European XFEL Theory Seminar

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

Keith Gilmore

European Synchrotron Radiation Facility

A many-body approach to X-ray spectroscopy including vibronic interactions

First-principles calculations of X-ray spectra typically adopt an independent particle approximation such as in core-hole density functional theory or multiple-scattering schemes. Such approaches can rigorously account for band-structure features and accurately reproduce spectra involving s-orbital core levels. However, this approach may fare poorly at the near-edge when the core-hole has non-zero angular momentum. To go beyond this limitation of the independent particle approximation, we include the interaction between the core-hole and the excited electron by solving the Bethe-Salpeter equation (BSE).

The first portion of this presentation introduces our BSE code OCEAN[1] (Obtaining Core Excitations using ab initio electronic structures and the NIST BSE solver) and presents a few recent calculations of X-ray absorption (XAS), emission (XES), and both resonant and non-resonant inelastic X-ray scattering (N/RIXS). Limitations of the method and ideas for going beyond a two-particle description will be discussed briefly.

The latter part of the presentation considers vibrational contributions to RIXS. With recent improvements to energy resolution, RIXS measurements can now reveal phonon loss features and the technique is increasingly used to quantify electron-phonon coupling strengths, particularly in strongly correlated materials. We consider whether RIXS truly probes electron-phonon coupling and the possibility of reproducing vibrational features in RIXS using a cumulant-derived spectral function[2].

[1] K. Gilmore et al., Comp. Phys. Comm. 197, 109 (2015).

[2] D.C. Langreth, Phys. Rev. B 1, 471 (1970).

Host: Evgeny Gorelov