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Band Structure and Optical Spectra of Double Perovskite $Cs_2AgBiBr_6$ for Solar Cells Performance

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The present study reports on the electronic band structure and optical properties of $Cs_2AgBiBr_6$ double-perovskite material using a pseudopotential plane-wave method within the generalized gradient approximation. Our results show that $Cs_2AgBiBr_6$ has a good absorption in the visible spectrum region, nevertheless, it has an indirect band gap of magnitude of 1.32 eV. This limits its application in photovoltaics. An alternative is proposed to overcome this shortcoming.

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1. Introduction

Perovskite-type materials have attracted much attention in the field of photovoltaic devices. This is due to their important optical and electronic properties [1–9]. As a matter of fact, the power conversion efficiencies of perovskite solar cells were improved by about 20% in ten years, which makes them comparable with polycrystalline silicon solar cells.

Generally, perovskite solar cells with excellent performance are based on lead which is toxic and are instable [10]. This severely limits their applications in photovoltaics. To overcome this shortcoming, a new generation of perovskites materials such as $Cs_2AgBiBr_6$ was proposed [11–14]. These materials are inorganic, stable, and non-toxic. Besides, they are regarded as useful materials for photovoltaic applications since they were reported to be successfully synthesized [15].

The fundamental properties of perovskite solar cell materials, mainly the electronic and optical properties play a crucial role in the design and fabrication of devices based on these materials. For that, the current contribution attempts to investigate the electronic band structure and absorption coefficient of the double perovskites material $Cs_2AgBiBr_6$ using first-principles calculations.

2. Computational method

The computations realized in this paper are based on a pseudopotential plane-wave method using the CASTEP code [16]. The exchange and correlation potential is described using the generalized gradient approximation (GGA) of Perdew et al. (PBE) [17].

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The plane wave cut off energy is taken to be 1400 eV. The Monkhorst and Pack k-point meshes [18] are used so as to perform the Brillouin zone integrations with a $10 \times 10 \times 10$ special k points mesh.

3. Results and discussion

The electronic band structure is an effective means for studying the electronic and optical properties of semiconductors [19–23]. The accurate knowledge of these parameters is an important information for synthesizing and fabricating devices based on these semiconductors [24–27]. In this regard, the electronic band structure of $Cs_2AgBiBr_6$ double perovskite has been computed using the GGA-PBE approach. Our findings are displayed in Fig. 1. The picture appears to be qualitatively similar to those of other semiconducting materials [28, 29]. A close inspection of Fig. 1 shows the absence of intersection points between the Fermi level and energy bands. This indicates that the material of interest is a semiconductor. By observing Fig. 1, one can note that the valence band maximum is located at the high symmetry point L in the Brillouin zone, whereas the conduction band minimum occurs at the Γ point. This suggests that the material in question is an indirect (L-Γ) band gap semiconductor. The computed magnitude of this band gap is found to be 1.32 eV. As a matter of fact, the nature of the band gap of $Cs_2AgBiBr_6$ limits its application in photovoltaics. In this case, we suggest replacing Bi by In in order to change the nature of the band gap. Work is in progress in this respect and will be reported in due course.

The optical properties of semiconductors are important physical parameters that are required to model quantum structures [30, 31]. Before being absorbed, the incident light of a given wavelength penetrates into a material and travels a certain distance. This distance

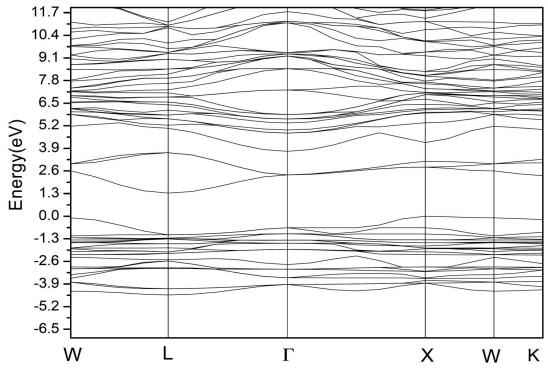

Fig. 1. Electronic band structure for $Cs_2AgBiBr_6$.

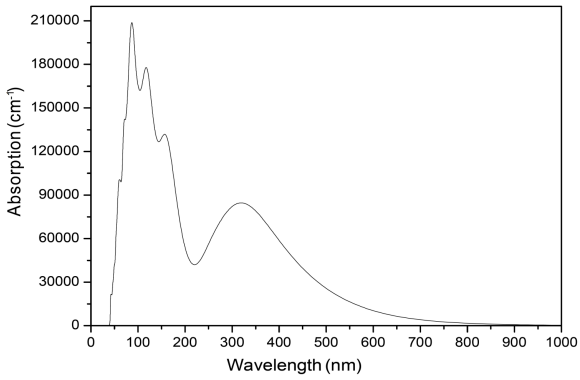

Fig. 2. Optical absorption coefficient spectrum for $Cs_2AgBiBr_6$.

is characterized by a physical parameter termed as the absorption coefficient [32–34]. Figure 2 illustrates the evolution of the absorption coefficient as a function of the photon incident energy. Note that the absorption coefficient is practically null for photon incident energies lower than the fundamental absorption edge and then it increases in magnitude. This is attributed to the increase in the number of electrons which have the energy that permits them to interact with photons. The magnitude of the optical absorption coefficient depends on that of the frequency of the electromagnetic wave. As far as the material of interest is concerned, the latter shows a good absorption of light in the visible spectrum region.

