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Abstract for an Invited Paper
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Simulations of nanoparticle ionic and organic hybrid materials¹

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We have used molecular dynamics simulations over microsecond time scales to study the structure and dynamics of coarse-grained models for nanoparticle-based ionic and organic hybrid materials [1]. The systems of interest consist of particles with charged surface groups and linear or three-arm counterions, which also act as the solvent. A comparable uncharged model of nanoparticles with tethered chains is also studied. The pair correlation functions display a rich structure resulting from the packing of cores and chains, as well as electrostatic effects. Even though electrostatic interactions between oppositely charged ions at contact are much greater than the thermal energy, we find that chain dynamics at intermediate time scales are dominated by chain hopping between core particles. We have also used molecular dynamics simulations and density functional theory to investigate the structure of solvent-free oligomer-grafted nanoparticles [2,3]. At low temperatures and moderate to high oligomer lengths, the qualitative features of the core particle pair probability, structure factor, and the oligomer brush configuration obtained from the simulations can be explained by a density-functional theory that incorporates the configurational entropy of the space-filling oligomers. In particular, the structure factor at small wave numbers attains a value much smaller than the corresponding hard-sphere suspension, the first peak of the pair distribution function is enhanced due to entropic attractions among the particles, and the oligomer brush expands with decreasing particle volume fraction to fill the interstitial space. At higher temperatures, the simulations reveal effects that differ from the theory and are likely caused by steric repulsions of the expanded corona chains.

[1] B. Hong, A. Chremos, and A. Z. Panagiotopoulos; Faraday Disc., DOI: 10.1039/c1fd00076d (2012).

[2] A. Chremos, A. Z. Panagiotopoulos, H.-Y. Yu, and D. L. Koch; J. Chem. Phys., 135:114901, 12pp (2011).

[3] A. Chremos and A. Z. Panagiotopoulos; Phys. Rev. Lett., 107:105503, 5pp (2011).

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