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Dynamical and Mechanical Behavior of Associating Protein Hydrogels[1] DARINA DANOVA, JAMES L. HARDEN, Johns Hopkins University, DAVID R. HEINE, GARY S. GREST, Sandia National Laboratories — Molecular dynamics simulation is used to study the dynamical and mechanical properties of hydrogels made from synthetic associating proteins. These proteins are triblock architectures composed of a central soluble, unstructured block flanked by associating helical ends. The ends are amphiphilic leucine zippers designed to reversibly assemble into trimeric bundles. Solutions of the triblock proteins reversibly self-assemble into hydrogels with predominantly trifunctional crosslinks. The hydrogel formation may be controlled by changes in temperature and pH, thus providing a switchable material with potential application in biomedical and environmental engineering. A coarse-grained model which mimics the alpha-helical secondary structure and amphiphilic properties of the leucine zipper domains is developed in order to accurately describe the structure and dynamics of the self-assembling hydrogel. Then, mechanical properties of the hydrogel under uniaxial and shear strain are presented and related to changes in the molecular level structure of the hydrogel in an effort to relate the protein structure to the hydrogel material properties.

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David R. Heine
Sandia National Laboratories

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