



CMCC *Mechanochemistry Discussions*

Online Seminar Series

Developing First-Principles Methods to Study Force- and Stress-enabled Mechanochemistry

Livestreaming at
10:00 AM (CT)

THURS., July 15, 2021

on the CMCC YouTube Channel:

[https://www.youtube.com/channel/
UC7eCYPKbGTKpgO7W2bNABxg](https://www.youtube.com/channel/UC7eCYPKbGTKpgO7W2bNABxg)



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ABSTRACT:

A wide variety of chemical transformations can be induced by the application of force or stress to reactive systems. In some cases, these reactions are undesired, including some tribochemical (friction-induced) reactions and bond-breaking in polymers under stress. A large and growing set of examples shows that mechanochemistry can be harnessed for useful chemical transformations, making the case for mechanochemistry as a general-purpose tool to advance chemical innovation. In order to realize this vision, we require greater understanding of how force and stress can be focused on particular bonds and reaction coordinates, and how this enhances chemical reactivity and selectivity. In this talk, I will outline strategies for applying stress to quantum-mechanical models of reactive chemical systems and for understanding the resulting mechanochemical reaction pathways. I will also describe the development of interatomic potential models that can enable larger-scale models of mechanochemical effects.



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