IIT KANPUR
PHYSICS COLLOQUIUM

UNDERSTANDING-DRIVEN DISCOVERY OF QUANTUM MATTER: A BOTTOM-UP DESIGN APPROACH

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ABSTRACT

Successful discovery of topological materials based on first-principles predictive theories has exemplified an unprecedented theory/design paradigm, which enables a systematic, understanding-driven realization of quantum matter, surpassing traditional reliance on fortuitous experimental discoveries. Such predictive theories largely rely on experimentally available materials, and so far, an inverse design of topological materials and associated responses has been explored only to a limited extent. In this talk, I will discuss our recent theoretical efforts in designing materials and engineering quantum states using an understanding-driven materials design approach. Specifically, I will demonstrate how passivating the high-energy surfaces of nonlayered nitrides or phosphides generates synthetic layered materials with tunable topological states and enhanced spin Berry curvature effects. I will also discuss topology, symmetry, and property relations, highlighting how these insights can facilitate the use of topological materials for quantum device applications.

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