CENTER FOR RESEARCH IN SOFT MATTER & POLYMERS

CRiSP SEMINAR

Monday, Sep. 16, 2019

10:00 a.m.

366 Colburn Lab

"Multiscale Modeling of Rubbery Elastomers: Mechanochemistry & Accelerated MD"

Rubbery elastomers are a versatile material used in a variety of consumer products (e.g. tires, seals). The first part of this talk focuses on the incorporation of mechanochemistry -- the study of chemical reactions induced by mechanical forces -- into multiscale models of rubbery elastomers. Transition states and reaction rates are calculated as a function of the load on a polymer chain, and incorporated into multiscale models. The second part of this talk focuses on the use of accelerated MD methods -- specifically, parallel replica -- to study the long-timescale behavior of rubbery elastomers.

Gopinath Subramanian

Scientist

Los Alamos National Lab

Gopinath Subramanian graduated with a PhD in Mechanical Engineering from Texas A&M University in college station. He is presently a scientist in the Computational Physics Division at Los Alamos National Laboratory. Prior to this, he was an Assistant Professor in the School of Polymer Science and Engineering at the University of Southern Mississippi.

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