ЦЕНТЪР ЗА ОБУЧЕНИЕ – БАН

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Basic Information:
Course Title: **Quantum chemical methods in catalysis**
Lecturer: Assoc. Prof. Valentin Alexiev, PhD
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Total Teaching Hours: 30 hours.

Annotation (up to 150 words)
The aim of the course is to allow the acquaintance of the PhD students with the actual quantum-chemical methods such as method of Hartree-Fock, Functional Density Theory, Correlation methods, hybrid methods such as molecular mechanics and the method of the strong bonding.The above mentioned methods will be applied to some simple molecular systems and surfaces. The students will get practical knowledge in the application of the quantum-chemical programs Demon, Gaussian -03 and Crystall-03

Course content (brief description by topics or modules)
Topic / Module 1: Introduction to computational chemistry. Models, approximations and reality.
Basic principles - energy, electrostatics, thermodynamics, quantum mechanics, statistical mechanics and atomic units.
Practical session 1: Virtual machine for this course. Installed software packages and interfaces. Working with the graphical interface Gabedit.

Topic / Module 2: Molecular Modeling Methods I. Molecular Geometry Models.
• Cartesian Coordinates and Internal Coordinates.
• Description and Modeling of Molecular Geometry.
Methods for Calculating the Electronic Structure of Molecular Systems. Hartree-Fock and Post-HF.

Topic / Module 3: Molecular Modeling Methods II. Density Functional Theory (DFT).
• Kohn-Sham Theorems. DFT.
• Exchange-Correlation Functionals (LDA, GGA, Hybrid Functionals).
• Potential Energy Surfaces (PES)
• PES Topology
• First and Second Derivatives of Energy
• Geometry Optimization: Molecules and Clusters.
Topic / Module 4: Molecular Modeling Methods III. Vibration of Molecular Systems
• Hessian Matrix and Vibrational Mode
• Vibration of Molecules and Clusters
• NMR and IR/Raman Spectrum (Raman Spectrum).
Exercise: Practical Session 4: Applications to Benzene Molecule and Clusters.
Calculation of IR and NMR Spectrum of Benzene in the Hartree-Fock Approximation.

Total Energy, Geometry Optimization and NMR of Benzene in the Framework of TFP (B3LYP).

Topic / Module 5: Molecular Modeling Methods IV. Transition States and Thermodynamics
• PES. Extreme Points (Local Minima and Maxima),
• Transition State Search.
• Methods for Finding Transition Structures
• Isomers - Formation Energies and Reactions
Thermodynamics of an Ideal Gas
• Ideal and Real Gas
• Sum of States and Chemical Potentials.
• Gibbs Free Energy.
• System Stability and Chemical Reactions
Exercise: Practical Session 5: Proton Transfer in Malonaldehyde Enol (B88-LYP / DZVP). Diels-Alder - trans-butadiene and ethylene (PM3). Modeling Other Reactions.

Topic / Module 6: Practical molecular modeling using installed utilities and molecular modeling installation packages. Methods
• Molecular mechanics. Semi-empirical methods (Mopac). Hartree-Fock and post-HF. Density functional theory.
• Choosing a theoretical method
• Basis functions - using available basis functions
• Molecular energy for a given geometry and optimizing molecular geometry
• Molecular orbitals and densities.
Exercise: Practical session 6:. General energy calculation and optimization of molecules within HF and DFT approximations. Molecular diagrams, graphical representation of molecular diagrams, orbitals and densities.

Teaching and assessment methods
Full-time and part-time forms of study.

Competencies acquired as a result of training (3–5 points)
1. Acquisition of basic knowledge in quantum chemical methods.
2. Acquisition of knowledge for using the Hartree-Fock method
3. Acquisition of knowledge about density functional theory.
4. Acquisition of knowledge about electronic calculation of the structure and methods for simulation of molecular dynamics, with applications in materials science.

Literature:
1. Introduction to Quantum Mechanics, David J. Griffiths, Cambridge University Press, 978-1-316-64651-9, 2017
2. The Physics of Quantum Mechanics, James Binney & David Skinner, J Binney, ISBN. 9780199688579, 2008

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ул. „Сердика“ № 4
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3. Квантова химия, Н. Тютюлков, Наука и изкуство, София, 1978 г.

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

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