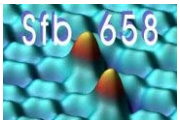
Freie Universität Berlin

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 – 13:30	Lunch Break
13:30 – 14:15	Klaus Hermann (FHI, Berlin) *Computational Core Electron Spectroscopy: Challenges and Success*
14:15 – 15:00	Frank de Groot (Utrecht University) *A personal view on the interpretation of transition metal L edges*
15:00 – 15:30	Coffee Break
15:30 – 16:15	Bernard Delley (PSI, Villigen) *Open Shell X-ray Spectroscopies Made Simple*
16:15 – 17:00	Sebastian M. Stepanow (ETH Zürich) *Spin and orbital magnetism of transition metal and rare earth atoms on surfaces*
17:00 – 17:45	Maurits W. Haverkort (MPI, Dresden) *From excitons with multiplets via edge singularities and resonances to empty density of states*
17:45 – 18:45	Poster Session