“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.