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Predicting the Anomalous Density of a Dense Fluid Confined within a Carbon Nanotube GERALD WANG, NICOLAS HADJICONSTANTINOU, MIT — The equilibrium density of fluids under nanoconfinement can be substantially smaller than their bulk density. Understanding the physical basis for and magnitude of these anomalous densities is key to many nanoengineering applications, such as constructing a sub-continuum model of nanoscale fluid flow. We provide here a theoretical description of this phenomenon in the most frequently, perhaps, studied system - a dense fluid confined within a carbon nanotube (CNT). We show that the reduced density is primarily due to repulsive interactions between the fluid and the CNT, which modify the fluid structure near the fluid-CNT interface and lead to a "stand-off" distance between the two materials. Using a mean-field approach to describe the energetic landscape near the CNT wall, we obtain closed-form analytical results describing the length scales associated with the layered fluid. Combined with empirical knowledge of the layered-fluid density, these results allow us to derive a prediction for the equilibrium fluid density as a function of the CNT radius that is in excellent agreement with molecular dynamics simulations. We also show how aspects of this theory can be extended to describe water confined within CNTs and find good agreement with results from the literature.

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