Abstract Submitted for the MAR13 Meeting of The American Physical Society

Heterogeneous nanoparticles at water-oil interfaces: Structure, Order, Diffusion, and Implications for the stability of Pickering emulsions¹ ALBERTO STRIOLO, XUAN-CUONG LUU, The University of Oklahoma, MOLECULAR SCIENCE AND ENGINEERING TEAM TEAM — Pickering emulsions find applications, e.g., in food processing, personal care products, and drug delivery. The emulsions stability is naturally related to the structural and dynamical properties of the nanoparticles adsorbed at oil-water interfaces. Such properties are investigated here by means of dissipative particle dynamics simulations, informed by atomistic molecular dynamics simulations results (Langmuir 2011, 27, (9), 5264-5274). Several nanoparticles are considered, including Janus and homogeneous, and of several different shapes (spherical, elliptical, discoid, etc.) Structural and transport properties are quantified as a function of surface density and system composition. Results for radial distribution functions, hexagonal order parameters, and self-diffusion coefficients are reported. We sometimes find unexpected behavior. For example, self-diffusion coefficient maxima are observed in mixed systems. Implications of such observations on macroscopic observables (i.e., the stability of Pickering emulsions) are discussed.

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