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Progress and challenges in the theory and interpretation of x-ray spectra

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There has been dramatic progress in recent years both in calculations and the interpretation of various x-ray spectra, ranging from extended x-ray absorption fine structure (EXAFS) and diffraction-anomalous fine structure (DAFS) to near-edge structure (XANES) and inelastic x-ray scattering (IXS). Using synchrotron radiation x- ray sources, these spectroscopies have become powerful probes of complex materials ranging from catalysts and minerals to bio-structures and aqueous systems. Together with advances in analysis techniques, these methods permit an interpretation of spectra in terms of structural, electronic, magnetic and vibrational properties. We summarize these advances first with a heuristic description of the real-space approach used in the electronic structure and spectroscopy codes developed by our group [1]. Our approach is based on real-space multiple-scattering Green's function techniques, rather than wave-functions. This simplifies calculations of excited states and x-ray spectra, particularly the inclusion of key many-body effects and relativistic corrections. The approach is illustrated with applications to various x-ray spectra of complex materials. For example, DAFS takes advantage of the fine structure in the intensity of Bragg diffraction peaks near an absorption edge, and provides unique information that combines EXAFS and XRD experiment. We also discuss some recent theoretical developments leading to a new generation of codes including FEFF9 [2] and extensions for treating strongly correlated systems.

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