Abstract Submitted
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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[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[2,3] to study the polar surfaces and interfaces of solid state systems such as GaAs (111) and $(\bar{1}\bar{1}\bar{1})$ polar surfaces. In our work, we apply this method to wurtzite CdSe to determine the energy of of various polar surfaces such as $(0001), (000\bar{1})$, and non-polar surfaces such as $(10\bar{1}0), (11\bar{2}0)$, 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. Rapcewicz, 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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