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Coarse-Grained Molecular Monte Carlo Simulations of Liquid Crystal-Nanoparticle Mixtures[1] RYAN NEUFELD, GRIGORIY KIMAEV, FRED FU, NASSER M. ABUKHDEIR, University of Waterloo — Coarse-grained intermolecular potentials have proven capable of capturing essential details of interactions between complex molecules, while substantially reducing the number of degrees of freedom of the system under study. In the domain of liquid crystals, the Gay-Berne (GB) potential has been successfully used to model the behavior of rod-like and disk-like mesogens. However, only ellipsoid-like interaction potentials can be described with GB, making it a poor fit for many real-world mesogens. In this work, the results of Monte Carlo simulations of liquid crystal domains using the Zewdie-Corner (ZC) potential are presented. The ZC potential is constructed from an orthogonal series of basis functions, allowing for potentials of essentially arbitrary shapes to be modeled. We also present simulations of mixtures of liquid crystalline mesogens with nanoparticles. Experimentally these mixtures have been observed to exhibit microphase separation and formation of long-range networks under some conditions. This highlights the need for a coarse-grained approach which can capture salient details on the molecular scale while simulating sufficiently large domains to observe these phenomena. We compare the phase behavior of our simulations with that of a recently presented continuum theory.

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