

Thursday, August 29, 2024

Refreshments at 3:15pm outside PSF 101
Colloquium from 3:30pm - 4:30pm in PSF 101

Data-Driven Discovery and Design of Materials' Surfaces and Interfaces

Professor Arunima Singh
Arizona State University



Abstract:

Materials and their surfaces and interfaces are at the heart of modern-day technology, playing a central role in a variety of fields such as biosensing, energy conversion, quantum computing, and nanoelectronics. Recent advancements in ab initio methods, materials informatics, and data science have dramatically expanded our ability to understand existing materials and discover new ones with greater ease, scope, and speed. In this talk, I will show how we have used a combination of ab initio simulations, high-throughput computations, and machine learning to discover and design materials, focusing specifically on ultra-wide band gap materials and photocatalytic materials.

Biography:

Arunima K. Singh is an Assistant Professor in the Department of Physics at Arizona State University (ASU) and a graduate faculty member in the Materials Science and Engineering Department at ASU. She earned her Ph.D. from Cornell University in 2014. Before joining the ASU faculty, she held postdoctoral positions at Lawrence Berkeley National Laboratory and the National Institute of Standards and Technology. Prof. Singh is a recipient of the Department of Energy (DOE) Early Career Research Program Award and serves as a Thrust co-Lead at ULTRA, a DOE Energy Frontier Research Center. Her research centers on accelerating materials discovery, synthesis, and application through first-principles computations and data science, with a particular focus on physical phenomena at material surfaces and interfaces.