Basic Information:
Course Title: Computer modeling of molecular structure and optical properties of single molecules and supramolecular aggregates
Lecturer: prof. Silvia Angelova, PhD
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Total Teaching Hours: 30

Annotation

The course is suitable for PhD students in chemistry or physics. The objectives of the course are: 1) PhD students to gain knowledge of the basics of computational chemistry and 2) to introduce the PhD students to modern computer modeling methods with application to the study of structure and properties of photoactive systems. Practical classes are planned, which aim to illustrate the lecture material, and on a number of topics - to expand the knowledge and skills of PhD students in the use of modern computational methods for the study of molecular properties and intermolecular interactions that determine the structure and properties of materials.

Course content (brief description by topics or modules)

Topic / Module 1: Principles and approximations in quantum chemistry (2 hours); Computational methods: ab initio methods, semi-empirical methods, molecular mechanics, molecular dynamics, Monte Carlo method, etc. Hierarchy of computational methods (2 hours)

Topic / Module 2: Density Functional Theory (DFT) (2 hours); Applications of DFT for modeling different levels of matter organization – atoms, molecules, solids, and nanostructures (7 hours); Methods for accounting for environmental effects – explicit and implicit approaches (2 hours)

Topic / Module 3: Practical exercises: Working with *ChemDraw* and *GaussView* graphical software. Preparation of input files for the *Gaussian* program. Construction of Z-matrices (8 hours); Working with *ChemCraft* and *GaussView* graphical software. Visualization of calculation result files using *GaussView* and *PyMol* (7 hours)

Teaching and assessment methods

Forms of instruction – lectures, consultations;

Assessment – written examination (test).

Competencies acquired as a result of training (3–5 points)

- Acquisition of knowledge of the fundamental principles and methods of computational chemistry and their application to the study of molecular systems.
- Skills in the use of modern computational methods and specialized software for modeling molecular structure, as well as the electronic and optical properties of single molecules and supramolecular aggregates.

- Ability to analyze and interpret intermolecular interactions and their relationship to the structure and properties of materials.
- Practical skills for conducting research using computational chemistry methods, including processing, analysis, and evaluation of the obtained results.
- Competence in the independent application of computational modeling methods in research activities in the fields of chemistry, physics, and materials science.

Literature:

1) E. G. Lewars, Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics 2nd ed., 2011.

2) Structure of Molecules, St. Kliment Ohridski University Press, 2007 (in Bulgarian).

3) F. Jensen, Introduction to Computational Chemistry, J. Wiley&Sons, 1999.

4) Methods of Electronic-Structure Calculations: From Molecules to Solids, J. Wiley&Sons, 2000.

5) J. B. Foresman and Æ. Frisch, Exploring Chemistry with Electronic Structure Methods, 3rd ed., Gaussian, Inc.: Wallingford, CT, 2015.

Additional information (optional) (e.g., special requirements, laboratory equipment, prior knowledge)

If possible, participants should have their own laptop computer for participation in the practical exercises and for working with specialized computational modeling software. Prior knowledge is not mandatory for PhD students specializing in the fields of chemistry or physics.