1161-82-275 **Wei Li** (wli52@utk.edu), Chemical and Biomolecular Engineering, University of Tennessee, Knoxville, Knoxville, TN 37996, and **Manolis Doxastakis*** (edoxasta@utk.edu), Chemical and Biomolecular Engineering, University of Tennessee, Knoxville, Knoxville, TN 37996. *Crossover from Rouse to entangled polyisoprene dynamics: a multiscale simulation approach.*

Topological constraints govern the dynamics of entangled macromolecules when polymers exceed a critical molecular weight. The crossover from the low molecular limit described by the Rouse model to dynamics prescribed by entanglements has long been the subject of extensive research with significant challenges present. Constraint release and contour length fluctuations are often introduced into phenomenological descriptions to capture dynamics that depart from the original Doi-Edwards tube theory. However, significant recent studies find that many of these features present chemically specific characteristics rather than a ubiquitous behavior questioning our comprehensive understanding of the fundamental underlying mechanisms. Polyisoprene melts have long served as a prototype experimental system to study the evolution of the end-to-end distance along with mechanical relaxation. In this study we present new results by a systematic investigation of the transition of polyisoprene molecules from the Rouse regime to dynamics dictated by topological constraints. We report findings on mean correlation times as well as a complete description of full relaxation spectra and contrast our data to experimental studies. (Received August 18, 2020)