291n Understanding Nanoparticle Aggregation Using Multi-Scale Simulations and Atomic Force Microscopy

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Nanoparticles find applications as pharmaceuticals, catalysts, paints, adhesives, photographic supplies, UV absorbers, inks, pigments, etc. The development of computational tools that predict the properties of nanoclusters formed at the end of the synthesis process is essential for efficient scale up of high-rate synthesis methods.

Monodisperse (20-60 nm) unmodified polystyrene nanoparticles and carboxylated polystyrene nanoparticles in water are chosen as systems of study. Using force curves obtained from atomic force microscopy measurements between two polystyrene particles, an interparticle potential is developed. This force field is used in Brownian dynamics simulations under quiescent conditions to characterize morphology in terms of fractal dimension and cluster size distribution, and to determine rate kernels for aggregation and breakage taking place during the simulation.

This work is part of an interdisciplinary project aimed at multi-scale simulation of nanoparticle aggregation for high-rate synthesis methods.