Pramana – J. Phys. (2017) 89:11
DOI 10.1007/s12043-017-1399-7

Density functional study of $AgScO_2$: Electronic and optical properties

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Abstract. This paper focusses on the electronic and optical properties of scandium-based silver delafossite ($AgScO_2$) semiconductor. The density functional theory (DFT) in the framework of full potential linearized augmented plane wave (FP-LAPW) scheme has been used for the present calculations with local density approximation (LDA) and generalized gradient approximation (GGA). Electronic properties deal with energy bands and density of states (DOSs), while optical properties describe refractive index and absorption coefficient. The energy bands are interpreted in terms of DOSs. The computed value of band gap is in agreement with that reported in the literature. Our results predict $AgScO_2$ as indirect band-gap semiconductor. Our calculated value of the refractive index in zero frequency limits is 2.42. The absorption coefficient predicts the applicability of $AgScO_2$ in solar cells and flat panel liquid crystal display as a transparent top window layer.

Keywords. Density functional theory; band structure; optical properties.

PACS Nos **71.15.Mb; 71.20.−b; 78.20.−e**

1. Introduction

The wide band-gap delafossites have emerged as a new family of transition metal oxide materials with a number of remarkable electronic and optical properties [1–4]. Among them, copper and silver-based delafossites are of particular interest because they have sufficiently wide band gap and can be used as window layer in a variety of optical devices. The unique feature of this semiconductor family is that they can be combined with N-type semiconductor to form PN junction [1] which can be used as an inner layer of solar cells for electricity generation. This peculiar characteristic has established a benchmark in invisible electronics and opened a new era in solar cell technology [5–9].

Dietrich and Jansen [10] synthesized and reported the 3R phase of $AgScO_2$. Shannon *et al* [11] reported the syntheses of various delafossite families including $AgScO_2$ and provided lattice parameters for the 3R phase. These lattice parameters are converted into 2H-type structure and then optimized by Kandpal and Seshadri using the CASTEP code [12]. They reported the influence of d10–d10 interactions and predicted the candidature of these structures for transparent conducting oxide (TCO) applications. Nagarajan *et al* [13] synthesized a series of compounds like $CuMO_2$ (Sc, Y, Cr, $Fe_{0.5}V_{0.5}$) and $AgMO_2$ (M = In, Sc, Cr, Ga) and reported the conductivity of these compounds. They predicted that Cu-based compounds show higher conductivity than Ag-based compounds. Sheets *et al* [14] synthesized $AgScO_2$ and observed the mixed phase of this compound. They predicted the optical band gap for $AgScO_2$ to be 3.8 eV. They also reported theoretical band gap (2.4 eV) using LMTO method at gamma point of Brillouin zone (BZ) which is in far agreement with the said optical value. Using minima hopping method combined with high-throughput calculations Cerqueira *et al* [15] explored the periodic table in search of novel oxide phases and predicted structure as well as band gap for vaious oxide structures. Cerqueira *et al* [15] reported the band gap for $AgScO_2$ as 2.1 eV which was appreciablly smaller than the band gap calculated by Sheets *et al* [14]. The debate over band gap and limited number of reports encouraged the present investigation on optical and electronic properties of $AgScO_2$.

Published online: 20 June 2017