Condensed Matter / Biophysics Seminar

Thursday

February 19

4:00 P.M.

Rm 184 NSH

Non-equilibrium Realtime TDDFT Simulations, and Stationary State Orbital Free Functional Development

Prof. John Parkhill, University of Notre Dame

I'll give a two-part talk discussing the application and development of two theoretical techniques related to density functional theory (DFT). In the first part of my talk I'll describe my group's efforts to understand electronic relaxation with TDDFT. The application for this theory is modeling the femtosecond to picosecond transient electronic dynamics of molecules and materials, especially photovoltaic materials (organics and perovskites). We have developed a code which allows us to simulate the non-radiative relaxation of an excited chromophore in real time, and visualize the electron density while it relaxes. We've also made theoretical improvements which allow the model to properly relax to a Fermi-Dirac distribution at long times, and even correct ground state DFT simulations which I will explain.

In the second part of my talk I'll discuss our work towards an accurate kinetic energy density functional (KEF). With a good approximation to the KEF, simulations of materials an order of magnitude larger than the largest DFT simulations being performed today would be routinely possible. However ever since Thomas and Fermi, development of KEF's has been a long and difficult process. I will discuss our radically different (although totally empirical) strategy for constructing a KEF and initial results. The crux of our approach is to exploit recent advances in computer vision technology to provide a model of the functional with more flexibility than is possible with traditional forms.