Department of Physics and Astronomy Colloquium

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Date: October 25, 2017
Time: 3:30 p.m.
Place: Rm. 103, Thirkield Hall, Howard University
Host: Dr. Pratibha Dev

Title: Computational Capabilities and Concepts for 21st Century Materials and Applications

Abstract: There is a dire need to design and discover energy-efficient materials to meet the challenges of modern technology. Alongside experiment and theory, computer simulations have provided insights into the properties of materials. Computational materials design aims to understand the fundamental origin of complex materials' behavior and use this information to make predictions to accelerate experimental processes. Low-dimensional materials are increasingly being explored for diverse applications such as high-electron-mobility transistors, photovoltaics, energy storage, etc. Because their properties emerge from a complex interplay among the electronic degrees of freedom often on different length/energy scales that can be tuned to improve device performance. In this talk, I will present recent works investigating the fundamental properties of materials, especially, low-dimensional nanostructures, which often contain intrinsic defects. These imperfections present both opportunities and challenges and to take advantage, we need a better understanding of their role, which is crucial in low-dimensional materials. I will discuss the complementary nature of the various atomistic simulation, e.g., first-principles density functional theory and multiscale, many-body methods with a focus on a first-principles, many-body approach that I pioneered to understand better, disordered nanostructures and materials in general.