



Research Article

Modification in photovoltaic and photocatalytic properties of bismuth ferrites by tailoring band-gap and ferroelectric properties

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ABSTRACT

Bismuth ferrite has recently been extensively studied as potential material for photovoltaic and photocatalytic applications as it provides wide opportunity to tune band-gap by site engineering with suitable elements. Further, this doping modified the optical and ferroelectric properties of bismuth ferrite for the applications. Rare-earth (Gd) and transition-element (Mn, Co and Cr) co-doped samples of bismuth ferrite have been synthesized by the sol-gel technique at low temperature. Structural characterization using X-ray diffraction reveals a phase transformation from rhombohedral to orthorhombic with co-doping in pure BFO sample. A reduction of grain size for doped bismuth ferrites samples is observed in SEM analysis. The dielectric properties get enhanced with co-doping due to decrease in the Fe^{2+} ions and oxygen vacancies. Increase in the remnant polarization was obtained in doped BFO samples and maximum $P_r \sim 1.615 \mu\text{C}/\text{cm}^2$ for Gd doped BFO sample. Decrease in band-gap values with doping has been observed from (2.35–1.90 eV). Power conversion efficiency has been calculated with doping of different substances which results in improved photovoltaic properties with respect to pure BFO ($\eta\% \sim 0.00039\text{--}0.026$). Also, photocatalytic studies have been done for all the samples of BFO. Enhanced values of photocatalytic efficiency ($\eta\% \sim 90.89\text{--}96.08$) has been observed with co-doping of rare earth and transition elements in bismuth ferrites. Thus, co-doping of rare-earth and transition-element in bismuth ferrite can improve multiferroic, ferroelectric, photovoltaic and photocatalytic properties for different applications.

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1. Introduction

The increasing global energy crisis and environmental issues related to fossil fuel usage poses a need to develop newer and unconventional sources of energy. Solar energy is considered as clean, pollution free, and renewable resource of energy. It provides a reliable and effective way for solving the problem of energy crises and environmental protection. Photovoltaic power generation and Photocatalytic mechanism is a key way to utilize natural source of light i.e. solar energy [1,2]. Photovoltaic power generation generally utilizes two step processes: (1) with the absorption of light (photons) electron-hole (e-h) pairs are generated and (2) electron-hole separation to generate voltage [3]. Silicon based solar cells has

occupied most of the market and crystalline silicon solar panels have been commercialized due to their high and stable power conversion efficiency (> 26%). One of the major drawbacks of silicon based solar cells is high manufacturing and installation costs [4,5]. Moreover, these solar cells have some limitations [10,11] as (1) small band-gap value limits absorption of light, major part of light is not utilized which may result in low open-circuit voltage (Voc); (2) photo-generated electrons and holes can't be separated efficiently (or recombination rate is more), which results low value of short-circuit current (Jsc); (3) their power conversion efficiency (PCE) is limited by the Shockley-Queisser limit (limit of maximum solar conversion efficiency that can occur in the band gap value of Silicon, 1.1 eV), which limits the conversion of incident light only to 33.7%. As a result, other solar cells such as organic-inorganic hybrid perovskite solar cells, amorphous silicon solar cells, dye-sensitized solar cells, quantum dot solar cells, organic solar cells, ferroelectric based solar cells etc. have been extensively studied [6–9] but could not resolved above mentioned issues. Therefore, ferroelectric (FE) photovoltaic

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