Colloquium

Department of Physics, Temple University

DEVELOPING AND APPLYING DFT TO STUDY/DESIGN MOLECULES AND MATERIALS FOR CLEAN ENERGY AND PHARMACEUTICALS

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Abstract

In modern society, solutions of many problems facing humanity (e.g., health, sustainability, etc.) require understanding, control, and design of molecules and materials at the electron level, which must be treated quantum mechanically. Due to its efficiency and reasonable accuracy, density functional theory (DFT) is one of the most widely used electronic structure methods in condensed matter physics, chemistry, and biology. I present here an advance in DFT, the recently developed non-empirical strongly constrained and appropriately normed (SCAN) meta-generalized gradient approximation (meta-GGA). It predicts accurate geometries and energies of diversely-bonded molecules and materials (including covalent, metallic, ionic, hydrogen, and van der Waals bonds), significantly improving over its predecessors, the GGAs that dominate materials computation, at comparable efficiency. Often SCAN matches or improves upon the accuracy of a computationally expensive hybrid functional, at almost-GGA cost. SCAN captures the intermediate-range van der Waals (vdW) interaction, which is largely missed by the conventional GGAs and hybrid functionals. The addition of the long-range vdW correction to SCAN results in a versatile vdW functional that is accurate and outperforms its competitors for a variety of vdW-dominated systems, including layered materials and organic molecules adsorbed on metal surfaces. These improvements in predictive power can have broad impact in many different fields, especially in the materials genome initiative for clean energy and in the design of pharmaceuticals. Possible applications will be discussed.

Monday, February 8, 2016 at 3:00pm
SERC, Room 116
Refreshments served at 2:45pm