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Dissipative Particle Dynamics modeling of nanorod-polymer composites SHAGHAYEGH KHANI, JOAO MAIA, Case Western Reserve University — Recent years have seen a plethora of experimental methods for fabricating nanorod-polymer composites with enhanced physical and mechanical properties. The macroscopic properties of the composites are directly related to the dispersion and organization of the nanoparticles in the matrix. For instance, a significant improvement in the properties of the nanorod-polymer composites is observed upon formation of a percolating network. Thus, controlling the structure of the nanoparticles in the matrix will advance the technology in the field. One way of doing this is by adjusting the chemical interactions which is done through grafting polymer chains on the surface of the rods. Although the enthalpic interactions play the major role in such systems other entropic variables such as the dimension of the rods, density of grafting and etc. may influence the final morphology of the system. The recent developments in the computational techniques have paved the road for further understanding of the controlled assembly of nanorods in polymer matrices. In this study, Dissipative Particle Dynamics (DPD) is employed in order to investigate the effect of enthalpic and entopic variables on the phase behavior of the nanorod-polymer composites. DPD is a coarse-grained mesoscale method which has been found very promising in simulating multi component systems. The interaction parameter between the components of the systems can be mapped onto the Flory-Huggins χ-parameter via well-known Groot-Warren expression. The main goal of this work is to provide a phase diagram that can be used to guide the experiments in designing new materials.

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