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MATERIALS AND BIOMATERIALS SCIENCE AND ENGINEERING

Listening to the Lattice: DFT Insights into Stress, Raman Signatures, and Defect Physics

ABSTRACT

Materials in their pure form are often far less functional than we imagine. For example, silicon becomes a useful semiconductor when doped with phosphorus or arsenic, pure gold is too soft for making ornaments unless alloyed with copper, and elemental iron becomes truly useful only when carbon transforms it into steel. These familiar examples highlight an important theme: materials reveal their functional behavior only when we perturb their lattices. External mechanical stress and internal modifications such as defects or dopants both distort local bonding, alter vibrations, and reshape electronic structure. In this talk, I present a unified perspective on how such perturbations influence materials at the atomic scale, using density functional theory (DFT) as a quantitative probe. First, I will present DFT-based phonon calculations that compute the IR and Raman spectra of a well-known perovskite solar-cell material ($MAPbI_3$) and show how Raman spectroscopy serves as a highly sensitive, non-destructive probe of local strain, revealing stress states and anisotropic lattice responses. As a second example, I will discuss defect formation energies and doping mechanisms, particularly Ca and Ti substitution in $TbInO_3$, in search of enhanced conductivity. Here, DFT provides insight into defect thermodynamics, local structural relaxations, and how these factors govern the possibility of activating transport pathways in a nominally insulating system. Finally, I will outline our ongoing efforts to scale these insights through AI-assisted autonomous DFT workflows that integrate literature reasoning, workflow generation, and automated analysis to accelerate materials discovery. Together, these efforts illustrate how stress, defects, and lattice vibrations form a coherent framework for understanding and engineering materials through first-principles computation.

BIOGRAPHY

Kuntal Talit is a Postdoctoral Research Associate in the Nowadnick Group at the University of California, Merced. He holds a Ph.D. in Physics from UC Merced and master's degrees in Materials Engineering and Applied Physics from IIEST, India. Before starting his Ph.D., he spent five years as a software developer at IBM in India. His research combines density functional theory, lattice dynamics, and defect physics to understand how strain, doping, and lattice perturbations shape the properties of functional oxides. His current focus is on developing AI-assisted autonomous DFT workflows to accelerate materials discovery.

Kuntal Talit

University of California, Merced

Refreshments: 1:45pm, **Seminar**: 2-3pm