CMCC Mechanochemistry Discussions

Online Seminar Series

Toward a Better Understanding of Liquid Additive Effects and Their Possible Mechanistic Roles: Three Types of Mechanochemical Reactions

Livestreaming at 10:00 AM (CT)

THURS., February 15, 2024

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

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ABSTRACT:

Mechanochemical reactions are driven by the combined action of temperature and mechanical energy; however, their chemical mechanisms are poorly understood, and in some cases, they are significantly different than those solely occurring under thermal activation. Since around ten years ago, new experimental techniques to study in situ mechanochemical reaction kinetics have been developed, based on synchrotron X-ray powder diffraction or/and Raman spectroscopy. These methods have already contributed to the elucidation of many aspects of mechanochemical reactions in ball mills, such as the formation and consumption of reaction intermediates, polymorphic changes, changes in mechanochemical reactivity with the temperature, and the effects of small quantities of liquid additives.

During recent years our laboratory has studied essentially three types of mechanochemical reactions, and our learnings will be discussed in this presentation. (1) Various electron transfer reactions of the electron donor tetrathiafulvalene and p-benzoquinone derivatives as electron acceptors, including the effects of liquid additives and the reactant polymorphism. (2) Proton-transfer reactions between acidic and basic compounds, typically using the ΔpK_a rule. The characterization of amorphous mechanochemical products by microcrystal electron diffraction and their recrystallization upon exposure to solvent vapors will be shown. (3) Diels Alder cycloaddition reactions with the objective of experimentally determining their rate law using in situ Raman spectroscopy measurements, which have used liquid additives to modify the rheology of the mixture of reactants often enabling measurements under homogeneous conditions.

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