Materials Chemistry and Physics 297 (2023) 127293

Contents lists available at ScienceDirect

Materials Chemistry and Physics

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

Electronic structure, stability, photocatalytic and optical properties of new lead-free double perovskites Tl_2PtX_6 (X = Cl, Br) for light-harvesting applications

Shakeel Ahmad Khandy [a,*], Ishtihadah Islam [b], Kulwinder Kaur [c], Atif Mossad Ali [d,e], Alaa F.Abd El-Rehim [d,f]

[a] ZJU-Hangzhou Global Scientific and Technological Innovation Center, School of Micro-Nano Electronics, Zhejiang University, Hangzhou, 311200, China
[b] Department of Physics, Jamia Millia Islamia New Delhi, New Delhi, 110025, India
[c] Department of Applied Sciences (Physics), Punjab Engineering College (Deemed to Be University), Chandigarh, 160012, India
[d] Department of Physics, Faculty of Science, King Khalid University, Abha, 61413, Saudi Arabia
[e] Department of Physics, Faculty of Science, Assiut University, Assiut, 71516, Egypt
[f] Department of Physics, Faculty of Education, Ain Shams University, Roxy, Cairo, 11771, Egypt

HIGHLIGHTS

- Electronic, photocatalytic and optical properties of lead-free Perovskites Tl_2PtX_6 (X = Cl, Br) are discussed.
- Shrinking gap from 2.37 eV (Cl) to 2.12 eV(Br) due to replacement of Cl to Br anions is observed.
- Exhibit a significant absorption coefficient α(ω) throughout the visible and ultraviolet spectrum (2–6eV) of light.
- Possible photoreduction of CO_2 by Tl_2PtX_6 is observed from simulated HER plots.

ARTICLE INFO

Keywords:
Electronic structure
Semiconductors
Optoelectronic properties
Perovskites
Photo catalysis

ABSTRACT

Metal halide perovskite materials are seamless applicants of photovoltaic and optoelectronic devices. First-principles computational approach is carried out in this work to explore the structural, electronic, and optical characteristics of Tl_2PtX_6 (X = Cl, Br). In structural details, the formation energy (H_f) exposes the studied materials as stable and the tolerance factor along with phonon spectrum decide the stability criterion for the certainty of structural stability of these alloys. The robust p-d hybridization between cations (Pt) and anions (Cl and Br) descent the semiconducting direct band gap from 2.37 eV (Cl) to 2.12 eV(Br), respectively in response to the decreasing size of halide atom. This shrinking gap owed to replacement of Cl to Br anions swings the absorption towards visible region. Also, the possible photoreduction of CO_2 by Tl_2PtX_6 is observed from simulated HER plots. The present materials exhibit a significant absorption coefficient α(ω) throughout the visible and ultraviolet spectrum (2–6eV) of light, which marks the experimental realization of photocell and optical device applications.

1. Introduction

Over the past few years, perovskite device materials have revolutionized the flexible electronics, solar cell fabrication and solid-state battery production as well as their fundamental topographies. In spite of many advantages, hybrid perovskite solar cells have some serious concerns and the main shortcomings, which primarily consist of stability and toxicity [1]. Across-the-board, stability/toxicity concerns need to be resolved and it seemingly hinters the largescale production of these photovoltaics. Stability originating from organic part of hybrid perovskite can be resolved by replacing this portion with inorganic cations. Lead toxicity is therefore being casted off by subsequent ad-atoms like bismuth, germanium, tin, copper and alkaline metal elements (e.g. Ca, Ba, Sr) during the fabrication of organic-inorganic halide perovskite

* Corresponding author.
E-mail address: shakeelkhandy11@gmail.com (S.A. Khandy).

https://doi.org/10.1016/j.matchemphys.2023.127293
Received 23 July 2022; Received in revised form 15 December 2022; Accepted 1 January 2023
Available online 5 January 2023