UNIVERSITY of MISKOLC
Faculty of Materials and Chemical Engineering

Antal Kerpely Doctoral School of Materials Science & Technology

Computational Spectroscopy and Thermodynamics

Prof. Dr. Milán SZŐRI

COURSE DESCRIPTION

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Computational Spectroscopy and Thermodynamics

Prof. Dr. Milán SZŐRI

Lecturer

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Recommendation

The lecture is proposed for all students of the Kerpely Doctoral School, with a special focus on students interested in chemistry and computer simulations.

Language

English.

Scope

The main goal of the course is to provide students with an overview of modern computational chemistry tools and to teach them how to utilize these techniques in various applications, complementing experimental methods.

Methodology

The course is conducted through in-person lectures and practical sessions. The lectures and practices are structured to provide a comprehensive understanding of theoretical chemistry methods. Students are then trained to apply these methods using various software packages, enabling them to apply their knowledge practically to systems of interest.

Topics

1. Quantum chemical calculation of spectra associated with molecular vibrations.
2. Quantum chemical computation of electronic excitation spectra of molecular systems: Absorbance and fluorescence spectra.
3. Determination of chirality through molecular computations.
4. Computation of NMR spectra.
5. Ab initio prediction of thermodynamic functions.

References

1. Höltzl Tibor, Veszprémi Tamás: *Kémiai szimulációk az atomoktól a vegyipari reaktorokig* Akadémiai Kiadó **2019** (ISBN: 9789630599726)
2. Martin Kaupp; Michael Bühl; Vladimir G Malkin: *Calculation of NMR and EPR parameters: theory and applications* Wiley-VCH, **2004** (ISBN: 3527307796)
3. Frank Neese: *ORCA An ab initio, DFT and semiempirical SCF-MO package* - Version 5.0.4 (https://www.orcasoftware.de/tutorials_orca/)
4. Yukihiro Ozaki, Marek Janusz Wójcik, Jürgen Popp(ed.): *Molecular Spectroscopy A Quantum Chemistry Approach.* **2019** Wiley-VCH Verlag GmbH & Co. (ISBN: 9783527344611).
5. Frank Jensen: *Introduction to Computational Chemistry* (3 ed.) John Wiley & Sons **2017** (ISBN: 9781118825983).

Exam

Project work.

Complex exam questions

1. What spectra contain signals corresponding to vibrational transitions? What effects influence the positions and intensities of spectral bands? How can these factors be accounted by using computational chemistry tools?

2. Describe theoretical methods used for the electronic molecular excitation spectrum. What spectra are associated with electronically excited molecular states?

3. What experimental and theoretical chemical methods are known for determining molecular chirality? What kind of additional information do quantum chemical calculations provide for interpreting experimental spectra?

4. How can NMR parameters be determined using computational chemistry tools? What information can be extracted by comparing experimental and computed spectra?

5. What are quantum chemitry based thermodynamic protocols used for? What thermodynamic functions can be estimated using quantum chemical methods? What level of accuracy do these protocols achieve?