

Advanced quantumchemistry

2 units (selection)

Eiji Kanazaki · PROFESSOR / PHYSICOCHEMISTRY AND MATERIAL SCIENCE, CHEMICAL SCIENCE AND TECHNOLOGY, EARTH AND LIFE ENVIRONMENTAL ENGINEERING

Target) Molecular science based quantum chemistry minded for current topics will be present both in experimental and theoretical fields with emphasis on molecular spectroscopy in relation to molecular structure and molecular properties

Outline) Basic studies on the electronic states of molecules are presented from aspects of molecular spectroscopy under outer stresses of electric, magnetic and of optical forces to molecules or molecular assemblies. Although discussion will be mainly focused onto some resonance conditions of the forces, their double resonance will be included if time is not pressed

Style) Lecture

Keyword) *molecular spectroscopy*

Fundamental Lecture) “Quantum Chemistry”(1.0), “Physical Chemistry”(1.0)

Relational Lecture) “Graduate Seminar in Chemical Science and Technology” (0.5), “Advanced experiments on chemical science and technology”(0.5)

Goal) To understand, at least, one of the current topics in quantum chemistry

Schedule)

1. about this lecture
2. basic concept of quantum chemistry
3. basic methods of quantum chemistry
4. advanced concept of quantum chemistry
5. advanced methods of quantum chemistry
6. basic concept for electronic states of molecule
7. advanced concept for electronic states of molecule
8. basic concept for the study in electronic states of molecule, a survey
9. basic methods for the study in electronic states of molecule
10. advanced concept for electronic states of molecule
11. introduction to interaction of molecules with outer field
12. basic concept for interaction of molecules with outer field
13. basic concept for calculation of interaction
14. advanced concept for calculation of interaction
15. more advanced concept for calculation of interaction
16. examination

Evaluation Criteria) レポート提出を求め、平常点を考慮して評価する

Textbook) ATKINS, PHYSICAL CHEMISTRY, 9th ed., 2010, Oxford University Press.

Contents) <http://cms.db.tokushima-u.ac.jp/cgi-bin/toURL?EID=216910>

Student) Able to be taken by only specified class(es)

Contact)

⇒ Kanazaki (G516, +81-88-656-9444, kanazaki@chem.tokushima-u.ac.jp)

MAIL (Office Hour: refer to the official HP)