Coarse-graining of slit-confined star polymers in solvents of varying quality

Reyhaneh A. Farimani, Christos N. Likos
Faculty of Physics, University of Vienna, Boltzmanngasse 5, A-1090 Vienna, Austria
reyhaneh.afghahi.farimani@univie.ac.at

We investigate star polymers with varying functionalities and under varying solvent conditions confined within a slit geometry. Our approach involves an accurate estimation and validation of the effective interaction by directly computing the force between a pair of star polymers and comparing the radial distribution function from monomer-resolved molecular dynamics simulations with that obtained through Monte Carlo simulations using the effective interaction. Our findings reveal significant sensitivity in the radial distribution function to subtle variations in the tail of the interaction potential, particularly in dilute regimes. Furthermore, we employ a morphological model to analyze the interpenetration of the star polymers, demonstrating that reducing the functionality leads to a marked increase in the interpenetration of these polymeric systems. We establish that solvent quality has minimal impact on the degree of interpenetration whereas the star functionality affects it markedly, leading to enhanced faceting and reduced interpenetration for as the number of arms grows. These results are particularly relevant for enhancing our understanding of polymeric materials' rheological and mechanical properties.

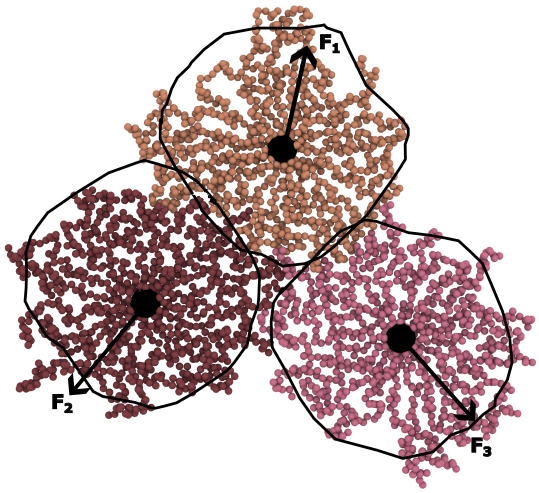

Figure 1: Graphical abstract of the study. It illustrates star polymers using a two-level coarse-graining approach. First, the polymers are simplified to point particles that interact based on pair potential. Second, a morphological coarse-graining is applied, which retains arm monomers and treats star polymers as deformable, interpenetrating soft colloids.