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Designing Reconfigurable Stimuli-Responsive Gel/Nanofibers Composites XIN YONG, OLGA KUKSENOK, ANNA BALAZS, Chemical Engineering Dept, University of Pittsburgh — Using dissipative particle dynamics (DPD), we model the response of a composite gel, which encompasses active nanofibers, to external stimuli, such as light and temperature. The gel is constructed by crosslinking polymer chains in a coarse-grained manner. We probe the volume phase transition and swelling kinetics of the gels in explicit solvents. Our model is validated through qualitative comparisons with Flory-Huggins theory, and the effects of solvent quality, crosslink density and temperature are analyzed. By incorporating nanofibers into the gel matrix, we utilize different responses of the fibers and gel to variations in external stimuli. We focus on the fiber-gel and fiber-fiber interactions and establish routes for modeling composites with multiple types of fibers, which enable greater control of materials functionality. Utilizing the adaptability of gel/nanofiber composites, we design composites that can dynamically reconfigure shape via external stimuli to achieve actuation and locomotion. Our findings provide fundamental insights into the dynamics of gel-based composites, as well as guidelines for designing re-programmable multi-functional materials.

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