Laboratoire des Solides Irradiés, UMR 7642

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Salle LMS (05-1026)

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13H30

Probing excited states of materials with theory and x-ray spectroscopy

There has been dramatic progress in recent years both in the theory and interpretation of various x-ray and electron spectroscopies, including x-ray absorption spectra (XAS), inelastic x-ray scattering (IXS), and electron energy loss spectra (EELS). Using synchrotron radiation x-ray sources and modern electron microscope techniques, 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 methods, these theoretical tools now permit an interpretation of spectra in terms of structural, electronic, magnetic and vibrational properties. We first summarize these advances, with a heuristic description of the real-space approach used in the electronic structure and spectroscopy codes such as the FEFF code of our group [1]. This theoretical approach is based on real-space Green's function techniques, rather than wave-functions, but this simplifies calculations of both excited states and x-ray spectra. The method also builds in key many-body effects including extrinsic and intrinsic losses, Debye-Waller factors to account for vibrations and disorder, and relativistic corrections including spin-orbit interactions. Dynamic structural effects can also be included, using DFT/MD methods. The approach is illustrated with applications to complex materials throughout the periodic table.

[1] J. J. Rehr and R. C. Albers, Rev. Mod. Phys.**72**, 621(2000).
[2] J. J. Rehr, J. J. Kas, M. P. Prange, A. P. Sorini, Y. Takimoto, F. Vila, Comptes Rendus Physique, **10**, 548 (2009).
[3] F. Vila, J. J. Rehr, R.G. Nuzzo and A. F. Frenkel, Phys. Rev. B**78**, 121404_R (2008).