



Colloquium

1st June 2011 - 15:00
FLASH HALL, Seminar Room (28c)

John J. Rehr

Department of Physics, University of Washington, Seattle

Calculations of X-ray Spectra in Real-space and Real-time^{*}

Real-time approaches are becoming increasingly important in understanding photon spectroscopies ranging from linear and non-linear optical response to x-ray absorption spectra (XAS). In this talk I will discuss several methods based on a real-time approaches.

First we discuss a real-time approach for calculating the dynamic structure of nano-scale materials base on finite-temperature density functional theory / molecular dynamics and the real-space Green's function approach in the FEFF9 code [1]. This approach exploits recent advances that permit parameter-free calculations of the key many-body effects in the theory. The method is illustrated for the case of Pt nanoclusters supported on gamma-alumina [2], and explain many of the unusual properties observed for such catalytic materials.

Second, I discuss our real-time, time-dependent density functional theory (RT-TDDFT) approach for calculations of frequency-dependent linear and non-linear optical response. This approach is based on calculations of the time-dependent Hamiltonian using SIESTA and an explicit Crank-Nicholson time-evolution of the wave-functions [3].

Finally, I discuss a generalization of this real-time approach for core-level x-ray response based on time-correlation functions and prospects for generalizations to case of high-field strengths.

^{*}Supported by DOE Grant DE-FG03-97ER45623 and NSF Grant PHY-0835543.

[1] John J. Rehr et al., *Comptes Rendus Physique*, 10, 548 (2009).

[2] F. Vila et al., *Phys. Rev. B* 78, 121404(R), (2008).

[3] Y. Takimoto et al., J. Rehr, *J. Chem. Phys.* 127, 154114 (2007).

