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Improving self-healing behavior of dually cross linked nanogels that encompass nanoparticles SOLOMON DUKI, GERMAN KOLMAKOV, University of Pittsburgh, Department of Chemical Engineering, Pittsburgh, PA 15261, KRZYSZTOF MATYJASZEWSKI, Carnegie Mellon University, Department of Chemistry, Pittsburgh, PA 15213, ANNA BALAZS, University of Pittsburgh, Department of Chemical Engineering, Pittsburgh, PA 15261 — Numerical studies of nanogels that are cross-linked by stable and labile bonds have shown that the material can withstand significantly high stresses before it undergoes fracture. The mechanical integrity of such materials is preserved through structural rearrangement of the nanogel particles; this structural rearrangement is facilitated by the making and breaking of the labile bonds. Apart from the bond properties, the stiffness and flexibility of the nanogel is crucial to determine the mechanical properties of these self healing novel materials. Our simulations show that the mechanical property of the entire sample is significantly improved by introducing hard core nanoparticles into the structural units. Through numerical modeling of hard core-soft shell nanogel material we identify the region of parameters (the nanogel size and core/shell ratio) at which the sample demonstrates optimal stability and self-healing behavior.

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