588b Modeling Spontaneous Formation of Precursor Nanoparticles in Clear-Solution Zeolite Synthesis

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Zeolites are nanoporous alumino-silicates used in industrial applications such as catalysis and separations. Understanding how zeolites nucleate and grow is of fundamental scientific and technological importance. In the past decade, silica nanoparticles have been found to play an important role in zeolite formation from clear solutions. To explore the properties of such nanoparticles, we have developed and applied a lattice model to simulate nanoparticle formation, structure and stability. Silica condensation/hydrolysis is modeled by a nearest neighbor attraction, while the electrostatics are represented by an orientation-dependent, short-range interaction. Using this simplified model, we show excellent qualitative agreement with experimental SAXS andn SANS observations. The nanoparticles are identified as a metastable state, stabilized by electrostatic interactions between the negatively charged silica surface and a layer of organic cations. Nanoparticle size is controlled mainly by the solution pH, through nanoparticle surface charge. The size and concentration of the charge-balancing cation are found to have a negligible effect on nanoparticle size. Increasing the temperature allows for further particle growth by Ostwald ripening. We suggest that this mechanism may play a role in the growth of zeolite crystals.