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CASTEP Study on Electronic and Optical Properties of Zinc Oxide

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Abstract

We investigate the effect of size on the electronic and optical properties of zinc oxide(ZnO). CASTEP simulations based on density functional theory has been performed to find the band structure, density of states and optical properties of zinc oxide(ZnO) bulk and nanocluster. The results show quantum confinement effect as band structure show discrete lines. The change in band gap has been observed from 0.822 eV to 0.013 eV. Band structure calculations show Fermi level shift towards conduction band. Optical properties display low value of absorption in nanocluster as compared to bulk. ZnO nanocluster show high value of dielectric function compared to bulk. The results demonstrate high response of ZnO cluster in electromagnetic waves.

Keywords: Castep; Electronic; Optical; Zinc Oxide

Abbreviations: ZnO: zinc oxide; 0D: zero-dimensional; DFT: density functional theory; GGA: generalized gradient approximation

Introduction

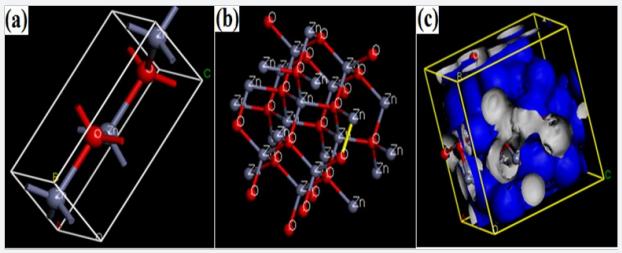

Figure 1: ZnO (a) unit cell (b) Nanocluster and (c) electron density around cluster.

Zinc oxide (ZnO) is a promising direct wide band gap semiconductor, which has many advantages such as good optical, electronic properties and low cost [1,2]. ZnO has received considerable attention as a potential solar material due to its photostability and excellent charge transport [3]. Currently, a significant amount of theoretical research is being devoted to ZnO nanoparticles (Figure 1). In particular, zero-dimensional (0D) ZnO nanostructures such as nanoparticles have attracted considerable attention because they would have improved applications for their large surface-to-volume ratio, controllable shapes and quantum confinement effect [4]. The 0D ZnO nanostructures have been synthesized by various methods and characterized to have some unique properties. In contrast to the large amount of experimental investigations, only few theoretical studies on the nano structural ZnO have been done so far (Figure 2). In this regard, ab-initio calculations have contributed to explore the electronic structures of ZnO nanocluster and bulk for their promising application in building nano devices [5-9]. Theoretically, their structure, electronic, and optical properties have also been investigated.

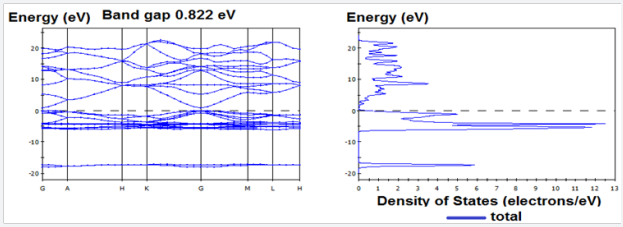

Figure 2: Band structure and density of states of ZnO bulk.

In this paper, we first calculated the band structure, density of states and optical properties of ZnO nanocluster and bulk by using CASTEP code based on density functional theory (DFT) (Figure 3). The electronic and optical properties were calculated with the optimized structures. The photo catalysts are often semiconductors that contain transition-metal or post-transition-metal ions with d0 or d10 electronic

configuration as cations and along with VA or VIA group ions as counter anions [4,10,11]. As a semiconductor of this type, ZnO is a low cost and environmentally friendly material with predominant chemical and physical properties, thus it has been widely used as photo catalyst (Figure 4). So, we also discussed the photo catalytic activity of ZnO nancluster following the part of optical properties.

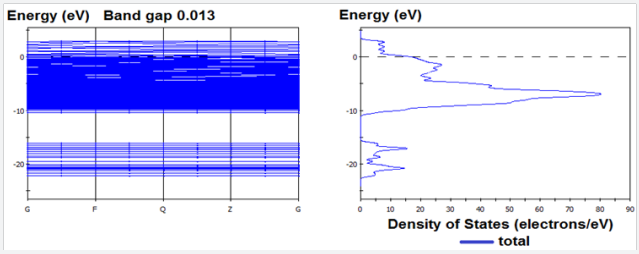

Figure 3: Band structure and density of States of ZnO nanocluster.

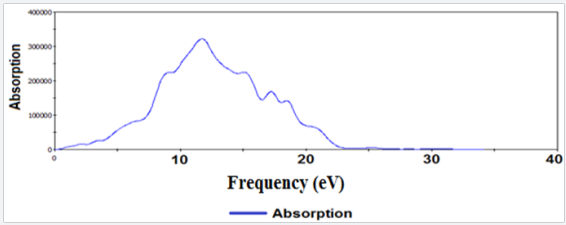

Figure 4: Absorption spectra of ZnO bulk.

