硒化鎘奈米晶粒結構與電子特性之尺寸相關性

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摘 要

奈米晶體對於介在其塊材與分子間的物理特徵具有科學研究與工業技術上引起廣泛的興趣。膠態製備的硒化鎘奈米晶體被使用來研究晶體結構與電子特性對於粒子尺寸的相關性,這是由於它們擁有穩定、可操控且單一分佈的特徵。隨著粒子的尺寸減小,四面體結構的鍵長 R⁽¹⁾顯示出延長而 R⁽²⁾則呈現收縮的行為,此結構上的變形歸因於表面應力以及原子堆疊錯位的平衡恢復。相較於硒化鎘塊材,光電子能譜在束縛能的變化不僅具有奈米晶體尺寸且具有表面包覆的相關性,此現象可由光電子末態效應所描述。此外,由硒化鎘奈米晶體呈現出螢光效率與表面特性的相關性,指示出非輻射結合路徑關聯於無包覆的表面硒原子。

Size Dependence of Structural and Electronic Properties in CdSe Nanocrystals

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ABSTRACT

Nanocrystals are of great scientific and technological interest in various physical properties between bulk and molecule. Colloidally prepared CdSe nanocrystals are used to study the dependence of crystalline structure and electronic properties on particle size, since they possess stable, controllable, and monodispersed characteristics. With a reduction in particle size, the bond length $R^{(1)}$ of tetrahedral structure shows an expansion, while $R^{(2)}$ reveals a contracted behavior; the structural distortion are owed to the increasing surface stress as well as atomic relaxation at the stacking fault. The energy shift of photoemission spectra, with respect to bulk CdSe, has the dependence not only on nanocrystal size but also on surface passivants, which can be described by an effect in the photoemission final state. In addition, CdSe nanocrystals exhibit the relation between photoluminescence efficiency and surface properties, indicating that the nonradiative recombination pathways are associated with the unpassivated surface Se atoms.