

## UCT&IOCB Theoretical Chemistry Seminars

University of Chemistry and Technology, Department of Physical Chemistry  
Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences

Seminars will be held in IOCB club (5th floor, main building of IOCB) and in the conference room of FChE (4th floor, building A of UCT, room A402): ***Fridays, 15.00h***

### ***Program (winter term 2016/2017):***

- 23.9. (I) Thomas Bally** (University of Fribourg): *Electron hole transfer through peptides*
- 30.9. (U) Nico van der Vegt** (TU Darmstadt): *Osmolyte effects on the water solubility of macromolecules: Computer simulations*
- 7.10. (I) Phil Mason** (IOCB): *Everything you wanted to know about alkali metals but were too ashamed to ask: 46 explosions in 45 minutes!*
- 14.10. (U) Ondřej Vopička** (UCT Prague): *Sorption of gases, vapours and their mixtures in glassy and rubbery polymers: Unified modelling with GAB model of multilayer adsorption*
- 21.10. (U) Jan Heyda** (UCT Prague): *Where simulation meets experiment, Kirkwood-Buff theory*
- 4.11. (U) Matthias Heyden** (MPI Mülheim a. d. Ruhr): *Extracting solvation entropies and free energies from equilibrium intermolecular vibrations*
- 11.11. (I) Julia Ortony** (MIT): *Water Dynamics from the Surface to the Interior of a Supramolecular Nanostructure*
- 25.11. (I) Martin Lepšík** (IOCB): *Recent Advances in Quantum Mechanics-based Protein-Ligand Scoring*
- 2.12. (U) Jan Macák** (Uni. Pardubice): *Self-assembled layers of TiO<sub>2</sub> nanotubes: Preparation, properties, and application.*
- 9.12. (I) Vladimír Špirko** (IOCB, AS CR): *Are physical constants constant?*

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**U** - conference room of FChE (4th floor, building A of UCT, room A402)

Jan Heyda

Petr Slaviček

Pavel Jungwirth

Lubomír Rulíšek