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**Simulations of Self-Healing Polymer Networks** ARUN KUMAR N, EVGENY STUKALIN, Department of Chemistry, The University of North Carolina, Chapel Hill, NC 27599, LUDWIK LEIBLER, Matière Molle et Chimie, CNRS-ESPCI, 75005 Paris, France, MICHAEL RUBINSTEIN, Department of Chemistry, The University of North Carolina, Chapel Hill, NC 27599 — Self-healing polymeric materials are systems that after damage can revert to their original state with full or partial recovery of mechanical strength. Using hybrid MD/MC simulations we study autonomic self-healing of reversible polymer networks. The self-healing mechanism of dangling chains in polymer networks which can form weak reversible bonds, e.g., hydrogen bond, is based on the slow-dynamics of re-association of the broken reversible bonds. The simulation protocol for self-healing process consists of three steps : (1) equilibration of the reversible network, (2) introduction of a fracture plane in the polymer network across which reversible bonds are not allowed to form, and simultaneous shifting of the fractured sections with respect to each other, while pulling the dangling chains back to their respective halves, and (3) after some waiting time, allowing chain penetration and bonding across fractured interface during the healing time period. The simulation model is used to capture the new features of the self-healing mechanism related to the renormalization of reversible bond lifetime and exchange of bonding partners and is compared to analytical models of this process that account for these features.

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