

Models of Synthesis of Colloids, Nanoparticles, and Nanostructures

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We describe recent advances in modeling of processes that lead to the formation of uniform size and shape nanoparticles, as well as nanosize surface structures. Formation of core-shell particles, particle sintering and certain other processes involving nanoparticles have also been modelled by these techniques. A recently developed kinetic Monte Carlo approach is utilized to reproduce growth morphologies realized in recent experiments on noble-metal nanoparticle synthesis and sintering. Specifically, we can identify growth regimes that yield useful particle properties. The developed modeling approach allows us to qualitatively study the effects of temperature and supply atoms on the resulting nanoparticle/nanostructure morphology.

