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Understanding the stability concerns and electronic structure of $CsYbX_3$ (X=Cl,Br) halidoperovskites for optoelectronic applications

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ABSTRACT

Here we discuss the electronic structure and optical properties of Yb based halide perovskites with keen interest on phonon and mechanical stability using the HSE06 approximated density functional theory calculations. The experimental structural parameters are exploited to calculate the semi-conducting band structures with energy gap of 4.32 eV and 3.68 eV for $CsYbCl_3$ and $CsYbXBr_3$ alloys, respectively. Cubic phase stability is guaranteed by the phonon dynamics and machinability of these structures. The observed relaxed structural parameters are in accord with the previous experiments. We found that the present halide perovskite compounds are semiconductors with tuneable band gaps and the f-states of Yb element play a significant role in defining the electronic structure. In addition to this, the sound velocities accompanied by the Debye temperatures (181 K for Cl and 141 K for Br) are evaluated. Furthermore, the dielectric constant optical conductivity, electron loss function, refractive index provide a fundamental basis of the feasible optical characteristics suitable for optoelectronic devices and applications.

1. Introduction

Stability guarantees and intriguing physical properties of high-quality materials are obligatory in smart device productions, e.g. dynamic memories, photodiodes, sensors, solar cells, thermoelectric generators etc. For the same, infinite materials are available but the practical limitations (synthesis, machinability, stability) restrict their use. Thus, time-consuming exhaustive studies undertaken by researchers to find the emergent low-cost materials with quality implications in maintaining the desired properties under extreme conditions are necessary [1–4]. Keeping this in mind, perovskite oxides or halides prove to be a dynamic choice to realize such technical projects [5,6]. These compounds include metal conductors, semi-metals, insulators, half-metals, semiconductors, Weyl or Dirac semi-metals and super conductors [7,8]. And these materials deliver noteworthy physical or chemical properties such as optical, magnetic, catalytic, sensing, ferroelectric, thermoelectric, magneto-resistive and electrode properties for multidimensional features in the field of industry and technology [9,10]. With these properties perovskites compounds are categorized as the desirable materials in driving the multifunctional device applications [11,12]. These innovative properties are linked to the phonon and charge-carrier dynamics or energetic landscapes. In the recent past, numerous theoretical approaches have been put forward to compute the desired properties of these materials. The accuracy of such reports is ascertained by comparing the data sets with experimental results and the methods like density functional approach, molecular dynamics, machine learning etc. are thought-out to be precise and accurate [13,14].

In the present case of $CsYbX_3$ (X=Cl and Br) kind perovskites, only few reports of experiments or theory are available with no discussion on electronic structure, phonon dynamics or mechanical properties [15–17]. *Meyer* in early 70′s reported the cubic structure of $CsLnCl_3$ (Ln=Sm, Eu, Tm, Yb) alloys [17] and his group later

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