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Computational Modeling of Polystyrene-b-(ethylene-co-butylene)-b-styrene and Mineral Oil Gels and Nanocomposites T.L. CHANTAWANSRI, M. BERG, R. MROZEK, K. STOKES, U.S. Army Research Lab, RDRL-WMM-A, B. HENZ, P. CHUNG, U.S. Army Research Lab, RDRL-CIH-C, F. BEYER, J. LENHART, J.W. ANDZELM, U.S. Army Research Lab, RDRL-WMM-A — There has been substantial interest in thermoplastic elastomer (TPE) gels composed of poly(styrene-b-(ethylene-co-butylene)-b-styrene)(SEBS) and hydrocarbon oils. Although the effects of adding nanoparticles on TPE gels is relatively unexplored, research in polymer nanocomposites have shown that the addition of nanoparticles enhanced physical properties. The microstructure of such a system is dependent on a variety of parameters such as block copolymer and nanoparticle concentrations, temperature, nanoparticle size, and nanoparticle interaction; thus to perform an extensive study of phase space, mesoscale modeling should be used in conjunction with the experimentation. To complement our experimental system, mesoscale modeling of this TPE gel and the corresponding nanocomposite are preformed using dynamic density functional theory and self consistent field theory through Materials Studio, where morphology of the system is studied as a function of various parameters and conditions. The validity of the computational methods has been confirmed for a number of experimental results, and subsequently has been used to explore a larger design space than is accessible solely through experimental methods.

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