



Contribution ID: 231

Type: **not specified**

Theory of X-ray spectroscopy of materials

Thursday, 21 November 2024 14:00 (30 minutes)

I will discuss X-ray absorption (XAS) and Resonant inelastic scattering of X-rays (RIXS). There is no practical unified theory for the interpretation of XAS spectra and one-particle models based on Density Functional Theory as well as multiplet model Hamiltonians are used for specific spectra [1,2]. In 2p3d resonant inelastic x-ray scattering (RIXS) one scans through the 2p X-ray absorption edge and measures the low energy excitations. The present experimental resolution of ~20 meV allows the detailed observation of the electronic and magnetic structure. Energy-resolved RIXS to determine the energy positions of the magnons and phonons [3]. Momentum-resolved RIXS can be used to determine the momentum dependence of these excitations, for example the electron-hole pair band structure of LaCoO₃ [4].

[1] Core Level Spectroscopy of Solids, Frank de Groot and Akio Kotani (2008)

[2] J. Elec. Spec. 249, 147061 (2021)

[3] Elnaggar et al. Nature Comm 14, 2749 (2023)

[4] Wang et al. Phys. Rev. B. 98, 035149 (2018)

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Session Classification: Plenary

Track Classification: AfLS