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The first-principle study on wide-gap semiconductor material $CuYO_2$

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Abstract. Using the first-principle method within the generalized gradient approximation, this paper study the bands structure, structural parameters, and state densities of wide-gap semiconductor material $CuYO_2$. The calculated results show that, the valence band of $CuYO_2$ mainly compose of 3d of Cu, and 2p of O; while the conduction band mainly compose of 3d of Y. Through the $+U$ correction, with the increasing of the value of U, the conduction band and valence band of $CuYO_2$ become split, the peak of 3d of Y move towards high energy area, which induce to the enlarge of conduction band area and band gap; in addition, the minimum of conduction band is transfer L point into Γ point when the value of U is 2eV, which show $+U$ method mainly correct the conduction band of $CuYO_2$ so that improve the calculated value of band gap.

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Key words: $CuYO_2$, band structure;first-principle method

1 Introduction

Transparent conducting oxides(TCO) are technologically important material with conduction and optical properties used in in solar cells, flat panel displays, electrochromic mirrors and window, and other optoelectronic devices [1]. The most of TCO such as ZnO, Ln_2O_3, and SnO_2 have n-type conductivity and have been widely applied in industrial materials as new type TCO materials [2–5]. However, without the high merit p-type TCO, the application n-type TCO is rather restricted because the active functions of many optoelectronic elements come from p-n junction. Even so, comparing with many

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n types TCO, P-type TCO is still lack, and the conductivity of p-type TCO is significantly lower than the conductivity of n-type TCO. In order to construct the transparent p-n junctions devices, it is essential to explore new p-type TCO so that the combination of the two types of TCO can be realizable. In 1997, Kawazoe *et al.* found that transparent thin films of copper aluminium oxide $CuAlO_2$ have p-type conductivity [6]. This research result attract attentions of many researchers. $CuAlO_2$ belongs to the family $CuMO_2$, which have $CuFeO_2$ structure, the conductivity is 0.95 S/cm under the room temperature, and Seebeck value is +138(means the materials have p-type conduction) [6,7]. Although the p-type conductivity of $CuAlO_2$ is still significantly low, it still becomes a hope that constructs transparent p-n junction devices in TCO. Since then, $CuAlO_2$ has become an important material, and other $CuMO_2$(Ga, In, Sc, Y, Cr, rare earths, etc) also present p-type conductivity in the last few years [8–14]. Among all the $CuMO_2$ family, $CuYO_2$ has attracted special attentions with wide band gap, in addition, $CuYO_2$ have particular physical and chemical properties due to Y belongs to rare earth element. Extensive experiments studies have been carried out in the past to understand and improve basic properties in the $CuYO_2$ [15–18], relatively little is known regarding its band/electronic structure. In particular, we notice that an *ab initio* investigation of band gap in $CuYO_2$ is still lacking. Only Shi *et al.* [19] investigated the band structure and optoelectronic properties of $CuYO_2$. Shi *et al.* found that the indirect band gap of $CuYO_2$ is 2.63eV by the local-density approximation (LDA) method, while direct optical band gap of $CuYO_2$ is 3.3eV [19]. It is well known that conventional density-functional method such as LDA or GGA (generalized gradient approximation) underestimate the band gap of semiconductor, as a result, fail to capture the accurate band structure of $CuYO_2$ because of ground state methods. These facts, as a consequence, inhibit further understanding of $CuYO_2$. Motivated by this observation, in order to better understand band structure properties of $CuYO_2$, in this study, we modify the intraatomic Coulomb interaction through the $+U$ approaches, in which the underestimation of the intraband Coulomb interaction is corrected by the Hubbard U parameter. It is expected that the present calculated results greatly help explain the structure properties of $CuYO_2$ from a microscopic perspective and can be a guide for applications of $CuYO_2$. The remaining part of this paper is organized as follows. In section II, we present our calculation methods. Section III present and discusses our calculated formation energies and transition energy level. Finally, we summarize the conclusion in Section IV.

2 Calculation methods and atomic model

The calculations are based on density-functional theory within the generalized gradient approximation(GGA) [20] as implemented in the VASP [21] code through the use of the PAW pseudo potentials [22]. In band structure calculations are performed with a four-atom unit cell, and the $4\times4\times4$ Monkhorst-Pack k-point set [23,24] has been used to sample the Brillouin zone. All atomic positions have been relaxed according to the calcu-