CMCC Mechanochemistry Discussions

Online Seminar Series

How does Mechanics Govern Chemistry?—

"Catalysis" by Force?

Livestreaming at
10:00 AM (CT)

THURS., September 19, 2024

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

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ABSTRACT:

"In his Bakerian lecture in 1862, H. C. Sorby addressed "mechanical force had been resolved into chemical action in the same way as, under other circumstances, it may be resolved into heat, electricity, or any other modification of force." Sorby argued that if mechanical force can be produced by chemical action, the converse should be possible. Since then, efforts to understand how mechanical forces facilitate chemical reactions and utilize such mechanisms for synthesis of new materials or better synthesis of existing materials have grown into an important subfield of chemistry, which is now called Mechanochemistry. One particularly interesting and relevant area is tribochemistry, which deals with chemical reactions facilitated by interfacial friction (or shear). At sliding interfaces, unconventional chemical reactions that do not take place in typical thermal conditions are often observed. Such reactions are known to be activated by mechanical shear action of the frictional interface. When reaction yield or rate is measured as a function of shear stress (which can be calculated from the applied load and friction coefficient) and plotted onto a semi-log graph, the slope is related to so called 'activation volume.' Although the activation volume can be readily determined experimentally, its physical meaning is still debated. We have investigated the shear-induced polymerization reaction of various types of organic molecules under vapor-phase lubrication (VPL) conditions. We found an empirical correlation between the magnitude of the activation volume and the molecular structure of reactant molecules (as well as the chemistry of solid surface). We hypothesized that the activation volume is associated with the physical deformation of reactant molecules and tested this hypothesis in collaboration with a reaction molecular simulation group (Ashlie Martini, University of California, Merced). In this talk, experimental and computational evidence supporting the hypothesis that the deformation of reactant molecule from its equilibrium geometry is the main driving force for shear-induced mechanochemical chemical reactions.

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