CMCC Mechanochemistry Discussions

Online Seminar Series

Pericyclic Reactions Under Pressure Studied by the Extreme Pressure-polarizable Continuum Model (XP-PCM)

Livestreaming at 10:00 AM (CT)

THURS., November 17, 2022

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

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ABSTRACT:
I will start with brief introductions to the field of what I call computational high-pressure organic chemistry and the essential method—extreme pressure polarizable continuum model (XP-PCM)—that enables the calculations of molecular properties and reactions under high pressure. I will then showcase applications of the method to typical pericyclic reactions under pressure, where interesting phenomena, such as transition state (TS) shifting along the reaction coordinate, conformational change becoming rate-determining, and possible TS turning into minimum will be discussed. The evolution of the cavity volume of the reactive system upon proceeding from the reactants to products, emerges as a useful diagnostic for analyzing the effect of the pressure on the reaction profiles. Finally, I will talk about a recent XP-PCM study on the thermal dimerization of 1,3-cyclohexadiene under pressure, which shows that accurate computation of activation volumes is a powerful tool in deciphering competing reaction mechanisms, and the analysis of partition of activation volume into physically meaningful contributions provides a new and extremely useful way to understand the origin of activation volume.

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