

DEPARTMENT OF PHYSICS & ASTRONOMY  
**CONDENSED MATTER SEMINAR**

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**Pressure-Mediated Band Gap Engineering of  
Sn – N, O Compounds**

The electronic structure of a material is one of the key fundamental properties to determine its interactions with light, its interfaces with the immediate surroundings, and its chemical, physical, and electronic interaction with other systems. The application of pressure allows systematic tuning of the charge density of a material cleanly, that is, without changes to the chemical composition via dopants, and exploratory high-pressure experiments can inform the design of bulk syntheses of materials that benefit from their properties under compression. I will present our work on the electronic and structural response of a number of tin binary compounds with technologically relevant properties. Specifically, tin nitride,  $\text{Sn}_3\text{N}_4$ , under compression, has a continuous opening of the optical band gap from 1.3 eV to 3.0 under pressure, corresponding to a 540 nm blueshift that spans the entire visible spectrum. The rate of decompression to ambient conditions permits access to recoverable metastable states with varying band gap energies, opening the possibility of pressure-tunable electronic properties for better tailored functional-specific materials. In rutile-structured  $\text{SnO}_2$ , we have correlated the observation of anomalous conductivity with structural disordering, that we predict to be universal for all materials undergoing a rutile to  $\text{CaCl}_2$  phase transition.

Tuesday, October 29, 2019

JFB 334

4:00 pm

Refreshments will be served in JFB 334 at 3:45 pm