



# SFB1242

Nichtgleichgewichtsdynamik kondensierter  
Materie in der Zeitdomäne

UNIVERSITÄT  
DUISBURG  
ESSEN

*Open-Minded*

**19.12.2017 / 10 Uhr c.t., Raum MG 272  
Campus Duisburg**

## **X-ray Absorption and Scattering Spectroscopy in Solids from Many-Body Perturbation Theory**

**Christian Vorwerk**

Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin,  
Germany and European Theoretical Spectroscopic Facility (ETSF)

X-ray absorption and inelastic scattering spectroscopy reveal the electronic and structural properties in crystalline materials on the atomic scale through the excitation of tightly-bound electronic core states. The determination of these spectra from first principles requires an accurate description of the electron-core hole interaction, which is typically screened by the surrounding many-electron system. In the approach [1] presented here, core excitations are determined through the solution of the Bethe-Salpeter equation (BSE), which includes the full non-local screened interaction between electron and core hole. Our implementation in the `exciting` [2] package makes use of Kohn-Sham single-particle energies and wavefunctions for both the core and conduction region, which are obtained from all-electron full-potential DFT calculations on equal footing. To demonstrate our approach, we discuss core spectra of selected bulk materials, ranging from simple oxides, like CaO [1], to complex systems, such as hybrid organic-inorganic perovskites. Our results, in good agreement with available experimental data, provide an in-depth analysis of the excitations, revealing their origin in the band structure and their real-space localization.

### **References**

- [1] C. Vorwerk, C. Cocchi, and C. Draxl, Phys. Rev. B **95**, 155121 (2017).
- [2] A. Gulans et al., J. Phys. Condens. Matter **26**, 363202 (2014).

**Für diese Zeit steht eine Kinderbetreuung nach vorheriger Anmeldung zur Verfügung.**

Contact: Prof. Dr. Björn Sothmann, Faculty of Physics  
Phone: +49 (203) 379-1578 / Mail: [bjoerns@thp.uni-due.de](mailto:bjoerns@thp.uni-due.de)