New developments in theoretical simulation of x-ray absorption spectra: Possibilities and applications

Program – 8 October 2015

10:50 – 11:00	Welcome and Introduction
11:00 – 11:45	Karsten Reuter (TU München) *First-Principles NEXAFS Simulations of Organic Adsorbates at Metal Surfaces*
11:45 – 12:30	Dimitrios Manganas (MPI, Mülheim) *Topics in Catalysis from a Theoretical Spectroscopy Perspective*
12:30 – 13:45	Lunch Break
13:45 – 14:30	Caterina Cocchi (HU Berlin) *All-electron many-body approach to X-ray spectroscopy*
14:30 – 15:15	Coffee Break
15:15 – 16:00	Bernard Delley (PSI, Villigen) *Open Shell X-ray Spectroscopies Made Simple*
16:00 – 16:45	Sebastian M. Stepanow (ETH Zürich) *Spin and orbital magnetism of transition metal and rare earth atoms on surfaces*
16:45 – 17:45	Poster Session