European XFEL Theory Seminar

Thursday, 17th May 2018, 17:00
Campus Schenefeld, main building (XHQ) room E1.172

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LDA+DMFT approach to core-level X-ray spectroscopy; application to 3d transition-metal compounds

We present an application of the local-density approximation (LDA) + dynamical mean-field theory (DMFT) to compute various core-level X-ray spectra of correlated materials. Anderson impurity model including the core states of the studied atom is constructed using the continuous LDA+DMFT hybridization function, which reflects the correlated dynamics of the valence electrons in the crystal. This allows us to obtain the fine structure of the spectra missing in the conventional cluster calculations, which capture only the metal-ligand hybridization. Technically, the calculations are enabled by a configuration-interaction-based impurity solver. We present a systematic comparison of 2p core-level X-ray photoemission spectra (XPS) of 3d transition-metal oxides MO (M=Ni, Co, Mn, Fe) and M_2O_3 (M=Ti, V, Cr, Fe) to recent high-resolution experiments [1]. We find overall a good agreement. We show how the fine structures in the XPS are related to specific microscopic processes. We also present selected examples of application to the L-edge X-ray absorption spectra and L-edge resonant inelastic X-ray scattering [2].

[1] Atsushi Hariki, Takayuki Uozumi, and Jan Kunes, Phys. Rev. B 96. 045111 (2017)
[2] Atsushi Hariki, Mathias Winder, and Jan Kuneš, arXiv:1803.03820 (2018)

Host: Evgeny Gorelov