

Structure Optimization of Low-Dimensional Quantum Dots via Anisotropic Surface Energy

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Semiconductor quantum dots (QDs) exhibit remarkable photostability, large absorption spectra, tunable emission peaks, and high quantum yields. These features originate from their low-dimensionality. It is necessary to control the shape of QDs because their specific characteristics are normally determined by their particular shape and size. We employed first-principle calculations to identify the optimal structures of CdSe quantum dots and investigated the shape-determining mechanism governing the formation of low-dimensional nanomaterials. The anisotropy of surface energy is a key factor determining the shape of nanomaterials and we suggest how to control their geometry and characteristics by adjusting the surface energy.

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I. INTRODUCTION

For more than 30 years, various semiconductor nanoparticles [1] have been synthesized [2–5] and their electrical [6–8] and optical [9] properties have been dramatically different from those of their bulk counterparts [10]. Semiconductor quantum dots (QDs) are usually described as fluorophores having remarkable photo-stability, large absorption spectra and tunable emission peaks [11, 12]. Furthermore, they have better optical properties with an exceptional resistance to both photo bleaching and chemical degradation. These nanoscale clusters are generally known to show highly size-dependent electronic and optical properties determined by variable energy band gap [13]. These features of QDs originate from their low-dimensional characteristics in nano-length scale. QDs in particular shapes and sizes can exhibit superior optical properties, but energetically favorable structures in nature could be differ-

ent from structures with optimal properties. To manage their performance systematically, it is necessary to explore the underlying characteristics determining the geometric structures associated with their electronic/optical properties.

For cadmium selenide (CdSe) QDs, synthesis Cd precursors, such as $\text{Cd}(\text{CH}_3)_2$ and, CdO, are generally used to synthesize the nanocrystals [2–5]. These precursors are not stable at high temperature and do not directly determine the nanocrystalline shape. However, the strong Cd ligands coordinate the complex with Cd, and this monomer concentration affects the shape step by step. At high temperatures, CdSe grows in a wurtzite (hexagonal) structure which is anisotropic. In particular, the (001) facet of CdSe is highly reactive compared to other facets due to the positively charged Cd ion, all electron-donating ligands in solution, and the dipole moment along the *c*-axis [14–17].

In recent studies by Peng *et al.* and other workers reported that the shape evolution from rods (1D) to dots (0D) occurs through an intra-particle monomer migra-

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