Abstract Submitted
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Atomistic Simulations of Hydrodynamic and Interaction Forces on Functionalized Silica Nanoparticles[1] J. MATTHEW D. LANE, AHMED E. ISMAIL, MICHAEL CHANDROSS, Sandia National Labs, CHRISTIAN D. LORENZ, King's College London, GARY S. GREST, Sandia National Labs — It is often desired to prevent the flocculation and phase separation of nanoparticles in solution. This can be accomplished either by manipulating the solvent or by tailoring the surface chemistry of the nanoparticles through functionalization with a monolayer of oligomer chains. Since it is not known how these functionalized coatings affect the interactions between nanoparticles and with the surrounding solvent, we present results from a series of molecular dynamics simulations of polyethylene oxide (PEO) coated silica nanoparticles of varying size (5 to 20 nm diameter) in water. For a single nanoparticle we determined the Stokes drag on the nanoparticle as it moves through the solvent and as it approaches a wall. Due to hydrodynamic interactions there are large finite size effects which we estimate by varying the size of the simulation cell. We also determined both solvent-mediated (velocity-independent) and lubrication (velocity-dependent) forces between two nanoparticles as a function of the coverage and chain length of the PEO chains.

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