field, and quantum mechanics/molecular mechanics. Evidence of some analytical and critical abilities and logical thinking, with ability to apply knowledge to familiar problems in physical chemistry.
D	Partial but limited command of knowledge on following topics: density-functional theory, Kohn-Sham equation, time-dependent density-functional theory, open system, molecular dynamics, force field, and quantum mechanics/molecular mechanics. Evidence of some coherent analytical and critical abilities and logical thinking, with limited ability to apply knowledge to practical problems in physical chemistry.
Fail	Little or no evidence of command of knowledge on following topics: density-functional theory, Kohn-Sham equation, time-dependent density-functional theory, open system, molecular dynamics, force field, and quantum mechanics/molecular mechanics. Lack of analytical and critical abilities and logical thinking, with very little or no ability to apply knowledge to practical problems in physical chemistry.

Course Type	Lecture with laboratory component course

Course Teaching & Learning Activities

Activities	Details	No. of Hours
Laboratory	lab sessions 6x4 hours of computational laboratory	24
Lectures		24
Tutorials		6
Reading / Self study		100

Assessment Methods and Weighting

Methods	Details	Weighting in final course grade (%)	Assessment Methods to CLO Mapping
Assignments	(continuous assessment)	40	CLO 1,2,3
Examination		60	CLO 1,2,3

Required/recommended reading and online materials	Attila Szabo & Neil S. Ostlund: Modern Quantum Chemistry (1st ed.) Robert G. Parr & Weitao Yang: Density-Functional Theory of Atoms and Molecules J.M. Haile: Molecular Dynamics Simulation Andrew R. Leach: Molecular Modelling - Principles and Applications
Course Website	NIL
Additional Course Information	This course is equivalent to CHEM6109 Computational Chemistry. CHEM4542 is offered every other year. Laboratory classes are mandatory. Students must complete ALL experiments and laboratory reports to pass this course.

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