Computational Method

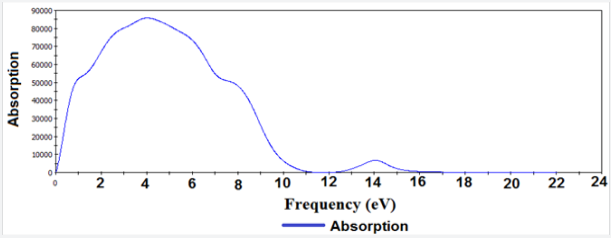

Figure 5: Absorption spectra of ZnO nanocluster.

In the present work, CASTEP module of Accelrys material studio based on density function theory and plane wave pseudopotential method was used to perform simulations [12]. Zinc oxide structure was imported and simulations were performed for band structure, density of states and optical properties. The (Figure 5) shows the imported structure of ZnO, build nanocluster and electron density around nanocluster. The ground state geometries for ZnO were relaxed using CASTEP (Figure 6). With CASTEP, the wave functions of valence electrons were expanded in a plane wave basis set with k vectors within a specified energy cutoff [13]. The core region and valence electrons of the atoms in the super cell of intrinsic ZnO are described within the generalized gradient approximation (GGA), employing the Perdew-Burke-Ernzerhof (PBE) functional form [14] (Figure 7).

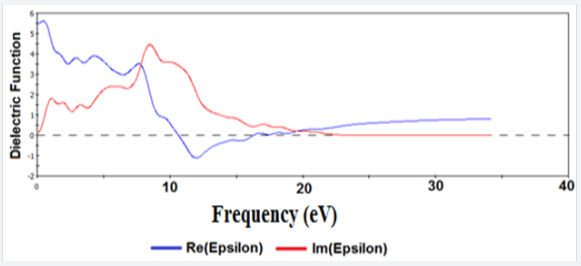

Figure 6: Real and imaginary dielectric Function of ZnO bulk.

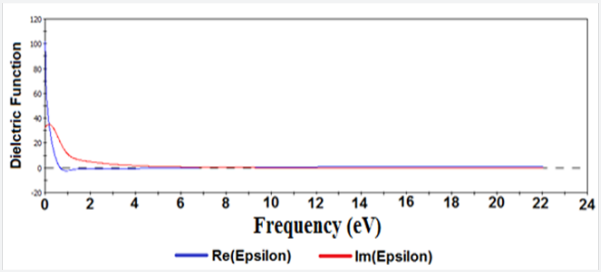

Figure 7: Dielectric Function of ZnO nanocluster.

Results and Discussion

Figure 2 and 3shows the band structure and density of states of ZnO bulk and nanocluster respectively. The results show reduction in band gap from 0.822 eV to 0.013 eV. The band structure calculations of ZnO nanocluster show splitting of energy levels and shift in Fermi level as shown (Figure 8 & 9).

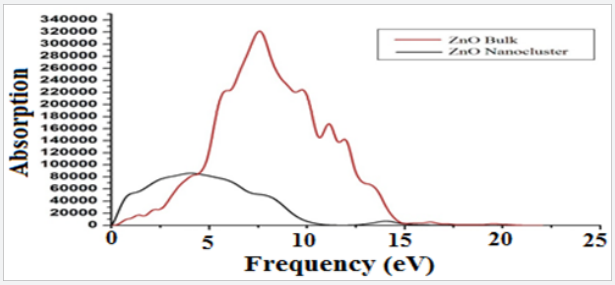

Figure 8: absorption spectra of ZnO bulk and nanocluster.

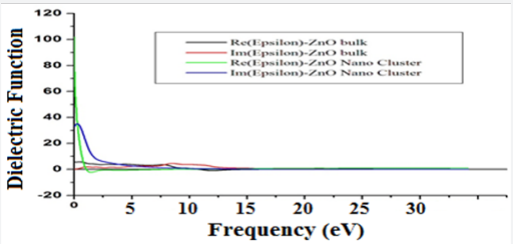

Figure 9: Comparison of dielectric Function of ZnO bulk and nanocluster.

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Conclusion

The CASTEP calculations based on the density function theory (DFT) have been carried out in studying the electronic and optical properties ZnO bulk and nanocluster. The results show reduction in band gap from 0.822 eV to 0.013 eV which means low energy required for transition between valence bands to conduction band. The ZnO nanocluster show low absorption as compared to bulk due to small band gap. The high dielectric function shows good response in electric field. The results show practical applications in nano fluids, photo voltaic sand solar cell.

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