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Molecular Dynamics simulations of Hydrogels DI XU, DIVYA BHATNAGAR, MIRIAM RAFAILOVICH, DILIP GERSAPPE, Dept of Materials Science and Engg, Stony Brook University, Stony Brook NY 11794 — Hydrogels are emerging as a widely used material, particularly with biological applications. In these systems, the solvent concentration and effects can have a profound effect on the overall properties of the network. The heterogeneous nature of the network requires detailed simulations to probe the physical properties. We have initiated a series of MD simulations to explore how the functionality of crosslinker monomers could affect the structure of gel network, and have included solvent effects on the swelling and the mechanical properties of the gel. We used coarse-grained molecular dynamic simulation with Monte-Carlo methods to simulate polymer network formation with crosslinker monomers of different functionality. Standard tests, such as calculating the stress correlation function, were used to analyze the cross linked network. We also used grand canonical simulations to study the swelling behavior by coupling the gel with an imaginary solvent bath. After equilibrium, mechanical properties were characterized in terms of stress relaxation by non-equilibrium molecular dynamic simulation.

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