174g Rational Fabrication of Nano-Electronic Devices Via Bottom-up Self-Assembly

Stephanie L. Teich-McGoldrick, Joydeep Mukherjee, and Sharon C. Glotzer

With the increasing pursuit for smaller dimensions and higher integration densities of functional devices on chips, self-assembly is being explored as a commercially viable fabrication tool. Synthetic chemists are able to synthesize a wide assortment of inorganic and organic nanoscopic building blocks of various shapes (core-shell, rods, tetrapods etc.) with a high degree of monodispersity and with specific inherent functionalities. The key challenge lies in organizing a large number of these functional elements into desirable ordered structures via self-assembly. The self-assembly process involves a complex interplay of geometrical parameters such as particle shapes and energetic parameters such as particle-particle interactions, particle-surface interactions etc. A rational design of the self-assembly process to fabricate precise structures with minimum defects necessitates appropriate tuning of these parameters. We present the results of Monte-Carlo simulations performed to understand the effects of various parameters on the self-assembly process. In particular we have investigated self-assembly of particles of different shapes such as core-shell, Y-shaped X-shaped etc. and with different interparticle interactions. We show that with suitable tuning of the shape and interaction parameters highly ordered assemblies of nanoparticles into 2-D superlattices such as honeycomb and square lattice structures can be achieved. Further, we quantify the degree of tolerance of the self-assembled structures with respect to relevant design parameters.