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Efficient method to calculate total energies of large nanoclusters MIN YU, University of Illinois at Urbana-Champaign, RAMPI RAMPRASAD, GAYANATH W. FERNANDO, University of Connecticut, RICHARD M. MARTIN, University of Illinois at Urbana-Champaign — We present a computationally efficient method to calculate total energies of very large nanoclusters based on first principles electronic structure techniques. The total energy of a cluster with well-defined facets can be separated into surface, edge, and corner energies, each a function of the chemical potentials, in addition to bulk contributions. Using density functional calculations we have verified that this separation describes the total energies of fcc Cu and zincblende $CdSe$ polyhedral clusters with up to 256 atoms. The calculated energies are then used to estimate the shapes of stable structures for large polyhedral nanoclusters. For sufficiently large clusters, only the surface and bulk terms survive. This method has been shown to be applicable to stoichiometric as well as non-stoichiometric clusters, containing polar or non-polar surfaces, and we are in the process of calculating the energies of various surfaces using total energy and energy density methods in order to predict equilibrium shapes of clusters as a function of size and chemical potentials.

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