

PHYSICS AND ASTRONOMY COLLOQUIUM

October 22, 2013

4:10 p.m.

Webster 17

Dr. John J. Rehr

Department of Physics, University of Washington

“Probing Excited States of Materials with X-ray and Electron Spectra”

There has been dramatic progress in recent years both in calculations and the 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 methods 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 developed by our group [1]. This approach is based on real-space Green's function techniques, rather than wave-functions, but this simplifies calculations of excited states and x-ray spectra. The method also builds in key many-body effects and relativistic corrections. 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).

Please meet our guest speaker and share in refreshments, 3:45-4:10pm in the foyer on floor G above the lecture hall.

Host: Dr. Susan Dexheimer