CMCC Mechanochemistry Discussions

Online Seminar Series

A Dynamical View of the Mechanochemical Reactivity of Solids

Livestreaming at 10:00 AM (CT)

THURS., August 17, 2023

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

Dr. Adam Michalchuk

University of Birmingham, UK
https://www.michalchukgroup.com/

ABSTRACT:

Mechanochemical reactions are phenomenally complex,[1] and require an understanding of the relation between processes spanning vast orders of magnitude in time and length scale. Understanding these complex reactions therefore requires a multi-faceted approach. I will briefly outline the different 'types' of mechanochemical reactions in relation to how these transformations can be studies,[2] before delving into our recent developments relating to probing mechanochemical transformations. I will discuss recent advances in studying macroscopic processes in mechanochemical reactions using time resolved synchrotron based methods.[3] I will subsequently discuss our efforts to use atomistic modelling as a means to understand at an elementary level how mechanical energy can drive chemical reactivity in crystalline solids.[4,5]

[1] AAL Michalchuk et al. (2021) Tribochemistry, Mechanical Alloying, Mechanochemistry: What is in a Name?, *Front. Chem.* 9, 685789

[2] AAL Michalchuk, Thermodynamics and Kinetics of Mechanochemical Reactions in Mechanochemistry and Emerging Technologies for Sustainable Chemical Manufacturing. *CRC Press*, 2023

[3] AAL Michalchuk and F Emmerling (2022) Time-Resolved In Situ Monitoring of Mechanochemical Reactions, *Angew. Chem. Int. Ed*. 61, 21, anie.202117270

[4] AAL Michalchuk (2023) The Mechanochemical Excitation of Crystalline LiN3, *Faraday Discuss*. 241, 230-249

[5] AAL Michalchuk et al (2022) Predicting the Impact Sensitivities of Energetic Materials Through Zone-center Phonon Up-pumping, *J. Chem. Phys*. 154, 064105

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