

Online Seminar Series

From Molecules to Functional Polymers - Multiscale Models in Mechanochemistry

Livestreaming at 10:00 AM (CT)

THURS., June 20, 2024

on the CMCC YouTube Channel: https://www.youtube.com/channel/UC 7eCYPKbGTKpg07W2bNABxg



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ABSTRACT:

When chemical substances are subjected to mechanical forces, geometrical, electronic and spectroscopic properties of the constituent molecules change. In most cases, however, it is not known how the mechanical force propagates through the material and how the structural changes at the molecular level arise. The reason for this is that several orders of magnitude, both in time and length, separate the macroscopic and molecular mechanochemical processes, which is a challenge for simulation methods in mechanochemistry. In this talk, scale-transcending approaches in computational mechanochemistry and high-pressure chemistry will be introduced and their application in the simulation of mechanochromic materials will be presented.

NST:

TEXAS A&M

HUNTER

CINCINNAT

ANDERBILT

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