Energy Density Method on semiconductor

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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 make this method work with modern plane wave codes, such as ABINIT[4]. The surface energy of the relaxed GaAs(110) surface is calculated as a test. we plan to apply this on wurtzite CdSe to determine the energy of various polar surfaces such as $(0001), (000\bar{1})$, and non-polar surfaces such as $(10\bar{1}0), (11\bar{2}0)$, and estimate the equilibrium crystal shape for large nanoclusters.

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