



First-principles investigation of structural, electronic and optical properties of quasi-one-dimensional barium cadmium chalcogenides Ba_2CdX_3 ($X = S, Se, Te$) using HSE06 and GGA-PBE functionals

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ABSTRACT

Structural, electronic and optical properties of quasi-one-dimensional barium cadmium chalcogenides Ba_2CdS_3 , Ba_2CdSe_3 and Ba_2CdTe_3 are studied using density functional theory. Structural properties of these materials are investigated by incorporating Van der Waals correction with PBE exchange correlation functional. Results of structural analysis are in good agreement with the previously reported experimental observations and confirm the quasi-one-dimensional structure of the compounds. Ba_2CdX_3 chalcogenide structures crystallize in orthorhombic phase with space group $Pnma-D_{2h}^{16}$. Band structure calculations with HSE06 show that Ba_2CdSe_3 and Ba_2CdTe_3 are wide bandgap materials with direct bandgap of 2.56 eV for Ba_2CdSe_3 and 2.16 eV for Ba_2CdTe_3 . Ba_2CdS_3 is an insulator with direct bandgap 3.16 eV. Optical properties are investigated by calculating the refractive index, birefringence, dichroism, dielectric function and absorption coefficient using the HSE06 method. Ba_2CdX_3 materials exhibit large optical anisotropy with considerable birefringence and dichroism. The comparatively high values of absorption coefficients, extinction coefficients, birefringence and dichroism make Ba_2CdX_3 materials suitable for applications as polarizers and sensing devices, while the large direct bandgaps indicate that they are promising candidates in photovoltaic applications.

1. Introduction

The compounds Ba_2CdS_3 , Ba_2CdSe_3 and Ba_2CdTe_3 belong to the general group of quasi-one-dimensional barium transition metal chalcogenides with the general formula Ba_2MX_3 ($M = Mn, Fe, Co, Zn, Cd$; $X = S, Se, Te$) [1], which have gained much attention recently due to their applications in solar cells [2], narrow wavelength optical devices [3], thermoelectric materials [4], room temperature γ and X-ray detectors [5,6], xerographic layers [7], scientific instrumentation, optical communication, laser industry and polarimetry [8].

Works on synthesis and analysis of the structural, optical and electronic properties of barium metal chalcogenides Ba_2MX_3 ($M = Cd, Zn$; $X = S, Se$) have been reported earlier [9–15]. These studies have established that these compounds crystallize in orthorhombic phase with space group $Pnma$ [16].

Synthesis of Ba_2CdTe_3 and its structure determination using powder X-ray diffraction data was first done by Y. C. Wang and F. J. DiSalvo in

1999 [16]. They reported that Ba_2CdTe_3 crystallizes in space group $Pnma$ (No. 62) of the orthorhombic system with lattice parameters $a = 9.8198 \text{ \AA}$, $b = 4.7436 \text{ \AA}$, $c = 19.0638 \text{ \AA}$ and is isotypic to Ba_2MnS_3 and K_2AgI_3 [17]. The synthesized structure consisted of one-dimensional ${}^\infty[CdTe_{2/2}Te_2]^{4-}$ chains of corner-sharing $CdTe_4$ tetrahedra running parallel to [010] separated by Ba^{2+} cations. Powder X-ray diffraction data indicated that each Ba atom is coordinated to seven tellurium atoms to form a distorted trigonal prism with one rectangular face capped by a Te atom. Later, Yang et al. synthesized single crystal of Ba_2CdTe_3 through a high temperature metal flux reaction and redetermined its structure from single crystal X-ray data [18]. They confirmed the earlier structure obtained through powder X-ray diffraction (but with some differences in bond lengths) and reported that Ba_2CdTe_3 is isotypic with Ba_2MnX_3 ($X = S, Se$) and crystallizes in the orthorhombic phase with space group $Pnma$ having lattice parameters $a = 9.8405 \text{ \AA}$, $b = 4.7502 \text{ \AA}$, $c = 19.1008 \text{ \AA}$.

Iglesias et al. synthesized single crystals of Ba_2CdS_3 and Ba_2CdSe_3 by

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