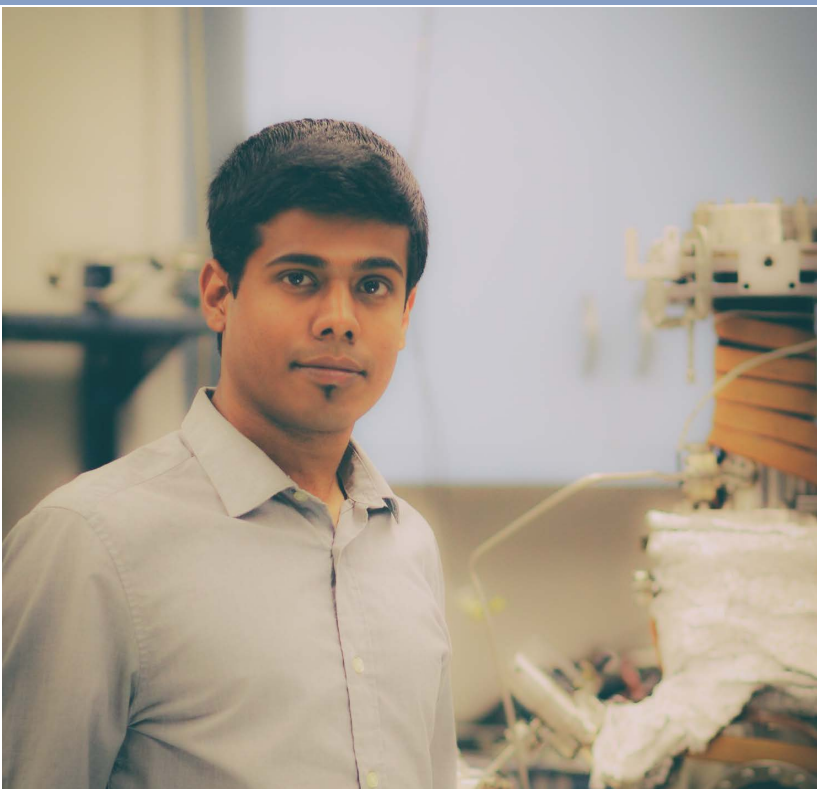


Computationally Guided Materials Discovery

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Dr. Prashun Gorai is currently a postdoctoral fellow in the Department of Metallurgical and Materials Engineering at the Colorado School of Mines and is also affiliated with the National Renewable Energy Laboratory. Dr. Gorai received his doctoral degree in Chemical Engineering from the University of Illinois at Urbana-Champaign in 2014 and his bachelor's degree from the Indian Institute of Technology Madras in 2008. His current research interests mainly focus on computationally guided discovery and design of materials, specifically for thermoelectric, photovoltaics, electronic, and piezoelectric applications. During his PhD, he studied oxygen diffusion in oxides through a combination of experiments (isotope diffusion in ultra high-vacuum) and first-principles calculation of defect energetics and kinetics.

The discovery and development of technologically useful materials has historically been a time-consuming and resource-intensive process. The role of computations in materials design has been traditionally limited to *ex post facto* explanation of the experimental observations. In recent years, a new paradigm for accelerated materials discovery has emerged: First-principles based computations are used to calculate the target properties of a large number of materials for a technological application and promising candidates are identified, which are then experimentally tested. This burgeoning new approach has been successfully implemented for the discovery of thermoelectric, photovoltaic, energy and gas storage, photocatalytic, and microelectronic materials.

In this talk, I will discuss how I use first-principles density functional theory calculations to guide the discovery of new functional materials and to identify new structure-property relations. These efforts have led to the identification of new thermoelectric materials: A_1B_1 compounds, quasi-2D layered structures, and *n*-type Zintl. As a by-product, new structure-property relations have also emerged that highlight the role of low valent cations in promoting thermoelectric performance and the degradation of thermoelectric performance from spin disorder. Besides thermoelectrics, I will also briefly discuss my computational work on identification of new high-efficiency, perovskite-inspired photovoltaic absorbers and quasi low-dimensional piezoelectric materials. Finally, I will introduce the open-access thermoelectrics materials database (www.tedesignlab.org) that I have created along with my team to share our computational results on discovery of thermoelectric materials.



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