

科目ナンバリング		U-LAS13 10006 LE60							
授業科目名 <英訳>	Basic Physical Chemistry (quantum theory)-E2 Basic Physical Chemistry (quantum theory)-E2				担当者所属 職名・氏名	エネルギー理工学研究所 講師 ARIVAZHAGAN RAJENDRAN			
群	自然科学科目群			分野(分類)	化学(基礎)			使用言語	英語
旧群	B群	単位数	2単位	週コマ数	1コマ	授業形態	講義 (対面授業科目)		
開講年度・ 開講期	2024・後期		曜時限	月2		配当学年	主として1・2回生	対象学生	理系向
【授業の概要・目的】									
We learn about the basics of quantum theory from the chemistry point of view. At first, we learn about the properties of electromagnetic waves and De Broglie wave of matter. Once we understand the wave particle duality, we move to the fundamental atomic models such as Bohr atomic model. Then we learn about the quantization of energy, the wave function and orbitals of atoms, and Schrödinger wave equation. We solve the Schrödinger wave equation to get an insight on the absorption and vibrational spectra of molecules. We then study the wave function and atomic spectra of hydrogen atom, and spin of electron in detail. Finally, we learn about the application of quantum chemistry in various fields.									
【到達目標】									
The aim of this class is to understand the basic principles of quantum chemistry.									
【授業計画と内容】									
1. Property of the electromagnetic wave 2. Bohr's atomic model 3. De Broglie wave of matter 4. Time independent Schrödinger wave equation 5. Time dependent Schrödinger wave equation 6. One dimensional potential wells 7. One dimensional harmonic oscillation 8. Wave equation of hydrogen atom 9. Wave function and energy eigenvalue of hydrogen atom 10. Angular momentum and Zeeman effect 11. Spin of electron 12. Spin-orbit interaction 13. Term symbols and revised Zeeman effect 14. Application of quantum chemistry 15. Assignment which is considered as a term examination 16. Feedback									
【履修要件】									
特になし									
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【成績評価の方法・観点】

Results will be evaluated by the submission of homework written in English (30%), attendance and discipline (20%), and assignment which is considered as a term examination (50%).

【教科書】

Donald A. McQuarrie 『Quantum Chemistry, 2nd Edition』 (University Science Books) ISBN:978-1-891389-50-4

Peter Atkins and Julio de Paula 『Atkins' Physical Chemistry, 10th Edition』 (Oxford University Press) ISBN:978-0-19-969740-3

【参考書等】

(参考書)
授業中に紹介する

【授業外学修（予習・復習）等】

I recommend that the students should review the points to be learned.

【その他（オフィスアワー等）】

Office hours are set at 15:00-17:00 in every Friday.