PHYSICAL/INORGANIC SEMINAR

Title: "Spectroscopy 'in Silico'"

JOINT SEMINAR W/ MATERIALS SCIENCE PROGRAM

Guest Speakers:

Professor Jochen Autschbach

SUNY Buffalo

Department of Chemistry

Monday, February 24, 4:00 PM

473 Hutchison Hall

Department of Chemistry

Abstract:

Computational chemistry has made tremendous progress since its inception. The energy of a molecule is a central quantity in computational studies, but certainly not the only important one. For example, the fundamental parameters defining virtually all spectroscopic and optical properties can be computed from first principles as derivatives of the energy, or the quasi-energy, taken with respect to electric and magnetic field amplitudes, electronic and nuclear magnetic moments, nuclear positions, etc. Frequency-dependent methods give access to excitation spectra and excited states properties. We will discuss selected applications from our group's research projects to organic molecules, transition metal complexes, and f-element complexes. Emphasis will be placed on molecular properties that are related to magnetic-field interactions, such as magnetic resonance parameters (NMR, EPR), and electronic and Raman optical activity. If time permits, we will briefly discuss certain shortcomings of Kohn-Sham density functional theory affecting various types of 'band gaps', and how to diagnose them and improve the calculations.

Host: Professor Michael Neidig, email: michael.neidig@rochester.edu