

An ab initio study of the silicon L_{2,3} near edge fine structure in electron energy loss spectroscopy

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Abstract

Electron energy loss spectroscopy (EELS) probes the angular momentum resolved information about the unoccupied local density of states of the underlying media [1]. Ideally, the ground state properties of conduction band calculated by the density functional theory (DFT) provide an approximate match to the EELS experimental results. However, in some cases, such as for cations in ionic insulators, DFT miserably fails. This discrepancy is mainly due to the excitonic effect: an electron excited to the conduction band sees an unscreened core-hole – the simplified picture of the many body effect that was not captured by DFT. Within the DFT framework, this effect can be approximated by the Z+1 strategy (creating a supercell of the material and add a proton to the center cation). One drawback of Z+1 approach is that it over exaggerates the excitonic effect because the life time of the core-hole in this approach is infinitely long. I will compare the simulation of the Si L edge (p electron → conduction band) with and without the Z+1 approach in this project. Some results in [2] will be reproduced.

[1] [Peter Rez and David A. Muller, The theory and interpretation of electron energy loss near-edge fine structure, *Annu. Rev. Mater. Res.*, **38**, 535-558 \(2008\)](#)

[2] [P. E. Batson, Distortion of the core exciton by the swift electron and Plasmon wake in spatially resolved electron-energy-loss scattering, *PRB*, **47**, 6898 \(1993\)](#)