

Course description

Course Title Quantum Chemistry Química Quântica		
Type/Attendance Time Lecture: 2 hours per week Tutorial: 2 hours per week	Credit points (ECTS) 5	Type of Examination Examination, Exercises
Recommended Prerequisites [Requirements prior to entrance to be entered]		
Content 1. Review of Fundamentals Axioms and theoretical background of quantum mechanics, H-atom and atomic orbitals, Pauli principle and Slater determinants 2. Ab initio Methods of Quantum Chemistry Born-Oppenheimer approximation, Hartree-Fock approximation (SCF), LCAO-MO-approximation, Roothaan equations, basis sets, correlation methods (CI, MP, et.al.) 3. Semi-empirical Methods of Quantum Chemistry Approximations (ZDO et.al.), Hückel method et.al. 4. Density Functional Theory Kohn-Hohenberg theorems, probability density functions 5. Potential Energy Surfaces for Chemical Reactions Scatterplots, adiabatic / diabatic potential curves, forbidden crossing of potential curves of the same symmetry, conical intersection Glossary SCF Method = Self consistent field method, LCAO-MO- = approximation of molecular orbitals as linear combinations of atomic orbitals, CI Method = Configuration interaction method, MP Methods = Møller-Plesset perturbation theory, ZDO Approximation = Zero Differential Overlap approximation		
Conteúdo 1. Revisão dos fundamentos; 2. Métodos <i>Ab Initio</i> de química quântica; 3. Métodos semi-empíricos de química quântica; 4. Teoria da Densidade Funcional; 5. Superfícies de energia potencial para reações químicas.		