CMCC Mechanochemistry Discussions

Online Seminar Series

Identifying Mechanochemically Accelerated Reactions Through High-Throughput Screening, Machine Learning Models, and Simplified Physical Models

Livestreaming at
10:00 AM (CT)
THURS., April 17, 2025

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

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Recent advances in mechanochemistry show that external mechanical forces can significantly accelerate reactions, such as Diels-Alder cycloadditions, offering greener synthetic routes. However, identifying reactions suitable for such acceleration remains a slow, manual process due to the absence of general design principles.

In this talk, I will present our efforts to uncover fundamental design principles for optimizing chemical reactions under external forces using a combination of high-throughput screening, optimization methods, and graph-based neural network potentials to conduct a broad search for reactions that can be significantly accelerated by external forces that are achievable in modern mechanochemical reactors. Our methods combine machine learning potentials with reaction path searching protocols (e.g., nudged elastic band and the growing string methods) to find potential transition states. We then examine candidate “activatable” coordinates (specific deformation modes that lead to enhanced reaction rates) by analyzing a mix of localized and normal coordinates. The most promising cases are then verified by higher-level calculations.

In addition, I will highlight the progress on the CMCC’s Mechanochemical Reaction Database (CMCCDB), a fork of the Open Reaction Database developed by the NSF Center for Computer-Aided Synthesis, with specific fields developed for mechanochemistry problems. This database, a collaborative effort involving researchers from Texas A&M University, Northwestern University, The City University of New York and Vanderbilt University, serves as a centralized platform allowing scientists to share reaction conditions and outcomes, to advance machine learning tools for more accurate predictions of mechanochemical reactions.

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