Simulations of the self-assembly of CdTe nanoparticles into large pitch helices

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Recent experiments have shown that CdTe nanoparticles can self-assemble into wires, sheets, or helical nanoribbons with a large pitch length (300-400 nm) depending on the amount and type of capping group used. While conventional Monte Carlo simulations of electrically charged truncated tetrahedrons successfully predict the formation of wires and sheets, they are inadequate to describe the formation of helical nanoribbons, which require a large number of particles and a long run time to observe their characteristic features. We use a newly developed energy minimization technique, "bottom up building block assembly," to predict the packing structure of tetrahedral CdTe nanoparticles within the helix. From this packing structure, we construct nanoribbons of various widths and minimize the energy to determine the width of the stable structure. We find the stable width of the ribbon is charge dependent with values that correspond to ribbons observed in experiments.

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