Brownian dynamics and dynamic Monte Carlo simulations of isotropic and liquid crystal phases of anisotropic colloidal particles: a comparative study

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We report on the diffusion of merely repulsive and freely rotating colloidal rods in the isotropic, nematic and smectic liquid crystal phases, to probe the agreement between Brownian and Monte Carlo dynamics under the most general conditions. By properly rescaling the Monte Carlo time step, being related to any elementary move via the corresponding self-diffusion coefficient, with the acceptance rate of simultaneous trial displacements and rotations, we demonstrate the existence of a unique Monte Carlo time scale that allows for a direct comparison between Monte Carlo and Brownian dynamics simulations. To estimate the validity of our theoretical approach, we compare the mean square displacement of rods, their orientational autocorrelation function, and the self-intermediate scattering function, as obtained from Brownian dynamics and Monte Carlo simulations. The agreement between the results of these two approaches, even under the condition of heterogeneous dynamics generally observed in liquid crystalline phases, is excellent.