Physics Colloquium

Chinedu Ekuma

"Computational Capabilities and Concepts for 21st Century Materials and Applications"

There is a long history of theoretical research into electron localization. The majority of this work focuses on either disorder-induced localization or localization due to electron interactions. These limiting cases were predicted by P. Anderson and N. F. Mott and are nowadays known as Anderson and Mott localization, respectively. We also know that both disorder and electron interactions coexists in physical systems and can be substantial in real materials. Alongside experiment and theory, computation has become an essential part of the development of an understanding of many properties of pristine systems. Despite the need, first-principles approach that "properly" characterizes electron localization have been elusive because both disorder and electron interactions break two of the fundamental assumptions in band theory, material homogeneity, and independent particles. In this talk, I will present a new computational approach overcoming these roadblocks by combining first-principles density functional theory, the Anderson-Hubbard model, and the typical medium dynamical cluster approximation within the dynamical mean-field theory. The computer simulations enabled by this method are expected to reveal new critical insight, e.g., simulations of monolayer hexagonal boron nitride predict that both disorder and electron interactions are essential for the material to undergo an insulator-to-metal transition.

Chinedu Ekuma *recently completed a two-year National Research Council Research Associateship in the Theoretical Chemistry Division at The U.S. Naval Research Laboratory, Washington, D.C. He obtained his Ph.D. in Computational Condensed Matter and Materials Physics from the Louisiana State University. Dr. Ekuma's research focuses on using density functional theory and various many-body approaches to design and study materials with the goal (1) to discover new materials with significantly useful technological applications; (2) to understand and control the interplay between the coexisting emerging functionalities; and (3) to explore how atomic defects affect these emerging properties. Of particular interest are promising materials for spintronic, energy-efficient, energy-conversion (photovoltaic, thermoelectric), and energy-storage applications and in advancing our knowledge on the decades-old problem of electron localization, where he pioneered the development of a first-principles-based approach that he currently applies to explore the role of atomic defects in materials.*

Physics Faculty and Search Committee Candidate

Thursday January 25th in LL 316 at 4:10
Refreshments available at 3:45