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Structure and Dynamics of Thin Polyacrylate Gel Films Supported on a Polymeric Substrate SRIRAMVIGNESH MANI, RAFIKUL ISLAM, RAJESH KHARE, Texas Tech University — Recently, we have used molecular dynamics (MD) simulations to demonstrate the viability of polyacrylate gel membranes for pervaporation based separation processes. In practice, these polymeric membranes are usually in the form of thin films that are supported on another polymeric substrate such as polysulfone or cellulose acetate. The structure and dynamics of the polymer constituting the membrane play an important role in governing the separation efficiency of these membranes. Since chain structure and dynamics in supported polymer thin films deviate significantly from their bulk values, it is necessary to understand the effect of the soft polymeric support on the properties of the polymer constituting the membranes. In this work, the structural and dynamic properties of polyacrylate gels that are supported on polysulfone are studied using molecular simulations. Specifically, three different networks formed by poly butyl acrylate (PBA), 50-50 random copolymer of butyl acrylate and 2-hydroxy ethyl acrylate (P(BA50-HEA50)), and poly 2-hydroxyethyl acrylate (PHEA) are considered. The properties of the supported thin film gel systems are characterized by determining the gel structure, glass transition temperature, and chain dynamics. The effect of the polysulfone support on the system behavior is determined by comparing the properties of the supported thin films systems with those of the bulk gel systems.

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