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Distinguished Seminar Speaker

A Journey from Atoms to Materials: Designing Functional Materials for Energy and Microelectronics

Prashun Gorai

**Research Assistant Professor | Metallurgical and Materials Engineering |
Colorado School of Mines | Golden, CO**



Abstract: Technological developments often rely on specifically designed materials and molecules. The increasing pace of technology development, coupled with rising energy needs and climate challenges, requires faster approaches for materials discovery. Historically, materials have been discovered by trial-and-error approaches that rely on chemical intuition. Designing materials with tailored properties is challenging because of the astronomical number of possible compounds and structures, and materials behaviors that do not adhere to standard chemical intuition. Computations have made great strides in accelerating materials development, but many challenges remain. We are addressing some of these challenges, including inverse materials design and bridging the gap between theoretical predictions and real materials. In this talk, I will share examples from our work on the computational discovery and design of functional materials, as well as modeling of defect and doping properties of semiconductors.

Biography: Dr. Prashun Gorai is a research assistant professor at the Colorado School of Mines (CSM) with a joint appointment at the National Renewable Energy Laboratory (NREL). He obtained his bachelor's degree in Chemical Engineering from IIT Madras (India), and his PhD, also in Chemical Engineering, from the University of Illinois at Urbana-Champaign. He was a postdoctoral fellow at CSM and NREL between 2014-2017. His research team uses quantum-chemical calculations, high-throughput computing, and machine learning to discover and design functional materials for energy conversion and storage, and next-generation microelectronics. The International Thermoelectric Society awarded him the Young Investigator Award in 2022 and the Royal Society of Chemistry (Materials Horizons) recognized him as an Emerging Investigator in 2020. He is a recipient of the Chemistry of Materials Lectureship and Best Paper Award 2023.