CMCC Mechanochemistry Discussions

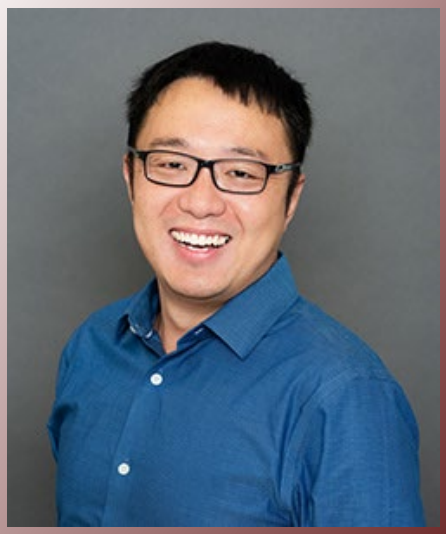
Online Seminar Series

Compressive Mechanochemistry of Molecular Compounds

Livestreaming at 10:00 AM (CT)

THURS., November 21, 2024

on the CMCC YouTube Channel:
https://www.youtube.com/channel/UC7eCYPKbGTKpgO7W2bNABxg



Dr. Hao Yan
University of North Texas
https://haoyangroup.com/

ABSTRACT:

In this talk, I will discuss the reactivity of molecular compounds under mechanical compression. Because of the anisotropic nature of molecules, they often deform in highly directional ways under hydrostatic (that is, uniform and static) pressure. In analogy to the Bell theory of tensile ("pulling force") driven mechanochemistry, we postulate that such directional deformations reduce the reorganization energy if they are aligned with a specific reaction coordinate of the molecule. We examine this postulate in several model systems including the topochemical polymerization of diynes and isomerization of metal oxo complexes. We further show that pressure encodes unique reaction selectivity by limiting the accessible conformations of the reactants. Lastly, I will share our prospects on using pressure for the quasi-static mapping of reaction pathways.

The CMCC is supported by the Division of Chemistry of the National Science Foundation under grants: 2023644 (Phase I) and 2303044 (Phase II).