

Unraveling the mysteries of complex systems with x-ray spectroscopy: theory and computation vs experiment

There has been dramatic progress in recent years both in ab initio calculations and in the interpretation of various x-ray and electron spectroscopies, especially x-ray absorption spectra (XAS) [1] and electron energy loss spectra (EELS). These developments have led to computer codes such as FEFF8, which are in semi-quantitative agreement with experiment and permit an interpretation in terms of structural and electronic properties of a material. Moreover, these developments have revolutionized experimental investigations of complex materials with the technique of extended x-ray absorption fine structure (EXAFS). We first summarize these advances, focusing on the theory underlying the real-space multiple-scattering approach used in FEFF8. This theory differs significantly from ground state electronic structure or quantum chemistry calculations based on density functional theory, and also includes many-body corrections to the independent particle approximation. In particular the theory treats excited states as quasi-particles and includes inelastic losses and the screened core-hole interaction. These developments are illustrated with a number of applications ranging from catalysts and minerals to bio-structures,

[1] J. J. Rehr and R. C. Albers, *Rev. Mod. Phys.* 72, 621 (2000).

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