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Structure and Transport Properties of Liquid Crystals under Nanoscale Confinement SHUYUAN WANG, GERALD WANG, Carnegie Mellon University — Significantly confined films of liquid crystals appear in a wide variety of technologies. The structure and transport properties of nanoconfined liquid crystals differ significantly from a bulk (unconfined) phase. In this work, we present theoretical and computational results on liquid crystals confined within slits whose sizes are ones to tens of the mesogen lengthscale. To study these systems, we perform molecular-dynamics (MD) simulations of fluids consisting of ellipsoidal particles, of a variety of aspect ratios, whose interactions are given by the Gay-Berne interatomic potential. While systematically varying the fluid density and temperature, we compute a number of fluid properties, including density, diffusivity, and statistics quantifying orientational order. Our results demonstrate the importance of adsorption effects induced by the solid boundaries, which significantly affect both the structure and transport, especially in the near-wall region, as well as the location of an isotropic-to-nematic phase transition for the system overall. We present an analytical model based on a mean-field theory, which enables us to characterize density inhomogeneities under confinement; the predictions of this model are validated by comparison with MD simulations

Gerald Wang
Carnegie Mellon University

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