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Forces between Functionalized Silica Nanoparticles[1] J. MATTHEW D. LANE, AHMED E. ISMAIL, MICHAEL CHANDROSS, GARY S. GREST, Sandia National Labs — Polymer-coated nanoparticles have a wide variety of applications, including drug delivery, adhesives, coatings, and magnetics. Although, the complexity of these nanoparticles precludes atomistic simulations of large numbers of nanoparticles in solution, it is possible to study the interaction between pairs of nanoparticles in an explicit solvent using molecular dynamics. From these simulations, we can compute the potential of mean force (PMF) between nanoparticles, which can be used in coarse-grained simulations at larger length and time scales. In particular, we present results for PMFs between polymer-grafted silica nanoparticles as a function of chain length, core size, and approach velocity. We report results for explicit-atom models of poly(ethylene oxide)-coated nanoparticles in water and alkylsilane-coated nanoparticles in decane.

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