232g Interfacial Properties for Polymer and Copolymer Systems by Density Functional Theory

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A non-mean field density functional theory (DFT) is proposed for interfacial properties of pure polymer and copolymer. The excess Helmholtz free energy functional is formulated in terms of a modified fundamental measure theory for short ranged repulsion and a density-gradient expansion for long ranged attractions. Analytical expression for the direct correlation function of Lennard-Jones fluid is utilized to take into account the effect of long ranged attraction on intermolecular correlations. With the predicted bulk properties as input, the interfacial properties including equilibrium density profile, surface thickness and surface tension are investigated.