



سمینار هفتگی گروه ماده چگال نرم

Phase separation in mixtures of thin and thick RE-Squared ellipsoids

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Phase separation of a 50:50 binary system composed of two prolate ellipsoids with different axis ratios is investigated through molecular dynamics simulation. Particles interact via the force-field RE-Squared, which can be used as a correction to Gay-Berne potential, conventionally used for ellipsoidal particles. The system can be considered as a coarse-grained model of a binary liquid crystal mixture. We have studied the system as a binary mixture lying in the isotropic phase which is then condensed through several stages. Phase separation has been detected in the system by changing the density as the control parameter. The system goes through two different phase changes, one being the phase change due to phase separation and the other one due to isotropic-nematic transition. For the latter case we have perceived a phase coexistence behavior in the orientational order parameter which has been done through a comparison between single-particle simulations and the binary mixture.

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