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Relativistic effects on the electronic and optical characteristics of $Cd_{1-x}Hg_xTe$ alloys-based solar cell materials

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ABSTRACT

The relativistic effects and compositional dependence on the electronic and optical properties of $Cd_{1-x}Hg_xTe$ alloys are reported by employing *ab-initio* self-consistent calculations based on full potential linear augmented plane-wave method (FP-LAPW) within the generalized gradient approximation (GGA). The electronic and optical characteristics are explored using the GGA combined with the modified Becke–Johnson (mBJ) potential, and spin-orbit coupling (SOC) is also incorporated. The mBJ-GGA + SOC scheme reveals the ability to alter the energy gap for $Cd_{1-x}Hg_xTe$ alloys by manipulating the Hg composition. The alloy undergoes a change from semimetal to semiconducting behavior. An accurate knowledge of the electronic band parameters is crucial in these mixed ternary alloys. For Hg-rich content of 75%, a band gap was found at around 0.15 eV. The direct energy band gap and significant absorption between the infrared and ultraviolet spans would suggest prominent optical activity in these promising systems.

1. Introduction

Among the II-VI semiconductor compounds, cadmium-telluride (CdTe), has received considerable interest because of its various technological applications. This promising semiconductor is suitable for photovoltaic functionalities for two reasons. The first one is the considerable optical absorption coefficient of $10^4\,cm^{-1}$ in the visible solar spectrum due to the direct band gap of CdTe. The second reason is the compound's optimal energy band gap of 1.6 eV for applications in the solar spectrum [1,2]. In the last four decades, this compound has become a prominent photovoltaic material that could be used in thin-film solar cells. This is a breakthrough in terms of solar cell efficiencies, as CdTe-based cells have an optimal thin-film cell performance of 16.5% [3]. Furthermore, these promising systems have valuable sector module efficiencies higher than 11% [2].

On the other hand, recent research works have been focused on the epitaxial processes of mercury tellurides (HgTe) by considering growth temperatures and lattice mismatch. Importantly, the lattice mismatch between CdTe and HgTe is insignificant at around 0.3%, because mercury has a larger atomic size than cadmium. This in turn makes the Hg–Te bond much weaker than the Cd–Te bond, leading to an enormous deviation in their formation energies and concomitant growth temperatures. The compounds CdTe and HgTe both crystallize in a zinc-blende (ZB) structure and constitute a series of alloys as $Cd_{1-x}Hg_xTe$ [3–9], where x represents the molar fraction of CdTe in the respective alloy. The mercury cadmium telluride (MCT) ternary alloys are characterized by the variation of the band-gap energy between 1.60 and −0.3 eV for CdTe and HgTe materials. It is noteworthy that earliest experimental scrutiny of these compounds was in the far infrared, close to the long wavelengths of 5–10 μm (corresponding to compounds with mercury compositions x = 0.7–0.8). Subsequently, $Cd_{1-x}Hg_xTe$ has become the typical compound for the usage in photovoltaic detectors applied to wavelengths in this energy widows [10,11]. Thus, the alteration of the band gap in $Cd_{1-x}Hg_xTe$ from semi-metallic HgTe to semiconducting CdTe, could lead to a practical system for emission in the mid-infrared (MIR) spectral regime. It has earlier been pointed out that CdTe and HgTe compounds can simply interdiffuse [12–17], although the solid solution $Cd_{1-x}Hg_xTe$ occurs for compositions spanning between x = 0 and x = 1. In this case, the variation of the energy band gap as a function of the changing Hg content is obtained using a sample

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