Liquid Crystal Phase Transition in Epitaxial Monolayers of DNA-Functionalized Nanoparticle Superlattices

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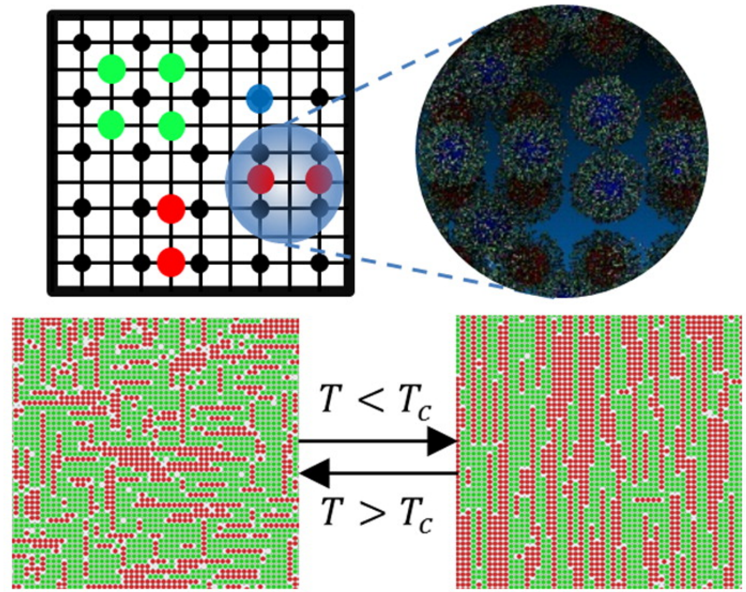
Epitaxial growth of DNA-functionalized nanoparticles is used to grow extended superlattices with a preferred orientation for optimizing the physical properties of metamaterials for real applications. Like any solid in nature, superlattices can contain different kinds of structural defects, which significantly alter their physical properties. Further development of these materials requires a deeper understanding of, as well as precise control over, structural defect formation. Here we use Monte Carlo simulations to conduct a systematic study of the equilibrium structures of the adsorbed nanoparticle monolayers by changing the binding energies of different attachment sites. The simulations show two main results. First, the structural defects form one-dimensional clusters with an exponential length distribution. Second, these linear defects exhibit spontaneous symmetry breaking and undergo a liquid crystal phase transition. Our work demonstrates that defects can be engineered to design two-dimensional superlattices with interesting physical properties.



Top: Schematic diagrams of the MC model (left) and the MD model (right); Bottom: Orientational disordered–ordered phase transition as a function of temperature.

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