Solar Energy 193 (2019) 799–805

Contents lists available at ScienceDirect

Solar Energy

journal homepage: www.elsevier.com/locate/solener

Role of $CuAlO_2$ as an absorber layer for solar energy converter

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ARTICLE INFO

Keywords:
Delafossite
Semiconductors
Solar fuel
Optical properties, efficiency

ABSTRACT

A delafossite semiconductor, namely $CuAlO_2$, with a lower band gap is a potential candidate for the absorption of solar radiation due to its excellent electronic and optical properties. In this paper, structural, electronic, vibrational and optical properties of delafossite $CuAlO_2$ have been calculated using state-of-the-art first principles calculations based on density functional theory (DFT). The optimized structural parameters, electronic properties and Raman active vibrational modes namely the E_g and A_{1g} are in good agreement with experimental and other theoretical data. The full phonon dispersion curves (PDC) together with the phonon density of states (PHDOS) of $CuAlO_2$ depict its dynamical stability due to non-existence of any imaginary phonon mode in the entire Brillouin zone (BZ). To understand the mechanism of optical transition properties, we have further calculated the dielectric functions, absorption coefficient and joint density of states (JDOS) for delafossite, $CuAlO_2$. The dielectric constant and absorption coefficient show a significant anisotropic nature in the components of polarization directions. Solar cell parameters of $CuAlO_2$ are also calculated and the highest theoretical efficiencies of 14.8% and 12.5% have been observed with Shockley-Queisser (SQ) limit and spectroscopic limited maximum efficiency (SLME) respectively. The SLME predicted efficiency agrees better to the experimental value as it includes the thickness dependent absorbance coefficient in account of non-radiative recombination and carrier loss mechanism.

1. Introduction

The past few decades were dedicated to the study of transition metal oxides for solar cell applications (Gao et al., 2018). Most of the solar cells and optical devices are based on the n-type materials (Nomura et al., 2002; Park et al., 2006; Popovich et al., 2003). However, applications such as light emitting diode (LED) and functional windows require both n and p-type materials. Recently, the p-type semiconductors are widely studied because they can combine with n-type to form a p-n junction diode useful in many applications including dye sensitized solar cells (DSSCs) (Zhang et al., 2017). The NiO based p-type semiconductor was studied which gives excellent results when combined with n-type materials such as TiO_2 (He et al., 2000; Odobel et al., 2010). However, NiO has some limitations due to its narrow band gap, significant absorption of sun light, and low hole mobility (Nattestad et al., 2010). The p-type semiconductors such as CuO (Sumikura et al., 2008), CuScN (Fernando et al., 1994), have been studied but they hardly show the solar cell power conversion efficiency (PEC). Therefore, the study of new p-type semiconductor materials in the form of complex oxides arises for DSSCs due to its tunable properties (Tan et al., 2007). In this context, copper (Cu) based delafossite type oxides having p-type conductivity are used for DSSCs applications (Ahmed et al., 2014). The Cu based delafossites are expected to have a small band gap due to higher energy valence band (VB) edge arising from d^{10} configuration of Cu^{2+} ions (Tablero Crespo, 2018). Amongst them $CuAlO_2$ with a delafossite structure is a first p-type semiconducting material which is useful in transparent conducting oxides (TCOs) (Kawazoe et al., 1997). Further, many delafossite type structure-based p-type materials such as $CuGaO_2$, $CuFeO_2$, $CuScO_2$, and $CuInO_2$ etc. were developed and their technological importance was highlighted. Among the different materials developed so far, $CuAlO_2$ is most fascinating and attractive delafossite due to the coexistence of p-type conductivity and transparency in visible light. Its different properties and related technological aspects have been investigated by many researchers, (Banerjee and Chattopadhyay, 2005). The lower band gap in $CuAlO_2$ makes it interesting for absorbing the solar radiation in solar conversion, photovoltaics or photoelectrochemical. Further, the delafossite type compounds are useful candidate for DSSCs. Recently, Tablero Crespo (2018) studied the possibilities of $CuFeO_2$ and $CuRhO_2$ as solar cell convertors, by calculating the absorption coefficient. The

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https://doi.org/10.1016/j.solener.2019.09.098
Received 11 April 2019; Received in revised form 27 September 2019; Accepted 30 September 2019
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