

A dynamical view of mechanochemical reactions

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Mechanochemical reactions – the ability to induce reactivity with mechanical force – offers an unparalleled opportunity for sustainable materials manufacture, removing solvent, reducing reaction times, and offering potential for highly scale-able reactions. Moreover, given the unconventional conditions of mechanochemical routes, they provide a route to synthesize materials that are otherwise impossible to make. Unfortunately, there remains very little understood about how mechanochemical processes occur, which greatly hinders their adoption by the wider community.¹

In this light we have been developing new experimental strategies to follow mechanochemical reactions in situ and in real time.² This includes innovations in time-resolved in situ (TRIS) diffraction³ and TRIS X-ray absorption spectroscopy.⁴ To date, these methods have provided exciting new insight into reaction profiles under various conditions, and both phase and microstructural evolution of materials within mechanochemical reactors. To supplement this work, we are developing fundamental new theoretical models to describe mechanochemical reactions, with the aim to understand at the atomic scale how mechanical energy is able to induce chemistry in solid materials.⁵ Together our experimental strategy to probe macroscopic dynamics of mechanochemical reactions, coupled with theoretical methods to probe microscopic dynamics, are providing unprecedented understanding of this potentially transformative technology.⁶ Through this talk we will highlight both experimental and theoretical developments and their applications to understanding the reactivity of solids under mechanochemical conditions.

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