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Coarse-grained explicit solvent simulation of the translational and rotational diffusion of a spherical particle in a polymer solution VICTOR PRYAMITSYN, Northwestern University, VENKAT GANESAN, University of Texas at Austin — We use an extension of DPD model to address the dynamical properties of a colloid particle in an unentangled semi-dilute polymer solution. Solvent and monomers are represented as DPD particles.The colloid particle is represented as a larger DPD particle with the rotational degrees of freedom and tangential component of the dissipative and random DPD interactions with the solvent and monomers. This allows us to model a finite slip length boundary condition at the particle fluid interface and study translational D_t and rotational D_r diffusivities of a spherical particle. For zero polymer concentration our results agree with the Stokes-Einstein (SE) theory. Fore dilute and semi-dilute polymer solutions we have found that polymer dynamic follow the Zimm model in a dilute regime and the Rouse model at high polymer concentration. For particles smaller than the polymer R_g observed D_t is much high than SE prediction for $R > R_g$ SE prediction recovers. We have found that increase of D_r relative to SE is rather correlated to the $\frac{R}{R_g}$ ratio than $\frac{R}{\xi}$, where ξ is the thickness of a depletion shell around the particle. D_r is very sensitive to the slip length at the particle fluid interface and insensitive to $\frac{R}{R_g}$.

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