Surface energies of semiconductors by the energy density method
MIN YU, RICHARD M. MARTIN — Energy Density formalism within the first-principles pseudopotential density functional theory has been proposed by Chetty and Martin\textsuperscript{1} in 1990s. Although the energy density function is non-unique, nevertheless integrals over surface regions provide unique results for surface energies, and calculations have been carried out by several groups\textsuperscript{2,3} to study the polar surfaces and interfaces of solid state systems such as GaAs (111) and (111) polar surfaces. In our work, we apply this method to wurtzite CdSe to determine the energy of various polar surfaces such as (0001), (000\bar{1}), and non-polar surfaces such as (10\bar{1}0), (1\bar{1}20), from which we can estimate the equilibrium crystal shape for large nanoclusters. 1. N. Chetty and Richard M. Martin, Phys. Rev. B 45, 6074 (1992). 2. K. Rapaewicz, B. Chen, B. Yakobson, and J. Bernholc, Phys. Rev. B 57, 7281 (1998). 3. N. Moll, A. Kley, E. Pehlke, and M. Scheffler, Phys. Rev. B 54, 8844 (1996).

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