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Dissipative particle dynamic simulations of solvent flow through nanometer sized smart channel coated with stimuli responsive polymer brush JIANHUA HUANG, Department of Chemistry, The University of Memphis, Memphis, TN 38152; Department of Chemistry, Zhejiang Sci-Tech University, Hangzhou, 310018, China, MOHAMED LARADJI, Department of Physics, The University of Memphis, Memphis, TN 38152, YONGMEI WANG, Department of Chemistry, The University of Memphis, Memphis, TN 38152 — Various efforts have been focused on the development of smart materials which can respond to environmental stimuli such as pH or temperature. Nanometer sized channels coated with such stimuli responsive polymers can serve as smart gating or smart valve that are of interest for applications such as controlled drug release and tunable permeation and separations of toxic solutes. These systems involve the interplay of solvent flow with the structure of polymer brush in response to the external stimuli. We applied dissipative particle dynamic (DPD) method to investigate solvent flow through such smart channels. The external stimuli are modeled by the change in solvent quality that causes polymers undergoing a coil-to-globular transition. We investigate the ability of such smart channel to control the solvent flow under different stimuli. The interplay of the solvent flow and the properties of polymer brush are studied at the molecular level. The effects of the grafted density and the layer thickness of polymer brush on its controlling ability have also been investigated.

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