



HARVARD

School of Engineering
and Applied Sciences

Friday, March 25 – 4:00 pm

Pierce Hall, Rm. 209

The Applied Physics Colloquium presents

Discovering new phenomena through the prediction of microscopic structure of matter

While most of the known materials have been discovered through experiments, one wonders if theory will ever become capable of leading materials discovery. The evolutionary methodology USPEX has been a major step towards this goal, as it provides, given just the chemical composition and pressure/temperature conditions, the stable and low-energy metastable structures. Recently developed formulation of the theory of energy landscapes improves the method and brings additional insight. Some of the applications are:



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1. New stable high-pressure phase of boron, γ -B₂₈. This superhard phase shows a surprising degree of charge transfer between boron sites, which affects many physical properties.
2. Transparent insulating phase of sodium, the band gap of which increases from ~2 eV at 200 GPa to >5 eV at 500 GPa.
3. New phases of calcium, CaLi₂.
4. Unusual high-pressure behavior of nitrogen, Mn CH₄, silane SiH₄, germane GeH₄ and stannane SnH₄.

It is now also possible to optimize the structure and chemical composition with respect to a given physical property. I will discuss newly predicted carbon allotropes with special properties.

Refreshments served at 3:30 in
LISE Open Space on the 3rd Floor.

A social hour will be held in the
Brooks Room (Pierce 213)
following the presentation.