UNIVERSITY of MISKOLC
Faculty of Materials Science and Engineering

AntalKerpely Doctoral School of Materials Science & Technology

Molecular Simulations of Complex Systems, Molecular Design and Calculations of Thermochemical properties

Milán Szőri, PhD

COURSE DESCRIPTION

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Molecular Simulations of Complex Systems, Molecular Design and Calculations of Thermochemical properties

Milán Szőri, PhD

Lecturer

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Recommendation

The lecture is proposed for all students of the AntalKerpelyDoctoralSchool, especially in the field ofInterfacial and Nanotechnologies, Materials Informatics, Materials Science and Technology in Space, High-temperature Equipment and Thermal Management, Chemical Processes and Technologies.

Language

Hungarian or English.

Scope

The main objectives of this course areto provide an overview of the modern computational chemistry tools for the students and to train students to use these techniques for wide variety of applications.

Methodology

The course is held in contact lectures. Lectures and practices are held in such a way that students can deeply understand the theoretical chemistry methods and then they are trained to use these methods implemented in software packages and they can transfer this knowledge in practice for system of interests.

Topics

Born-Oppenheimer approximation and its consequences: concept of molecule. Exploring the potential energy surfaces.

Quantum Theory of the Atoms in Molecules (AIM). Mathematical analysis of the electron density of the molecules and solids. Bond Theories.

Virtual combinatorial chemistry: generation and applications of graph representation of molecules. Exploring chemical space by theoretical chemistry methods.

From molecular properties to macroscopic properties: estimation of the thermodynamic properties and partition functions, contributions of molecular movements to the partition

functions.Calculation of Molecular Thermodynamic Properties: From Estimation to Prediction.

Highly accurate model chemistries and their applications and limitations.

Exploring reaction mechanisms and theoretical background of the absolute rate constant calculations based on the calculated potential energy surface. SWOT analysis of the computed rate constants. Study of complex reaction systems. Case studies for combustion and atmospheric oxidation processes.

Force field description of complex molecular systems. Adsorption phenomena as seen from molecular dynamic and grand canonical Monte Carlo simulations.

References

1. Christopher J. Cramer: E*ssentials of Computational Chemistry: Theories and Models* (2nd Edition), Wiley, 2004.
2. VeszprémiTamás, FehérMiklós: *A Kvantumkémiaalapjaiésalkalmazása,*MűszakiKönyvkiadó, 2002.
3. Frank Jensen: *Introduction to Computational Chemistry. Second Edition.* Wiley & Sons, Ltd. 2007.
4. + If a student intends to applyany method linked to this course for her/hisdoctoral research, then she/he will be able to request specific articles.

Exam

Oral exam.

Complex exam questions

1. Advantages and limitations of computational chemistry in structural characterization.
2. Virtual combinatorial chemistry studies.
3. Applied model chemistries for estimating thermochemical properties. Discussion about the performances of these model chemistries.
4. Theoretical background of the absolute rate constant calculations based on the calculated potential energy surface. Advantages and limitations of the computed rate constants for modelling experiment.
5. Theoretical background for molecular models of adsorption processes. Benefits and limitations.