General Information			
Course name	Molecular Structure and Chemical Bonding	**ECTS Credits**	6
		Semester	S

Aims

Attendees will learn actual methods used for computer simulations of molecules. By using practical examples, he/she will get hands-on experience with standard methods.

Content

Born-Oppenheimer approximation. Methods and approaches of classical molecular mechanics. Force fields and force constants for polyatomic simulations. Force fields for biomolecular simulations (CHARMM, AMBER, MM2-4, MMFF, CVFF,...). Independent electron approximation. Hartree-Fock self-consistent field method. Post Hartee-Fock methods. Density functional theory (DFT) - basic principles and implementation. LSDA approximation and gradient corrected methods. Hybrid methods. Wavefunction and electron density analysis. Limits and perspectives of classical and quantum molecular mechanics. Alternative methods. Ab initio computations and experimental observables. Experimental and computational observables. Molecular dynamics and stochastic methods. Integration algorithms. Car-Parinello dynamics.

Assessment Methods and Criteria

Elaboration of the project - characterization of the chosen molecule using methods mentioned in the course. Exam.

Grading Scale (in %):
A: 91% - 100%
B: 81% - 90%
C: 71% - 80%
D: 61% - 70%
E: 51% - 60%
F: 0% - 50%

Grading System:
The University recognises the following six degrees for the evaluation of the study results:
a) A – excellent (excellent results) (numerical value 1)
b) B – very good (above average results) (1.5)
c) C – good (average results) (2)
d) D – satisfactory (acceptable results) (2.5)
e) E – sufficient (results meet the minimum criteria) (3)
f) FX –failed (requires further work) (4)

Bibliography

1. Leech: Molecular Modeling: Principles and Applications, Longmann, 1996.

2. M.P. Allen, D.J. Tildesley: Computer Simulation of Liquids, Oxford University Press, 1989.

3. Polák, Zahradník: Kvantová chemie, SNTL/Alfa , 1985 or Zahradník, Rudolf, and Rudolf Polák. *Elements of Quantum Chemistry*. 1980 edition. New York : Prague: Springer, 1981.

4. P. W. Atkins, R. S. Friedman: Molecular Quantum Mechanics.Oxford University Press, 1997