**Course title:** Interactive Physical Chemistry – selectable / ~~regular course~~

**Number of contact hours:** 105 hours (45h lectures/15h Ex/45h seminar)

**ETCS credits**: 8

**Course description:** Students shall be introduced into the principles of microscopic and macroscopic modelling of physicochemical systems. The concepts of the underlying theories will be explained; available open software shall be used and understood. By use of social platforms and interactive matehmatics and graphics, students will interact and thus shall reinforce the understanding of the concepts needed. Final aim is to demystify the software and methods available and reduce the barrier for students to apply advanced mathematical methods.

Contents: Molecular modelling: hierarchy of computational methods, fundamentals of quantum chemistry, Hamiltonians, Born-Oppenheimer approximation, H-like atoms, molecular orbitals and Aufbau principle, Pauli's principle, LCAO method, Hartree-Fock approximation, basis sets, semiempirical approximations, density functional theory, molecular mechanics, molecular dynamics; Statistical Thermodynamics: Macrostates and microstates, probabilities and entropy, Fermi-Dirac, Bose-Einstein and Boltzmann distribution, partition functions, degeneracy, thermodynamic functions, translation, rotation and vibration, Debye's model of the solid state, metals, Fermi energy; Quantitative equilibrium relations and calculations: systematics of excess functions in mixtures, activity coefficients, regular models, calculation of excess functions, phase diagrammes and McCabe-Thiele diagrammes, models of local composition in non-regular mixtures, NRTL-model, miscibility gaps, UNIQUAC, UNIFAC, (extended) Debye-Hückel-model; Lab: (small) projects in measuring and modelling of liquid/vapour equilibria with various models, or molecular modelling with semiempirical, ab-inition or DFT methods are available and can be worked on in groups. Students are asked to perform physichochemical measurements or calculations, work out models from these data, compare them with literature data and present them in a consistent manner.(oral presentation) in front of the class.

**Education effects** (P6S_UW, P7S_WG)**:**

Learning outcome: Students can develop and understand physico-chemical models of real systems with emphasis on vapour/liquid-equilibria, molecular modelling and statistical thermodynamics. They are able to evaluate results of modelling critically, balancing assumptions, limits and effort in a rational way. They have developed the necessary skills to work with quantum chemical computational packages and relevant graphical, mathematical and statistical software.

**Literature:**

Basic literature
1. Atkins: Physical Chemistry
2. Wedler: Physikalische Chemie
3. Gmehling, Kolbe: Thermodynamics
4. Reinhold, Quantentheorie der Moleküle
5. Trevena: Statistical Mechanics

Additional literature
1. Hunter: Introduction to Modern Colloid Science
2. Lehn: Supramolecular Chemistry

**Assessment method:** written exam

**Prerequisites:** Bachelor degree in Chemical Engineering, Chemistry or closely related
Topics of Physical Chemistry from a B.Sc.-programme in chemistry, chemical engineering or similar course programmmes

**Primary target group:**

**Lecturer:** Michael Bredol - Münster University of Applied Sciences