4. Conclusion

The electronic band structure and optical properties of $Cs_2AgBiBr_6$ double perovskite have been investigated using a pseudo-potential plane-wave method within the GGA-PBE approach. The material of interest showed a good absorption in the visible spectrum region. However, its fundamental band gap energy was found to be indirect. This suggests that its application in photovoltaics is limited. We propose to replace Bi by In in order to change the nature of the gap. Work is in progress in this regard.

References

[1] A. Kojima, K. Teshima, Y. Shirai, T. Miyasaka, *J. Am. Chem. Soc.* **131**, 6050 (2009).

[2] R.F. Service, *Science* **344**, 458 (2014).

[3] H.J. Snaith, *J. Phys. Chem. Lett.* **4**, 3623 (2013).

[4] N.-G. Park, *J. Phys. Chem. Lett.* **4**, 2423 (2013).

[5] K.T. Butler, J.M. Frost, A. Walsh, *Mater. Horiz.* **2**, 228 (2015) and references therein.

[6] X. Lu, D. Yang, *Emerg. Mater. Res.* **6**, 234 (2017).

[7] R. Kusum, M. Chhikara, S.P.K. Shishodia, *Emerg. Mater. Res.* **5**, 259 (2017).

[8] N.B. Singh, M. Gilan, D. House, R. Yanamaddi, V. Razdan, B. Arnold, *Emerg. Mater. Res.* **2**, 344 (2013).

[9] H. Sampath, T.I. Jayaraj, R. Oommen, U.R. Parthasarathy, *Emerg. Mater. Res.* **4**, 286 (2015).

[10] A. Walsh, *J. Phys. Chem. C* **119**, 5755 (2015).

[11] Z. Zhang, C. Wu, D. Wang, et al., *Org. Electron.* **74**, 204 (2019).

[12] L. Schade, A.D. Wright, R.D. Johnson, et al., *ACS Energy Lett.* **4**, 299 (2019).

[13] J. Yang, P. Zhang, S.H. Wei, *J. Phys. Chem. Lett.* **9**, 31 (2018).

[14] R. Fu, Y. Chen, X. Yong, Z. Ma, L. Wang, P. Lv, S. Lu, G. Xiao, B. Zou, *Nanoscale* **11**, 17004 (2019).

[15] G. Garcia-Espejo, D. Rodríguez-Padrón, R. Luque, L. Camacho, G. de Miguel, *Nanoscale* **11**, 16650 (2019).

[16] S.J. Clark, M.D. Segall, C.J. Pickard, P.J. Hasnip, M.I.J. Probert, K. Refson, M.C. Payne, *Z. Krist.* **220**, 567 (2005).

[17] J.P. Perdew, K. Burke, M. Ernzerhof, *Phys. Rev. Lett.* **77**, 3865 (1996).

[18] H.J. Monkhorst, J.D. Pack, *Phys. Rev. B* **13**, 5188 (1976).

[19] N. Bouarissa, *Mater. Sci. Eng. B* **86**, 53 (2001).

[20] M.L. Cohen, J.R. Chelikowsky, in: *Electronic Structure and Optical Properties of Semiconductors*, Springer-Verlag, Berlin 1989.

[21] N. Bouarissa, *Phys. Status Solidi B* **231**, 391 (2002).

[22] A. Bechiri, F. Benmakhlouf, N. Bouarissa, *Mater. Chem. Phys.* **77**, 507 (2003).

[23] R.M. Martin, *Electronic Structure: Basic Theory and Practical Methods*, Cambridge Univ. Press, 2004.

[24] N. Bouarissa, *Mater. Chem. Phys.* **73**, 51 (2002).

[25] I. Vurgaftman, J.R. Meyer, L.R. Ram-Mohan, *J. Appl. Phys.* **89**, 5815 (2001).

[26] S. Adachi, *Properties of Semiconductor Alloys: Group-IV, III-V and II-VI Semiconductors*, Wiley, Chichester 2009.

[27] N. Bouarissa, F. Annane, *Mater. Sci. Eng. B* **95**, 100 (2002).

[28] N. Bouarissa, *Phys. Lett. A* **245**, 285 (1998).

[29] L. Hannachi, N. Bouarissa, *Physica B* **404**, 3650 (2009).

[30] F. Mezrag, W. Kara Mohamed, N. Bouarissa, *Phys. B* **405**, 2272 (2010).

[31] S. Saib, N. Bouarissa, P. Rodriguez-Hernández, A. Muñoz, *Physica B* **403**, 4059 (2008).

[32] S. Djaili, A. Gueddim, A. Guibadj, N. Bouarissa, *Optik* **200**, 163421 (2020).

[33] A. Bouarissa, A. Gueddim, N. Bouarissa, S. Djellali, *Polym. Bull.* **75**, 3023 (2018).

[34] A. Khaldi, N. Bouarissa, L. Tabourot, *J. Supercond. Nov. Magn.* **31**, 1643 (2018).