Computational Mechanochemistry

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Mechanical force can dictate reaction pathways, reshape energy landscapes, and control bond scission and formation. Molecular-scale mechanochemical transformations can, in turn, drive supramolecular reconfiguration and the emergence of mesoscale material architectures. The intrinsically non-equilibrium and multiscale nature of these processes makes their theoretical description particularly challenging. In this presentation, I will discuss state-of-the-art computational approaches for modeling systems subjected to external forces or generating internal stresses, with examples ranging from molecular switches and polymer networks fracturing under strain to mechanochemical reactions induced by mechanical milling.