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Quantum and classical simulations of nanowire self-assembly ZHIGANG WU, JEFFREY GROSSMAN, University of California, Berkeley — The ability to control the synthesis of nanostructures such as nanowires and nanotubes is crucial to the success of next-generation nanotechnology devices. One promising approach for efficiently controlling fabrication is to functionalize nanoscale building blocks such that they will self-assemble under the appropriate conditions. We employ a combination of ab initio total energy calculations, classical molecular dynamics (MD), and classical Monte Carlo (MC) calculations to investigate the possible self-assembly of nanoscale objects into chains and wires. The ab initio calculations provide key information regarding selective chemical functionalization for end-to-end attraction and the subtle interplay of the energy landscape, which is then used to fit classical potentials. Using these potentials, MD simulations are carried out to predict short- time (i.e., ps and ns timescales) dynamical properties of nanoparticle assembly as a function of particle shape, chemical functionalization, and temperature. Finally, both static and dynamical data from these calculations are used in MC simulations to predict large time- and length-scale assembly under a variety of synthesis conditions. Our results suggest a new technique for bringing nanoscale objects together to form ordered, ultra high- aspect ratio nanowires.

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