

## Modeling Conformational Properties of Branched Polymers from iSAFT Density Functional Theory

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A new density functional theory (DFT) formalism is designed to study the thermodynamic properties of branched polymers, such as star polymers, comb polymers, bottlebrush polymers, hyperbranched polymers, and dendrimers. Branched polymers are of great research interest because they have properties and phase behavior that are very different from those of linear polymers of similar chemical composition and molecular weight. As a consequence, branched polymers have potential applications in many areas, such as medicine, catalysis, and surface coating. The prediction and interpretation of these properties and phase behavior is generally difficult due to the complexity and variety of molecular structures. A new DFT formalism based on inhomogeneous statistical associating fluid theory (iSAFT) is proposed. The theory is capable of predicting surface adsorption for branched polymers of all architectures. The theoretical prediction is in qualitative agreement with simulation results. Taking advantage of symmetry of certain types of branched polymers (such as star polymers, dendrimers, and bottlebrush polymers), radial density profiles of individual beads are readily obtained from the theory. This knowledge allows us to study radii of gyration and other conformational properties in addition to solute and solvent distributions in the polymer. We believe this theory to be a powerful tool to model branched polymers with advantages over simulation (less computational expense) and other theories (more detailed information).