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The Role of Multiple, Reformable Parallel Bonds on the Self-healing Behavior of Dual Crosslinked Nanogel Materials 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 — Using computational modeling, we design novel self-healing materials composed of nanoscopic polymer gel particles, or nanogels. The particles are interconnected via both labile bonds (e.g., disulfide bonds) and stronger, less reactive bonds (e.g, C-C bonds) and therefore the nanogels form a "dual crosslinked" network. The stable bonds provide a rigid backbone while the labile bonds allow the material to undergo a dynamic reconfiguration in response to stress. We adapt the Hierarchical Bell Model (HBM) to describe the labile bonding interactions. The HBM effectively allows us to model cases where the ligands on neighboring nanogels interact through multiple sites. We show that the introduction of a small number of labile bonds that lie in parallel significantly increases the strength of the material relative to samples crosslinked solely by the stable bonds. We also isolate an optimal range of labile interconnections that provide high-strength, tough materials that are capable of self-repair.

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