# MATERIALS ENGINEERING SEMINAR

"Coupling Nanomechanical and Chemical Characterization for Evaluating Properties of Small-Scale Molecular Crystals"

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**Purdue MSE MS Final Exam**

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## ABSTRACT

Molecular crystals are used in a wide variety of applications, from pharmaceuticals and sweeteners to energetic materials. Understanding their chemical and mechanical properties provides insight into their performance and use. These properties are especially critical for energetic material systems, which may be sensitive to impact and require specific handling and storage practices. The mechanical properties of energetic molecular crystals are typically determined using nanoindentation by measuring elastic modulus, hardness, yield point, and fracture behavior. Reports of the properties and mechanical behavior of as-grown molecular crystals are limited due to the relative difficulty of performing good quality measurements. This work's contributions include the first known measurements of elastic and plastic properties for crystals of DAAF, CL-20, NTO, ETN, and R-salt.

When studying molecular crystalline systems, some important assumptions and behaviors typical to metallic and ionic systems begin to break down. The energetic material diaminoazoxyfurazan (DAAF) exhibits highly irregular mechanical behavior, which is likely explained by a complex combination of chemical and material attributes. This work investigates and compares the irregular mechanical response in DAAF—including high variance in mechanical properties, broad range of load-depth behavior, and non-conforming indentation impression geometries—to other energetic molecular crystals. The yield points (i.e., onset of plasticity) for several energetic materials, whose elastic modulus values range from 9.6 to 25.5 GPa, are also compared to identify the parameters that govern the onset of plasticity. This includes an investigation into yield point dependence on (or independence from) elastic modulus, hardness, near-neighbor spacing, and activation volume. When these materials reach the onset of plasticity, the maximum shear stress in each material ranges from 2-7% of their elastic modulus value. Analysis of the yield behavior in these materials suggests that there is not a strong correlation between yield stress and hardness, thus establishing that the mechanisms governing dislocation nucleation are not associated with (and cannot predict) hardness, and vice-versa. By recognizing and accounting for the added complexities associated with inherently non-spherical molecules in a crystal lattice, this work advances the comprehension of mechanical response in molecular crystal systems.

**Date: Wednesday, July 5, 2023**
**Time: 10:00 A.M.**
**Place: ARMS 1028 or via Webex:** https://purdue.webex.com/meet/dfbahr

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