CIRC Symposium Series 2025-2026

Designing Quantum Materials for Next-Generation Technologies

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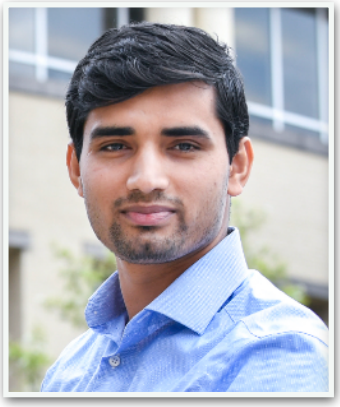

The rapid discovery and design of new materials is transforming the way we think about energy, nanoelectronics, and quantum technologies. At the heart of this transformation lies our ability to understand how the behavior of electrons can give rise to extraordinary properties such as superconductivity, exotic magnetism, ferroelectricity, and even entirely new topological states of matter. In this talk, I will highlight how my research group uses advanced computational methods, simple theoretical models, and close collaborations with experiments to uncover and control these quantum phenomena. I will share examples ranging from two-dimensional van der Waals materials that can be stacked like Lego blocks to design new functionalities, to electrides where electrons themselves act as building blocks of the crystal. These discoveries not only deepen our understanding of fundamental science but also open pathways toward applications in faster computing, more efficient energy devices, and next-generation quantum technologies.

A Structural Similarity Based Data-Mining Algorithm for Modeling Multi-Reactant Heterogeneous Catalysts

Jin Zeng | Department of Chemical Engineering

DFT simulations are powerful tools for studying heterogeneous catalyst systems. However, their high computational cost and large configuration space hinder their application in understanding multi-reactant catalysis on geometrically diverse surfaces. Our work introduces an innovative similarity algorithm that quantifies the structural differences between atomic configurations to address this challenge. The quantification effectively identifies structurally dissimilar configurations with minimal human intervention. Consequently, data mining the configurational phase-space through the similarity algorithm drastically reduces the number of DFT simulations required to identify the stable atomic models of interest.

Friday, October 17, 2025
11:30 am - 1 pm
Wegmans Hall 1400

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