



CMCC Mechanochemistry Discussions

Online Seminar Series

Prediction of Mechanosusceptible Reactions Using Molecular Distortions

Livestreaming at
10:00 AM (CT)
THURS., October 23, 2025

on the CMCC YouTube Channel:

<https://www.youtube.com/channel/UC7eCYPKbGTKpgO7W2bNABxg>



Prof. Mateusz Marianski
Hunter College, CUNY
<https://marianski-lab.github.io/>

Replacing solvothermal synthesis with mechanically-activated chemistry—where force, rather than heat and solvent, drives the making and breaking of covalent bonds—can help to solve the waste and energy challenges of chemical industry. Embracing mechanochemical synthesis, however, requires understanding how applied forces translate to acceleration of the chemical reactions and which classes of reactions, and specific reagents, will be susceptible to such effects. Herein, I will present our recent efforts to develop such theoretical framework for prediction of mechano-susceptible reactions. First, I will discuss how a relatively small, uniaxial force is able to accelerate the chemical reaction due to mechanical distortion along a specific molecular coordinate altering the reaction path. Second, this idea of molecular distortion along a productive coordinate will be exploited to screen a chemical space of Diels-Alder reactions to identify reactions that will be accelerated under distortion and provide insights into the origin of the mechanism.



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