Dynamic Simulations of Rod-Shaped Colloidal Particles: Phase behaviour, self-assembly, diffusion and electrophoresis

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Here, we present a coarse-grained model for dynamic simulations of rod-shaped colloidal particles. Individual rods are represented by a rigid linear chain consisting of overlapping spheres which interact through a pseudo-hard-core. Non-adsorbed polyremes are modelled as freely inter-penetrable spheres with respect to each other, while there is the pseudo-hard-core repulsion between the polymer and rod spheres. Solvents are considered implicitly or explicitly with a dissipative particle dynamics (DPD) model. The phase behaviour of this model, obtained from continuous compression and expansion simulations, reproduces previous predictions based on theoretical calculations and Monte Carlo simulations (Fig.1). The brute-force simulations and forward-flux-sampling simulations are performed with this model to investigate the nucleation mechanism and to predict the nucleation rate/barrier for the self-assembly process of hard-rod colloidal particles in non-adsorbed polyreme solutions (Fig.2). The diffusion coefficients of a single rod-shaped colloidal particle measured with this model are in good agreement with the predictions based on the continuum theory (Fig.3). We also use this mode to study the motion of a single charged rod-shaped colloidal particle in the electric-filed to reveal the orientation of the particle in electrophoresis (Fig.4).

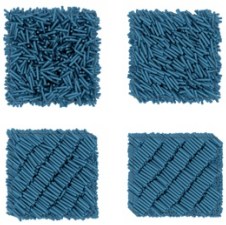

Fig.01 Isotropic, Nematic, Smectic, and Crystal phases in hard-rod suspensions.

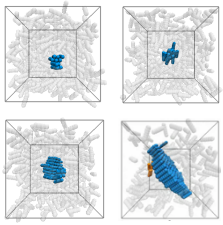

Fig.02 Nucleation-growth process in a hard-rod/polymer suspension.

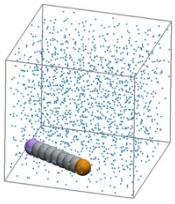

Fig.03 A rod-shaped colloidal particles in DPD solvent.

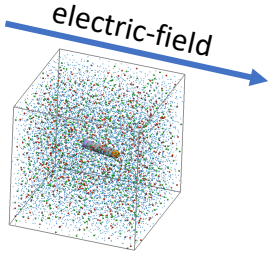

Fig.04 Electrophoresis of a rod-shaped colloidal particles.

Our model and method are suited to study various dynamic processes in rod-shaped colloidal suspensions, including nucleation, self-assembly and other kinetic processes, and can be readily extended to colloidal particles of different shapes and chemistry.

References

1. Liu, Y. & Widmer-Cooper, A. (2019) A Versatile Simulation Method for Studying Phase Behavior and Dynamics in Colloidal Rod and Rod-Polymer Suspensions. J. Chem. Phys., 150, 244508.