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The Effect of Multiple Parallel Bonds on the Self-healing of Labile Crosslinked Nanogel Networks ISAAC G. SALIB, GERMAN V. KOLMAKOV, CHET N. GNEGY, Chemical Engineering Department, University of Pittsburgh, KRZYSZTOF MATYJASZEWSKI, Department of Chemistry, Carnegie Mellon University, ANNA C. BALAZS, Chemical Engineering Department, University of Pittsburgh — We develop a hybrid computational approach to examine the mechanical properties and self-healing behavior of nanogel particles that are crosslinked primarily by highly reactive bonds that can break and readily remake (labile bonds). The individual nanogels are modeled via the lattice spring model (LSM). The crosslinks between the nanogels are simulated via a modified Hierarchical Bell Model (HBM), which allows us to capture both the rupturing and reforming of multiple, parallel bonds due to an applied force. Using our hybrid HBM/LSM, we simulate the behavior of the crosslinked nanogels under a tensile deformation. In these simulations, each labile linkage between the nanogels contains at most N parallel bonds. We reveal that while numerous parallel bonds within a linkage enhance the strength of the material, these bonds diminish the ductility and the ability of the material to undergo the structural rearrangements that are necessary for self-repair.

Isaac G. Salib
Chemical Engineering Department, University of Pittsburgh

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