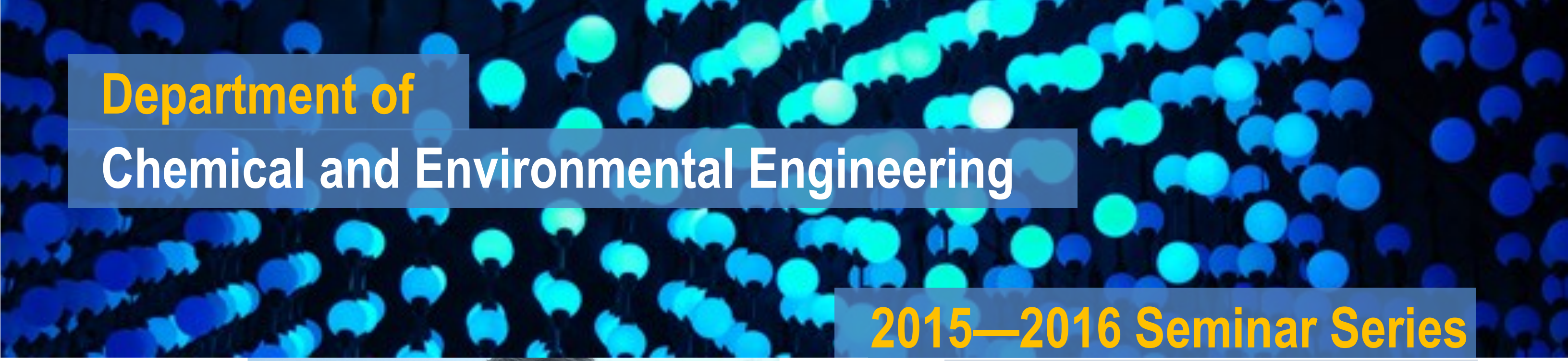


Department of
Chemical and Environmental Engineering

2015—2016 Seminar Series

Friday, October 23, 2015
9:30-10:30am
WCH 205/206

Mark Pederson

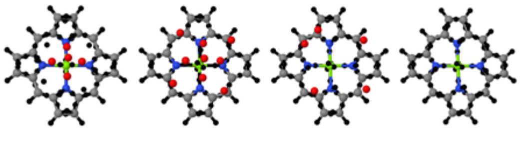
Professor

Department of Chemistry

Johns Hopkins University

Self-Interacton Corrected Density-Functional Theory with Unitary Invariance: Applications to Inorganic Molecular Magnets

Molecular magnets generally consist of a collection of transition-metal ions that have five to six nearest-neighbors. Due to this high-coordination, the d-level filling associated with the transition metal centers is often unambiguously determined by the ligands surrounding the metal center. As such, gradient corrected density-functionals, such as PW91 and PBE GGA, have proved to be very successful for describing such molecules. However, improvements in these functionals are necessary if one is interested in obtaining quantitatively accurate spin excitations in molecules containing low-coordination 3d transition metal ions or, for other reason, one is interested in understanding electronic transport across such molecules. In this talk, I review some of the general improvements that have been offered by the Perdew-Zunger self-interaction correction (SIC) and past approaches to solving these equations. A new version of the self-interaction correction to density functional theory, based upon Fermi Orbitals, is briefly introduced which seems to be simpler to use and which provides two formal improvements over the original version. Further, the formalism identifies quasi-classical electron positions that seem to be in accord with conventional classical models for electrons in molecules. Applications of this self-interaction-corrected theory, within the local spin-density approximation, give improvements to atomization energies of molecules, total energies and ionization energies in atoms, and the uniform electron gas is obtained. By example, it is shown that the method is fast enough to apply to systems with open metal centers.



BioSketch: Mark Pederson received his PhD in Theoretical Physics at the University of Wisconsin Madison where he performed very early work on an improvement of the density-functional-formalism through the inclusion of self-interaction corrections. After leaving Madison he spent 22 years at the Naval Research Laboratory in Washington DC where he developed and applied massively parallel computational methods for the density-functional-based simulations on molecules, clusters and nanoscale materials. His computational and mathematical algorithms and computer code (NRLMOL) have been used to test the first widely used gradient-corrected density functional to calculate infrared and Raman spectra, and to calculate spin-dependent phenomena in molecular magnets and molecular-scale circuits composed of such systems. Pederson has published over 220 papers on applications of NRLMOL to a diverse assortment of chemical and physical systems. Pederson moved to the Department of Energy in 2008 to start a program in Computational and Theoretical Chemistry and continues to do research as Research Professor in the Department of Chemistry at Johns Hopkins University. Most recently he has returned to the problem of developing a formulation of density-functional theory that is explicitly free of the self-interaction errors. He is a Fellow of the American Physical Society and has taken sabbaticals at the National Science Foundation as a program officer, and at the Max-Planck Institute as a visiting researcher.

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