Title of the course: Computational Chemistry

Credits: 2

Coordinator/Department: Fogarasi, Geza / Inorganic Chemistry

Terms for joining: at least two semesters of physical chemistry and one semester of theoretical chemistry

Topics covered by the course:
Molecular mechanics: theoretical basis, fields of applications, assessment of limitations. Electronic structure of molecules: an overview of methods of quantum chemistry; practical aspects: basis sets, treatment of electron correlation; semiempirical methods; density functional theory (DFT). Structural research by computational methods. Symmetry and molecular structure, with a brief introduction to group theory. Studying chemical reactions: transition state theory and statistical mechanics; reaction mechanisms, qualitative theories. Computer simulation of dynamic phenomena.

Literature*:
Compulsory:
1. Frank Jensen: Introduction to Computational Chemistry, John Wiley & Sons, Chichester, New York; 1999. ISBN: 0 471 98425 6.

Suggested:
2. Christopher J. Cramer: Essentials of Computational Chemistry, John Wiley & Sons, Chichester, 2002. ISBN: 0 471 48552 7.
3. Errol Lewars: Computational Chemistry, Kluwer Academic, Boston/Dordrecht/London, 2003. ISBN: 1-4020-7285-6.