

Semi-Plenary Lecture



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Title: Electronic Structure of Defects and Macroscopic Properties of Materials

Defects are responsible for a number of important and interesting properties of materials even when they occur at dilute concentrations. Defects interact over long distances through slowly decaying elastic, electric and other fields whose strength is determined by the electronic structure of the core. Thus the study of defects requires electronic resolutions with continuum range. This talk will describe ongoing work on a method -- Quasicontinuum Density Functional Theory -- to enable density functional theory calculations of defects in crystals. The main idea of the current method is a numerical discretization that adapts the resolution to the structure of the solution with no a priori ansatz or ad hoc patches. This is based on joint work with Michael Ortiz, Vikram Gavini, Thomas Blesgen and Phanish Suryanarayana.

Brief Biography:

Dr. Kaushik Bhattacharya is a Professor of Mechanics and Materials Science at the California Institute of Technology. His research concerns the mechanical behavior of solids, using theory to guide the development of new materials including active materials. He received his B.Tech from IIT Madras, India in 1986 and his Ph.D from U Minnesota in 1991. He joined Caltech in 1993 after a post-doctoral stay at the Courant Institute. He has held visiting positions at Cornell University, Heriot-Watt University, Max-Planck-Institute Leipzig, Cambridge University, Indian Institute of Science and the Jet Propulsion Laboratory. He received the SES Young Investigator Award in 2004 and the ASME Special Achievements Award in Applied Mechanics in 2004. He is currently an Editor of the Journal of the Mechanics and Physics of Solids.