

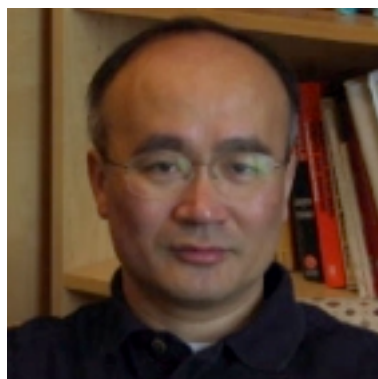
Physical Chemistry Seminar

Tuesday,
March 6, 2012

11:00 a.m.

Room 1315
Chemistry Building

The Wonder of Electron Density: From Fractional Charges, Fractional Spins to Non-covalent Interactions of Macromolecules



Professor Weitao Yang
Department of Chemistry
Duke University

Host: Professor JR Schmidt

Interactions between electrons determine the structure and properties of matter from molecules to solids. To describe interacting electrons, the extremely simple three-dimensional electron density can be used as the basic variable within density functional theory, negating the need in many cases for the massively complex many-dimensional wave function. This lecture will review the concept of electron density and many of its remarkable features, including latest developments. Electron density determines the energetics of chemical and physical changes, such as in electron transport, solar energy harvesting and conversion, drug design in medicine, catalytic processes in enzymes, and many other challenges in science and technology. Electron density can be used to visualize not only covalent chemical bonds, but also non-covalent interactions such as hydrogen bonds, van der Waals attraction and steric repulsion. Electron density also naturally leads to the concepts of fractional charges and fractional spins, which are key to the understanding and analysis of approximations in density functional theory.

Refreshments will be available prior to the seminar at 10:45 a.m. outside room 1315

Graduate Students may meet with the speaker at 1:00 p.m. in Room 8335