

Introductory info

Quantum Chemistry

Lesson 0

Staff and cast

Teacher

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Students

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Content

Quantum chemistry

- quantum theory (mechanics) applied to electrons moving around atomic nuclei
- inter-atomic interactions: potential energy and its derivatives (gradients, Hessian matrices)
- other properties: charge distribution in space (electric and magnetic multipole moments), polarizability, probability of radiative and non-radiative transitions, ...

Troublesomes

- many particles involved
- electrons (= fermions), specific conduct (Pauli exclusion principle)
- complex equations → numerical solution (computationally demanding) → (super)computers

Content

Focus of the present course

- basic concepts and methods

Goal(s)

- learn the language of QC (basics)
- become able to communicate with specialists in QC
- be ready to use third-party QC codes

Content

1. Basics of quantum theory
2. Angular momentum, spin
3. Hydrogen atom
4. Many-particle systems
5. Approximate methods – variational approach
6. Approximate methods – perturbation theory
7. Helium atom
8. Born-Oppenheimer approximation, potential energy surface
9. Hartree-Fock methods
10. MO-LCAO methods, basis sets of atomic orbitals, VB methods
11. Beyond the HF methods (correlation energy)

Course implementation

Lectures

- 2+ attendees
 - face-to-face meetings (lectures)
 - PDF presentations (itemized explanations + links)
- 1- attendee
 - home reading (meetings according to your needs)
 - recommended literature (selected chapters)

Seminar

- 2+/1- attendees = face-to-face / correspondence form
- tasks assigned in advance, presentations of / reports on prepared solutions

Literature

„Obligatory“

- lectures presentations
- and links provided therein

Obligatory (EDISON)

- Skála, L. *Kvantová teorie molekul*, Karolinum, Praha 1995
- **Pilar, F. L., *Elementary Quantum Chemistry*, McGraw-Hill, New York 1990**

Recommended

- Formánek, J. *Úvod do kvantové teorie I a II*, Academia, Praha 2004
- Fong, P. *Elementary Quantum Mechanics*, World Scientific, Singapore 2005
- Fišer, J. *Úvod do molekulové symetrie*, SNTL, Praha 1980
- Foresman, J.B., Frisch, A. *Exploring Chemistry with Electronic Structure Methods*, Gaussian Inc., Pittsburgh 1993

Communication, consultations, ...

The main communication channel

- lectures presentations and seminar tasks assignments at https://home1.vsb.cz/~kal0063/vyuka_kvch.htm

Consultations

- lectures, seminars
- e-mail (rene.kalus@vsb.cz)
- collective/individual consultations (by appointment)

Passing the course (with success)

EDISON

- report on an assigned topic and its (oral) defense

Credit

- report = presentation of assigned tasks at seminars
- (if needed, additional tasks)

Exam

- oral exam (discussion on selected topics with lectures presentations at hand)

Other business

Collisions with other ventures

- April 25 – the Day of Sports at the VSB-TUO – regular lecture/seminar preferred

Questions

- ???