< >	Basic Physical Chemistry (quantum theory)-E2 Basic Physical Chemistry (quantum theory)-E2			PARK Jaehong
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Course overview: We will discuss basics of quantum chemical theory

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1. Review of physical chemistry II and introduction of quantum chemistry
Schrodinger equation, operators, harmonic oscillator, particle in a box

2. Angular momentum

3. Theorems of quantum mechanics
Hermitian operators, eigenfunction expansion, commuting operators, parity

4. Approximation method
Variation method, and perturbation theory

5. Hydrogen, helium, many-electron atoms
hydrogen and helium, many electron atoms

6. Electronic structure of molecules

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Topics week Note

Quantum theory: Introduction and principles 1-2 Energy quantization, wave-particle duality, Schrodinger equation, Born interpretation of the wavefunction, operators, the uncertainty principle, the postulates of quantum mechanics

Quantum theory: techniques and applications 3-6 A particle in a box, harmonic oscillator, a particle on a ring, a particle on a sphere

Atomic structure and spectra 7-10 The structure of hydrogenic atoms, atomic orbitals and their energies, spin-orbit coupling, term symbols, selection rules

Molecular structure 11-14 Born-Oppenheimer approximation, valence-bond theory, molecular orbital theory, homonuclear diatomic molecules, heteronuclear diatomic molecules, polyatomic systems

Final/survey 15 Final exam for Wk 1-14 contents

Basic Physical Chemistry (quantum theory)-E2(2)

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Grades: One final exam (60%), 6 quizzes (30% = 6× 5%), attendance and class participation (10%)

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P. Atkins and J. de Paula.   Physical Chemistry, 9th ed 2014   Oxford University Press   ISBN: 9780199697403   8th or 10th edition is also OK, but students are responsible to check the differences between editions

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Homework: During the semester, you will have four homework assignments and the sum of four grades, will count 20% towards the final grade. Problem sets of homework will be assigned from the textbook(see the course textbook).Only legible and intelligible answers will be considered, and otherwise, you will lose some or all credits for the problem. No late homework turn-in will be accepted, unless the late return is excused.

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Instructor: Jaehong Park (email: j.park@moleng.kyoto-u.ac.jp)

Course meeting: (Yoshida South campus, XXX, XXX), 1 session/week, 90 mins/session

Office hour: (Location and Time: Katsura campus, A4-205, appointment by email).

Exams: There will be one 90-min final exam. The final exam will be held during the final exam schedule (XX-XX), which will be announced later.

Quizzes: There will be six quizzes. The sum of 6-quiz grade will count 30% towards the final grade.