USC Dornsife College of Letters, Arts and Sciences
Department of Physics and Astronomy

Ming Hsieh Institute - Physics

Joint Seminar Series

USC Viterbi School of Engineering
Ming Hsieh Department of Electrical and Computer Engineering

Recent Advances in Pushing Back the System-Size and Accuracy Limitations in Density Functional Theory

Vikram Gavini

Department of Mechanical Engineering,
Department of Materials Science and Engineering
University of Michigan, Ann Arbor

MONDAY, November 18
12:00pm-1:00pm
DMC 202
(previously the CPA building)

Abstract

Electronic structure calculations are widely used in understanding various materials properties. This talk will discuss recent progress in addressing the long-standing size and accuracy limitations in density functional theory (DFT), the workhorse of electronic structure calculations over the past few decades. In particular, the development of computational methods and numerical algorithms for conducting fast and accurate large-scale DFT calculations using adaptive finite-element discretization will be presented, which form the basis for the recently released DFT-FE open-source code. The computational efficiency, scalability and performance of DFT-FE will be presented, which demonstrates a significant outperformance of widely used plane-wave DFT codes. Some recent application studies that highlight the capabilities of DFT-FE will be presented. In improving the accuracy of DFT calculations towards quantum accuracy, recent progress in accurately solving the inverse DFT problem will be presented, which has enabled the computation of exact exchange-correlation potentials for polyatomic systems. Ongoing efforts on using the exact exchange-correlation potentials to develop a data-driven approach for improving the exchange-correlation functional description in DFT will be discussed.

Biography

Vikram Gavini is Professor of Mechanical Engineering and Materials Science & Engineering at the University of Michigan. He received his Ph.D. from California Institute of Technology in 2007. His interests are in developing methods for large-scale and quantum-accurate electronic structure calculations, numerical analysis of partial differential equations, and scientific computing. DFT-FE, a massively parallel open-source code for large-scale real-space density functional theory calculations, has been developed in his group. He is the recipient of NSF CAREER Award in 2011, AFOSR Young Investigator Award in 2013, Humboldt Research Fellowship for Experienced Researchers (2012-14), USACM Gallagher Award in 2015, and 2023 ACM Gordon Bell Prize (aka Nobel Prize of supercomputing).

Hosted by:
Aiichiro Nakano