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Phase behavior and clustering of nanoparticles with approximate polymer interactions ANDREW RAHEDI, FRANCIS STARR, Wesleyan University — In nanoparticle polymer composite (NPC) materials, the clustering or dispersion of the nanoparticles strongly influences the material properties. The purpose of this study is to better understand the factors that influence nanoparticle clustering as a step towards developing more efficient simulation approaches. To understand the clustering of nanoparticles in an NPC, we simulate both pure nanoparticles and nanoparticles with approximate polymer interactions and compare our results with simulations that include explicit polymer interactions. We find that pure nanoparticles without polymeric interactions undergo ordinary phase separation. Thus the previously observed lack of nanoparticle phase separation in an NPC is due to interactions with the polymer matrix; this interaction includes short-range attractions due to monomer interactions and long-range repulsions due to the excluded volume of the chains. We approximate this interaction by including a Yukawa potential as a weak long-ranged repulsion acting between nanoparticles. Since the simulation of an NPC is computationally expensive due to the polymer-polymer interactions, this approach improves the efficiency of our simulations and enables us to study the thermodynamic properties over a much broader range of conditions.

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