Theory and Calculations of Inelastic X-Ray Scattering

Juha Aleksi Soininen, *Department of Physical Sciences, University of Helsinki, Finland.* E-mail: aleksi.soininen@helsinki.fi

Non-resonant inelastic x-ray scattering (IXS) can be used to study the dynamics of the electronic excitations of the sample. Although in many cases the ground state of the sample is well described with the standard computational methods the excited states still pose a challenge. We will present computational results for IXS from core and valence electrons in solids. The behavior of the core excited states is dominated by the localization of the core-hole. In practice this means that the problem can be written as an effective single-particle problem for the final state electron. Since valence excited states are a combination of two delocalized states the problem cannot be reduced to an effective single-particle approach. One is forced to consider the whole complexity of the two-particle problem.

We will analyze recent experimental IXS results for core and valence excited states using band structure based approaches [1,2] and a real space multiple-scattering approach [3]. The role of the electron-hole interaction and quasiparticle effects in IXS will be reviewed. For the core-excited states an analysis of the momentum transfer dependence of the IXS cross-section respect to the final state local density of states will be presented. Calculated dispersions of valence-excitations will be compared to experimental results for selected cases.

[1] Soininen J.A., Shirley E.L., *Phys. Rev. B*, 2001, **64**, 165112. [2] Soininen J.A., Shirley E.L., *Phys. Rev. B*, 2000, **61**, 16423. [3] Soininen J.A., Ankudinova A.L., Rehr J.J., *to be submitted.*

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