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A DFT study of optical, elastic, mechanical, and overall water-splitting photocatalytic properties of pristine and Cd substituted $BaZrO_3$: A lead free environment friendly material

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Abstract

First principle calculations are taken into account to investigate different properties like overall water splitting, elastic, mechanical, optical, electronic, and structural, of pure along with cadmium-induced $BaZrO_3$ which is an oxide-based perovskite. Ultra-soft pseudo-potential is integrated within Cambridge Serial Total Energy Package to explore these properties. Generalized gradient approximation suggested by Perdew-Burke Erzenhoff and hybrid functional is taken into account for exchange–correlation potential. Cadmium introduced at Ba site is more successful rather than Zirconiumas brand new gamma points appeared that also influenced the electronic formation of pure BZO minimized band gap from 3.114–0eV and 4.203–0.470eV by using GGA-PBE and HSE03 respectively. In Cd substitution case, Fermi level shifted to near valence band which reveals property of semiconductor material called p-type before showing conducting behavior at full replacement of Ba with Cd. Furthermore, mechanical properties derived from elastic constants i.e. Bulk modulus, Shear modulus, Young modulus, Poisson ratio, and finally these materials were established to justify born stability requirements. In addition, Cauchy's pressure along with Pugh's ratio also proved brittle nature of these material compositions. We explored and compared optical properties for example absorption spectra, refractive index (3.1), dielectric function, and reflectivity, as an energy loss function of pure BZO in comparison with Cd loaded BZO. Cd based BZO transforms optical performance considerably therefore this material is more effectivefor optoelectronic devices. Overall water splitting was studied for pure and Cd substituted $BaZrO_3$. The pure and two and Six atoms doped material play a vital role for overall water splitting. It is proposed that the said materials are not only lead free for green energy applications in photocatalytic activity but also that the bandgap range is suitable for solar cell applications.

Introduction

Industrial revolutions and utilization of fossil fuel energy pose a very dangerous threat to global environment [1]. Therefore, hydrogen production from abundant water resources is a great concept, which is environmental friendly along with economically eye-catching [2], [3]. Despite many technologies based on electrolysis, thermo-chemical procedure, and bio-hydrogen production via bacteria/algae, have also been engaged in overtime production of hydrogen, for example starting work of Honda and Fujishima based on TiO_2 in the 1970s [3]. Water molecules splitting from a photocatalytic process in visible solar range is still a focus of researchers which is based on solar radiations. Photocatalytic water splitting by using sunlight and reusable photocatalyst material will not only overcome global warming but also have potential to reduce reproduction of unwanted/harmful by-products or toxic waste [2], [4]. Overall water splitting requires a photocatalyst for redox reactions that should proceed by hole reduction and water oxidation. Hence, phosphide, chalcogenide, nitride, numerous solid-state oxide, and carbide materials have been reported in literature [3], [5], [6], [7]. Now researchers are looking forward to Perovskite for Photocatalytic properties.

Hydrogen production via photocatalysis is derived from photo-generated holes and electrons inside the material that swift oxidation along with reduction process. Therefore, photocatalyst efficiency is based on given sites of valance band (VB) and conduction band (CB) edges relative to water redox potential. CB edge value must be lesser than hole reduction potential that is conduction band energy $H^+/H_2 \leq 0$eV; similarly, VB edge value should be greater than oxidation potential of water, that is valance band energy $H_2O/O_2 \geq 1.23$eV. Any material having a bandgap > 1.23eV and a lesser recombination rate for photogenerated electron-hole pairs can be a potential candidate for swift mentioned reactions as performing overall water molecules splitting [8]. An economical and energy-efficient photocatalyst should have superior absorption properties within visible to ultraviolet range of electromagnetic spectra, so plentifully solar radiations can be practised successfully.

