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Dynamics of suspension of interacting yolk-shell particles LUIS

E. SANCHEZ DIAZ, Oak Ridge National Lab, ERNESTO CORTES MORALES, Universidad Autonoma de San Luis Potosi, XIN LI, WEI-REN CHEN, Oak Ridge National Lab, MAGDALENO MEDINA NOYOLA, Universidad Autonoma de San Luis Potosi — In this work we study the self-diffusion properties of a liquid of hollow spherical particles (shells) bearing a smaller solid sphere in their interior (yolks). We model this system using purely repulsive hard-body interactions between all (shell and yolk) particles, but assume the presence of a background ideal solvent such that all the particles execute free Brownian motion between collisions, characterized by short-time self-diffusion coefficients D_s^0 for the shells and D_y^0 for the yolks. Using a softened version of these interparticle potentials we perform Brownian dynamics simulations to determine the mean squared displacement and intermediate scattering function of the yolk-shell complex. These results can be understood in terms of a set of effective Langevin equations for the N interacting shell particles, pre-averaged over the yolks' degrees of freedom, from which an approximate self-consistent description of the simulated self-diffusion properties can be derived. Here we compare the theoretical and simulated results between them, and with the results for the same system in the absence of yolks. We find that the yolks, which have no effect on the shell-shell static structure, influence the dynamic properties in a predictable manner, fully captured by the theory

Luis E. Sanchez Diaz
Oak Ridge National Lab

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