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Metal-like behavior in nanoparticle assemblies

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Nanoparticles are studied for their tunable uses and properties as individual particles. They can also self-assemble into a wide variety of structures, which further increases potential for different applications. Traditionally, these structures have been static ionic-compound-like lattices where all nanoparticles are fixed at lattice points; however, a set of metal-like phases was recently predicted computationally and observed experimentally. The metal-like phases are composed of two species of nanoparticle, one much smaller than the other and, in these phases, the small particles are delocalized within the crystal, roaming the lattice while still maintaining the structural stability of the crystal. In this talk, I will discuss a simplified computational model we developed to study the transition from the compound-like to metal-like structures, as a function of temperature and other properties. We find that the properties of the nanoparticles determine the overall structure into which they assemble. Some nanoparticle properties simply shift the temperature at which transitions between phases takes place, whereas others play a much more fundamental role in determining the assembled structure.

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