



Theory Seminar at European XFEL

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Spectroscopy of strongly correlated materials: Many-body approaches

Campus Schenefeld, main building (XHQ) room E1.172

The materials with strong electronic correlations are one of the most fascinating problems in modern solid state physics. They exhibit a variety of intriguing properties and phenomena, that are very sensitive to a change of control parameters (e.g. magnetization, temperature, pump-probe time delay, pressure). This remarkably rich physics is a consequence of competing kinetic and Coulomb energies of electrons, which makes a theoretical description of these materials and their electronic structure a challenging problem.

In the present talk I will discuss recent progress in theoretical methods that can help to interpret results of spectroscopic experiments and obtain a deeper understanding of the underlying physics. I will discuss recently developed approaches based on combination of material-specific density-functional-based model parameters and explicitly solvable many-body model Hamiltonians, capturing effects caused by electronic correlations.

Using these methods we can calculate X-ray absorption spectra (XAS) and X-ray photo-electron spectra (XPES) of LaCoO_3 and its surface effects. I will also show XAS calculations for magnetite Fe_3O_4 and X-ray emission spectroscopic calculations (XES) for metal-organic framework CPO-27-Ni.

We also apply modern computational methods, such as out-of-equilibrium dynamical mean-field theory and time-dependent density functional theory in order to treat strongly correlated materials in presence of strong electric fields.

