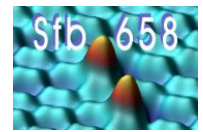


# New developments in theoretical simulation of x-ray absorption spectra: Possibilities and applications



## Program – 8 October 2015

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