# ME Seminar

## Ab initio studies of dislocations using large-scale electronic structure calculations

**Vikram Gavini, Mechanical Engineering, University of Michigan**

### ABSTRACT

Defects play a crucial role in influencing the macroscopic properties of solids—examples include the role of dislocations in plastic deformation, dopants in semiconductor properties, and domain walls in ferroelectric properties. These defects are present in very small concentrations (few parts per million), yet, produce a significant macroscopic effect on the materials behavior through the long-ranged elastic and electrostatic fields they generate. Notably, the strength and nature of these fields, as well as other critical aspects of the defect-core are all determined by the electronic structure of the material at the quantum-mechanical length-scale. However, carefully converged electronic structure studies on extended defects, such as dislocations, have been out of reach due to the cell-size and periodicity limitations of the widely used electronic structure codes.

This talk will discuss the recent developments that have enabled large-scale density functional theory (DFT) calculations, paving the way for electronic structure studies of defects. The first part of the talk will introduce orbital-free density functional theory (OFDFT), an electronic structure theory for materials systems whose electronic structure is close to a free electron gas such as Aluminum and Magnesium. The real-space reformulation of OFDFT, its accuracy for Al-Mg materials systems will be discussed. Using OFDFT, energetics of isolated dislocations in Al will be presented, which have provided new insights into the core size and core energies of these defects. Interestingly, the core energy is found to be dependent on the external macroscopic strain, which in turn results in an additional force on the dislocation beyond the Peach Koehler force. The implications of this additional force on interacting dislocations will be discussed. In the second part of the talk, the development of methods and algorithms for large-scale Kohn-Sham density functional theory (KSDFT) calculations will be presented, which is the most widely used electronic structure theory for ab initio studies. These efforts have led to the development of DFT-FE, a massively parallel GPU ported open-source real-space DFT code, which provides new capabilities for conducting fast and accurate large-scale DFT calculations on many thousands of atoms. The accuracy and performance of DFT will be presented and compared with widely used plane-wave based DFT codes. Finally, the energetics of $< c + a >$ dislocations in Mg using KSDFT will be presented showcasing the utility of DFT-FE for studying extended defects in materials.

This is joint work with Sambit Das, Balakrishnan Radhakrishnan, Mrinal Iyer and Phani Motamarri.

### ABOUT THE SPEAKER

Vikram Gavini is a Professor of Mechanical Engineering and Materials Science Engineering at the University of Michigan. He received his PhD from California Institute of Technology in 2007, and BTech from IIT Madras in 2003. His interests are in developing methods for first-principles based materials calculations, defect mechanics, numerical analysis of PDEs and scientific computing. DFT-FE, a massively parallel open-source code for large-scale density functional theory calculations, originated from his group. He is the recipient of the NSF CAREER Award in 2011, AFOSR Young Investigator Award in 2013, Alexander von Humboldt Foundation's Humboldt Research Fellowship for Experienced Researchers (2012-14), and the USACM Gallagher Award in 2015. His team was nominated as a finalist for the 2019 ACM Gordon Bell prize (supercomputing).

**June 10, 2022, 4:00 pm, A R Auditorium, ME@IISc**