

茨城工業高等専門学校	開講年度	令和05年度 (2023年度)	授業科目	Quantum Chemistry
科目基礎情報				
科目番号	0132	科目区分	専門 / 選択	
授業形態	講義	単位の種別と単位数	学修単位II: 2	
開設学科	国際創造工学科 情報系	対象学年	5	
開設期	前期	週時間数	前期:2	
教科書/教材	1) Quantum Mechanics for Chemists, by David Howard.			
担当教員	アッバス アルシハビ			
到達目標				
1) understand the difference between classical and quantum mechanics. 2) understand the idea of wave function. 3) understand the uncertainty relations. 4) solve Schroedinger equation for simple potentials. 5) understand the Schroedinger theory application to Hydrogen atom. eigenvalue problems for energy, momentum, angular momentum and central potentials explain the idea of spin. 6) solve the 7) understand the Schroedinger theory application to many-electron atoms. the Orbital Molecular Theory. 8) become introduced to				
ルーブリック				
	Ideal Level	Standard Level	Minimum achievement level standard (Pass)	Unacceptable Level
Understand the principles of quantum mechanics	Treat wave functions in linear algebra.	Understand the atomic wave function.	Know the difference between classical and quantum mechanics	Does not understand the postulates of quantum mechanics.
Understand the Schroedinger Theory of Quantum Mechanics	Define the equation for the well, and barrier potential applications.	Define the equation, and define components.	Understand the component of the Schroedinger equation.	Does not understand the Shroedinger equation components.
Understand the Schroedinger application to the Hydrogen atom.	Define the equation and calculate the eigen values.	Calculate the eigen values from the Schrodinger Equation.	Define the Hydrogen atom eigen values in the Schrodinger equation.	Does not understand the eigen values in the Schroedinger equation.
Understand the Molecular Orbital Theory application.	Can write the electronic configuration of the molecular orbital.	Make a Molecular Orbital energy level diagram of an elemental molecule.	Understand the bonding mechanism in the Molecular Orbital Theory.	Does not understand the Schroedinger application to the multi-electron atom.
学科の到達目標項目との関係				
学習・教育到達度目標 (A)				
教育方法等				
概要	Lecturing: Slide show, blackboard explanation.			
授業の進め方・方法	Tutorial: solving backboard questions, homework			
注意点	This class is held in English.			
授業の属性・履修上の区分				
☐ アクティブラーニング		☐ ICT 利用	☐ 遠隔授業対応	☐ 実務経験のある教員による授業
授業計画				
		週	授業内容	週ごとの到達目標
前期	1stQ	1週	Principles of quantum mechanics; revision	Understand the principles,
		2週	Postulates of Quantum mechanics	Understand the wave function.
		3週	Postulates of Quantum mechanics	Undertsnad linear operators, Hamiltonian.
		4週	Schroedinger theory of quantum mechanics 1	Undesrand Born`s Interpretation, Infinite square well potential
		5週	Schroedinger theory of quantum mechanics 2	Understand The Time-Independent Schroedinger Equation
		6週	Schroedinger theory of quantum mechanics 3	Understand the solutions to the Time-Independent Schroedinger Equation; zero and step potentials.
		7週	Midterm Exam	
		8週	Schroedinger theory of quantum mechanics 4	Understand Zero potential and step potentials.
	2ndQ	9週	Schroedinger theory of quantum mechanics 5	Understand barrier potential and harmonic oscillator potential.
		10週	The Hydrogen atom 1	Understand the application of Shroedinger`s equation to the Hydrogen atom.
		11週	The Hydeogen atom 2	Solve the Shroedinger`s equation for the Hydrogen atom.
		12週	Multi-electron atom	Understand the application of Shroedinger`s equation to the multielectron atoms.
		13週	Molecular Orbital Theory	Become introduced to Hartree Fock approximation
		14週	Molecular Orbital Theory	Become introduced to molecular orbital theory, Hydrogen molecule bonding
		15週	Final Exam	
		16週	Review	Review
評価割合				

	Presentation	Homework/Report	Mutual Evaluations between students	Behavior	Portfolio	Quiz	合計
総合評価割合	0	45	0	0	0	55	100
Basic Proficiency	0	15	0	0	0	15	30
Specialized Proficiency	0	15	0	0	0	25	40
Cross Area Proficiency	0	15	0	0	0	15	30