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Interaction between Polymer Grafted Particles: Self-Consistent-Field Study[1] JAEUP KIM, MARK MATSEN, University of Reading — Recently, there has been an ongoing debate regarding a possible attraction between two polymer grafted nanoparticles. Using numerical self-consistent field theory (SCFT) we investigate the inter-particle potential, showing that only a monotonically increasing repulsive force is expected between the two particles regardless of the particle size and brush thickness. We also compared the exact mean-field result to approximate solutions using the Derjaguin approximation. The previously reported attraction is thought to be an anomaly caused by the use of bispherical coordinates. We avoid this problem by developing a new SCFT scheme using two separate spherical coordinate systems centered on each particle. The idea of using multiple coordinate systems is applicable for many polymeric problems involving complicated geometries. In this scheme, two or more coordinate systems share an overlapping volume. Then the statistics of the polymers belonging to a certain coordinate system are solved in trial fields, and the resulting polymer concentration is shared by all coordinate systems to find a self-consistent solution. This method has been tried for other problems such as the behavior of a Janus nanoparticle (solved in spherical coordinates) in block copolymer lamellar phase (solved in cylindrical coordinates).

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Jaeup Kim
University of Reading

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