



March 23–27, 2025 MGM Grand Las Vegas Hotel & Casino Las Vegas, Nevada, USA #TMSAnnualMeeting



SUBMIT AN ABSTRACT FOR THE FOLLOWING TMS2025 SYMPOSIUM:

MECHANICS OF MATERIALS

Structure-Property Relationships in Molecular Crystal Deformation

Molecular crystals, solids consisting of individual molecules, rather than just atoms, sitting on ordered lattice sites, find use in applications ranging from pharmaceuticals, energetic materials, battery electrodes, to organic electronics, and may be encountered in exotic environments like the cryogenic conditions of moons, comets, or exoplanets. A vast richness in molecular structures gives rise to a wide range of intermolecular bonding possibilities, which in turn result in crystalline materials with fascinating properties. Bonding and molecule shape often vary with direction within a single crystal, leading to anisotropy in defect structures and behaviors. These factors pose unique challenges to understanding the mechanical properties of these materials, and consequently the understanding of deformation and fracture remains generally less developed than in other classes of materials. However, recent years have seen a substantial increase in both interest and investigations. This symposium aims to capture these recent advances in a venue that brings together investigators from a range of communities: pharmaceuticals, energetic materials, organic electronics, solid mechanics, and any others interested in deformation of these materials. Talks are solicited that discuss the roles of microstructures and defects in the deformation process, from elasticity, to plastic deformation, and on to fracture. Talks are solicited across time scales from quasi-static to shock regimes, and from experimental, theoretical, and computational modeling disciplines.

Specific topics of interest include, but are not necessarily limited to:

- Predictions of crystal structure and mechanical properties (e.g. elastic constants)
- Defect behavior and plasticity under mechanical loading
- Crack initiation and propagation
- · Relationship of single crystal behaviors to bulk processing like milling and compaction
- Chemical reactions driven by mechanical deformation

ORGANIZERS

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