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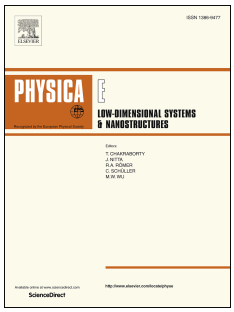

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S. Saidi, S. Zriouel, L.B. Drissi, M. Maaroufi

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A DFT study of electro-optical properties of kesterite Ag_2CdSnX_4 for photovoltaic applications

S. Saidi[1], S. Zriouel[2,3,†], L.B Drissi[2], M. Maaroufi[1]

1- Equipe de Recherche en Energie Electrique et Commande,

Ecole Mohammadia d'Ingénieurs, Université Mohamed V, Rabat, Morocco

2- LPHE, Modeling & Simulations, Faculty of Science, Mohammed V University, Rabat, Morocco

3- Department of Physics, Polydisciplinary Faculty,

Sultan Moulay Slimane University in Beni Mellal, Morocco and

Corresponding authors: † sanae.zriouel@usms.ma

Abstract

Given the importance of quaternary semiconductors in the solar cell applications, we present in this study the interesting structural and electro-optical properties of kesterite Ag_2CdSnX_4 for $X = S$, Se, Te. To accurately and comprehensively investigate the properties of these compounds, we use the full potential linearized augmented plane wave (FP-LAPW) method, based on the generalized gradient approximation (GGA) and the modified Beckee Johnson (mBJ-GGA) as exchange correlation functionals. The total and partial densities of states, the band structures, the band gap values and the linear optical properties namely, dielectric function, absorption coefficient, optical conductivity, reflectivity, refractive index and extinction coefficient are all presented and discussed in details from the photovoltaic aspect. The PBE-GGA and mBJ-GGA results show that the studied compounds possess direct energy band gap situated at the Γ point of the Brillouin zone. Moreover, a number of characteristic behaviors are found, such as the existence of obvious optical anisotropy, the occurrence of the peaks in the optical spectra that are assigned to interband transitions and the high absorption coefficient of $> 10^5 cm^{-1}$ in the visible and ultraviolet energy regions, indicating that kesterite Ag_2CdSnX_4 $(X = S, Se, Te)$ are well suited for use in solar energy-conversion applications.

Keywords: Kesterite Ag_2CdSnX_4 $(X = S, Se, Te)$; FP-LAPW ; Electronic structures ; Optical properties ; Solar energy materials.