Rigidity transition with increasing crosslinking of a single macromolecule

JIWU LIU, PHILLIP DUXBURY, Michigan State University — A nanoparticle can be formed by the intramolecular crosslinking of a polymer chain. In this process the rigidity of the system increases with the crosslinking density. We carried out extensive molecular dynamics simulations of the intramolecular crosslinking on six different models to study their rigidity transitions. It was found the crosslinking satisfiability of the system is greatly affected by its rigidity. A facile analysis of floppy modes of the system was employed to determine the rigidity transition threshold and a good agreement with simulation data was obtained.