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Self-healing in dually crosslinked nanogels: Computational modeling SOLOMON DUKI, VICTOR YASHIN, GERMAN KOLMAKOV, ANNA BALAZS, University of Pittsburgh, Department of Chemical Engineering, Pittsburgh, PA 15261, USA — We report the results of computational modeling of materials composed of dually crosslinked nanogels. In such materials, permanently crosslinked nanogel particles are bound together through two kinds of crosslinks, namely, the stable and labile ones. Under sufficiently high stress, the strong, stable bonds undergo irreversible rupture, whereas the weak, labile bonds can reform after breakage. We demonstrate that presence of the labile interparticle bonds makes possible the structural rearrangements inside the deformed material. As a result, the catastrophic failure of the material is postponed, and the defects (cavities) in the strained material heal themselves when the stress is released. The mathematical model used in the simulations was developed by us through a bottom-up approach, which allows us to capture the viscoelastic and plastic properties of the material under various deformation regimes.

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