Perovskite has gained focus in photocatalysis field because of its larger band edge positions which are also appropriate for reactions involved in photo-induced [9]. Cubic perovskite oxide ABO_3 can be tuned electronic band structure which is appropriate for working in solar radiation electromagnetic spectra [10], [11]. Barium zirconate (BZO) is a potential candidate for water splitting. BZO cubic perovskite doesn't undergo structural change up to 1600K [12]. It has eye-catching attention because of its optoelectronic properties which are tuned via chemical doping at the A-site. BZO have a 3193K melting point [13], good mechanical and chemical properties, high dielectric constant [14], and enlarged bandgap [15]. This makes BZO a potential applicant for many enthralling applications for example crucibles for vacuum induction melting experiments [16], high-temperature proton conduction [17], humidity sensors [18], and solid oxide fuel cells [19] thermal barrier coating for supersonic air jets [20]. Moreover, BZO in a UV range can also perform photocatalyst for hydrogen production without any catalyst [15]. Enhanced photocatalytic activity for BZO has been reported via Ce [21], Ta [22], Mg [23], and Cu_2O/Bi_2O_3 [24] doping.

Including doped BZO, photocatalysis in visible range spectra has not been reported yet. This may be due to CB/VB of BZO having Zr^{-4}d, O^{-2}p phases, and possess a larger energy band gap. Therefore, BZO photocatalysis by solar radiation needs band gap engineering. For this, inclusion of a non-metal with lesser electrons in valence orbit can shift VB [25]. The visible light performance of TiO_2 shows that phosphorous inclusion at the oxygen site can enhance photocatalysis due to its impact on VB edge [25]. This also eliminates uncompensated electronic charges and enhances photoactivity in visible light. Cd-BZO is also suitable for solar cell applications along with other optoelectronic applications because of its band gap engineering. This predicted material will open doors for a new era of optoelectronic devices. In this work different concentration of Cd-$BaZrO_3$ is presented. Trends of bandgap, optical, and elastic properties of all these materials for pure and Cd-induced BZO are also demonstrated. In density of state (DOS), shifting of states

towards high energies is observed. Overall water-splitting efficiency of 2-atoms Cd doped $BaZrO_3$ is very attractive. A detailed discussion on structural, electronic, elastic, mechanical, and optical responses is part of relevant sections.

The following discussion is catalogued as follows. In Section No. 2, computational details of work are described. Next section which is results and discussion completely elaborates on electronic band structures, total and partial density of states, elastic and mechanical properties. Next section carries overall water splitting property. A final section contains optical response against Cd substitution. The last part of this work concludes the achieved research findings.

Section snippets

Computational method

First-principles study has been finalized by using “generalized gradient approximation” (GGA-PBE) along with HSE03 implemented in CASTEP using USP that indeed assists in obtaining swift and precise results and also saves computational cost [26], [27]. Kohn-Sham series of equations engaged to learn outcome of Cd loaded $BaZrO_3$ lying on materials characteristics, for example, structural, optical, electronic, mechanical and elastic [28] At room temperature, structure of pure $BaZrO_3$ is “cubic” which …

Structural analysis

Geometry optimization is completed rooted on supercell of reducing exterior influence well before single point computation for considering different properties like structural, optical, electronic, mechanical, and elastic. Through a proper modification of the Birch-Murnaghan equation of state [34], Lattice parameters are achieved for pure $BaZrO_3$ that are equal to a=b=c=4.243 Å which is taken into consideration as a precise result. Theoretically calculated lattice parameters of our work…

Conclusion

The present work presented substitutional effect of Cd in $BaZrO_3$ at Ba site. Inclusion of Cd showed an impact on different properties like elastic, mechanical, optical, electronic, and structural of $BaZrO_3$. It was concluded that both end materials are cubic in nature and stable as well. $BaZrO_3$ shows a semiconducting behavior with a band gap of 3.114 eV which tends to decrease with an increase in concentration of Cd and final product showed a conducting behavior. With the assistance of total and …

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.…

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Data Availability Statement

We provide readers with information on where they can obtain the research data required to reproduce the work reported in the manuscript.…

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