SCIENTIFIC AND METHOD MODULES

Module name	Basic Concepts in Chemistry
Number	2012-B1
Aims	This module for non-chemists introduces the basic concepts in chemistry needed for actively participating in the thematic and advanced modules (T1–T6, A1, A2). The doctoral researchers will be given an introduction into the way chemists interpret atomic properties, structures and bonding and an overview on methods in theoretical chemistry.
Basics	
Contents	1. Periodicity atomic models, orbitals, electron configuration, periodic table and associated properties of the elements: atom and ion size, ionization energy, electron affinity, electronegativity, oxidation number, groups and rows 2. The chemical bond concepts, characteristics, breaking chemical bonds, and experiments. Ionic bonds, covalent bonds, d- and f-orbitals in chemical bonding, van der Waals bonds, hydrogen bonding, hydrogen bonds in bio-systems, electronic and IR-spectroscopy to probe chemical bonding, chemistry: the change of chemical bonds 3. Coordination chemistry d electrons, ligands & ligand types, coordination number, complex composition and structure, bonding, valence bond theory, Lewis-acid/ -base theory, crystal field theory, crystal field splitting parameter Δ_o, spectrochemical series, high-spin & low-spin complexes, spin-only paramagnetism 4. Theoretical Chemistry Introduction to computational chemistry, basic concepts, intermolecular forces, basic quantum chemistry of electronic structure and diversity of methods, density functional theory, force fields, molecular dynamics simulations, applications and examples from the computer
Methods	Seminars
Type	Two-day block course/ yearly recurrence with modification
Date (month/year)	March 22-23, 2012
Time	9:00 a.m.
Work load	15 hours presence/ 45 hours self-study
Examination	Written, 4 short tests
Credit points	2
Responsible scientists	Abel, Kersting, Kirchner, Krautscheid
Industrial partners	
Recommendations for literature, e-learning	C. E. Housecroft, E. C. Constable: "Chemistry", Pearson; P. W. Atkins: "Physical Chemistry"; Jensen: "Introduction to Computational Chemistry"; Frenkel and Smith: "Understanding molecular simulations"; Allen and Tildesley: "Computer simulation of liquids"; Szabo and Ostlund: "Modern Quantum Chemistry"

SCHEDULE for Module 2012-B1

Time	Lecturer	Programme	Location
Day 1			
9:00-10:30	Krautscheid	Periodicity	
10:45-11:30		Discussion and Test	
		Lunch break	
13:00-14:30	Abel	The Chemical Bond	
14:45-15:30		Discussion and Test	
Day 2			
9:00-10:30	Kersting	Coordination Chemistry	
10:45-11:30		Discussion and Test	
		Lunch break	
13:00-14:30	Kirchner	Computational chemistry	
14:45-15:30		Discussion and Test	

Didactic elements:
Lecture, discussions, practical training – lab demonstration, etc.

Expected performance:
Active participation in discussions during lab demonstration etc.

Doctoral candidates from the Chemistry field are allowed to take part in the module but will not receive any credit point or mark for attendance.