Physics Colloquium

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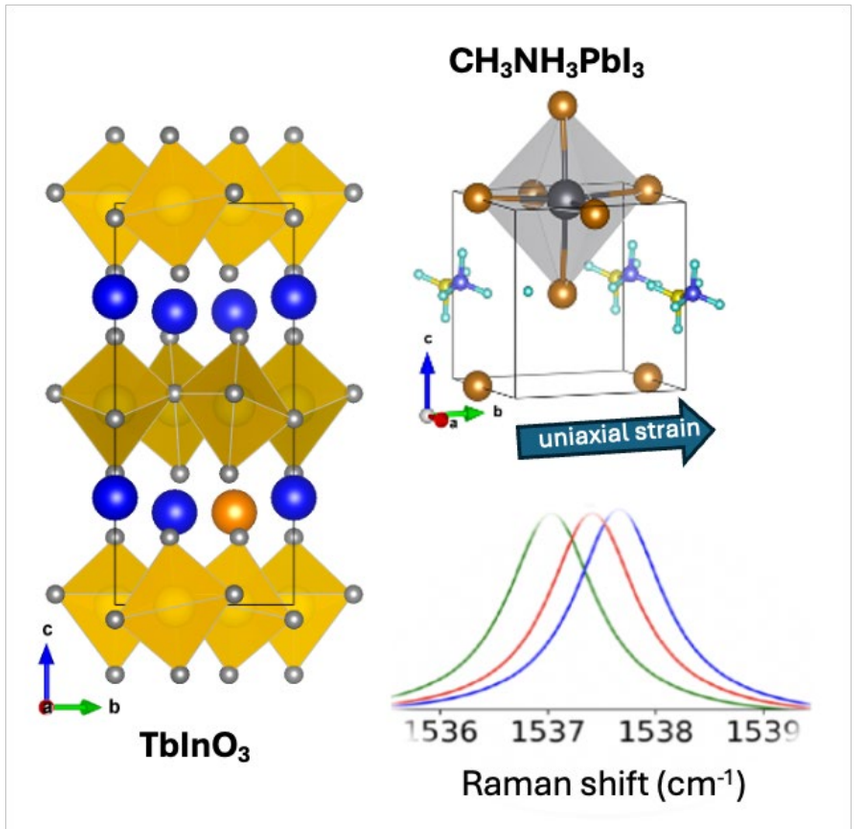
Engineering Function Through Imperfection: A First-Principles Perspective

ABSTRACT

Materials in their pure form are often far less useful than we might expect. Silicon only becomes a useful semiconductor when doped, pure gold is too soft for jewelry, and iron becomes strong and practical only when carbon transforms it into steel. These familiar examples point to a central idea in materials science: useful properties emerge when a crystal lattice is disturbed. In this talk, I will show how such disturbances, such as defects, dopants, or mechanical stress, slightly rearrange atoms inside a solid and lead to observable changes in material behavior using density functional theory (DFT) as a quantitative probe. I first focus on chemical doping in the oxide material $TbInO_3$. By studying calcium and titanium substitution, I show how DFT reveals defect formation energies, local structural relaxations, and how these factors govern the possibility of activating transport pathways in a nominally insulating system. I then turn to lattice vibrations as a sensitive probe of structural change. Using the perovskite solar-cell material $MAPbI_3$, I will demonstrate how IR and Raman spectroscopy capture subtle signatures of strain in vibrational spectra, providing a powerful and completely non-destructive way to detect local stress in materials. Finally, I briefly outline our ongoing efforts to scale these ideas using AI-assisted autonomous DFT workflows, which combine literature reasoning, automated simulation setup, and data analysis to accelerate materials exploration. Together, these efforts illustrate how stress, defects, and lattice vibrations form a coherent framework for understanding and engineering materials through first-principles computation.



3:00 - 4:00 p.m., Friday, January 23rd, 2026

In-person in McLane Hall 162