UNIVERSITY of MISKOLC
Faculty of Materials and Chemical Engineering

Antal Kerpely Doctoral School of Materials Science & Technology

Organic Chemistry and Computations

Dr. Zoltán Mucsi

COURSE DESCRIPTION

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Lecturer

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Recommendation

The course is recommended for PhD students of Kerpely Doctoral School, especially those working in organic chemistry, medicinal chemistry, photochemistry, or reaction mechanism analysis. It is particularly useful for students aiming to integrate computational chemistry into experimental research.

Language

English.

Scope

The primary aim of the course is to provide a comprehensive understanding of computational methods applied to organic chemistry. The course focuses on quantum chemical approaches to reaction mechanisms, molecular structure, reactivity, and photochemical processes. Students will gain insight into how theoretical calculations support experimental design, interpretation, and prediction in modern organic chemistry.

Methodology

The course consists of lectures and hands-on computational sessions. The theoretical background of quantum chemistry is introduced and directly connected to practical applications using widely used software (e.g., Gaussian, etc). Students will learn how to build molecular models, perform geometry optimizations, calculate reaction pathways, and analyze electronic structures. Emphasis is placed on interpreting computational results in a chemically meaningful way.

Topics

1. Fundamentals of quantum chemistry in organic systems (wavefunction, DFT, basis sets)
2. Geometry optimization and conformational analysis
3. Potential energy surfaces and reaction coordinate analysis

4. Transition state theory and reaction mechanism elucidation
5. Thermodynamics and kinetics from computational data
6. Solvent effects and implicit solvation models (PCM, SMD)
7. Electronic structure analysis (NBO, charge distribution, frontier orbitals)
8. Aromaticity and reactivity descriptors (e.g., NICS)
9. Photochemistry and excited states (TD-DFT, S0/S1/T1 states, ISC)
10. Case studies: organic reactions, catalysis, and functional molecule design

References

1. Essentials of Computational Chemistry: Theories and Models – C. J. Cramer, 2nd Edition, Wiley (2004)
   → Comprehensive theoretical foundation with strong relevance to organic chemistry applications.
2. Introduction to Computational Chemistry – F. Jensen, 3rd Edition, Wiley (2017)
   → Practical and method-oriented overview, widely used in graduate-level education.
3. Exploring Chemistry with Electronic Structure Methods – J. B. Foresman, Æ. Frisch, Gaussian Inc. (latest edition)
   → Application-focused guide, especially useful for hands-on computational work (e.g., Gaussian).

Exam

Project work.

Complex exam questions

1. **Reaction mechanism analysis**
   Describe how a full reaction mechanism can be elucidated using computational chemistry. Include the identification of intermediates, transition states, and the construction of a potential energy surface. How can competing pathways be quantitatively compared?

2. **Transition state verification**
   Explain the criteria for confirming a transition state structure in quantum chemical calculations. Discuss the role of frequency analysis, intrinsic reaction coordinate (IRC) calculations, and the connection between the transition state and reactants/products.

3. **Method selection and limitations**
   Compare Density Functional Theory (DFT) and wavefunction-based methods (e.g., MP2, CCSD). Under what conditions is DFT reliable for organic reaction modeling, and where can it fail? Provide specific examples related to organic chemistry.

4. **Solvent effects and realistic modeling**
   Discuss how solvent effects influence reaction energetics and mechanisms in organic chemistry. Compare implicit (e.g., PCM, SMD) and explicit solvent models, and evaluate their advantages and limitations in practical applications.

5. **Excited-state reactivity and photochemistry**
   Explain how computational methods can be used to study photochemical reactions. Describe the roles of S_0, S_1, and T_1 states, intersystem crossing (ISC), and conical intersections. How can these concepts be applied to understand photochemical bond cleavage or fluorescence quenching mechanisms?