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Synthesis of $Sr_{1-x}Ba_xBi_2B_2O_7$ glass ceramics: A study for structure and characterization using experimental techniques and DFT method

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ABSTRACT

In this investigation, the synthesis of glass ceramics of $Sr_{1-x}Ba_xBi_2B_2O_7$ (for $0 \leq x \leq 1.0$) and its structural, morphological and vibrational properties are presented. $Sr_{1-x}Ba_xBi_2B_2O_7$ glass ceramics are fabricated through standard melt-quenching method followed by annealing at temperatures below its glass transition temperature. The fabricated glass ceramic compounds are studied through X-ray diffraction technique for the structural characterization where the glass like nature with an indication of crystalline peak is observed. There is a shift in the observed peak with the increase in the barium concentration indicating the changing local crystal lattice parameters. The samples were studied through Scanning Electron Microscopic imaging to visualize its morphology, where it is evident that large grain are grown indicating mixed glassy and crystalline nature. The structure of synthesized glass ceramics was determined using quantum chemical calculations carried out by density functional theory (DFT) employing B3LYP functional in conjunction with SDD basis set. FTIR and Raman spectra were recorded and vibrational analysis of these materials was made using potential energy distribution (PED) obtained in DFT computations. NLO behaviour and HOMO-LUMO energies of these glass ceramics were also evaluated.

1. Introduction

Glasses play a vital role in designing solid state electronic and ionic devices, such as wave guides, lasers, magneto-optic couplers, fast ion-conductors, optical switches, etc. They are supercooled liquids which are transparent and amorphous in nature. They are formed by fusion without any crystallization. The important difference between glass and crystal is the existence of long-range order in the crystal structure [1]. The characterization of glasses as a function of composition and other properties needs a comprehensive knowledge on their microscopic structure. For the past few decades, glasses have been focussed to explore the different materials suitable for prominent applications as electrochemical, electronic, electro-optic and magneto-optic devices. Borates, a class of such glasses, are great resources for functional materials, mainly for non-linear optical (NLO) application devices. They are easily quenched for a wide range of composition with alkali content, and continuation variations of their structure and properties [2]. Borate glasses containing alkaline earth oxides along with ZnO, PbO, TeO_2, Bi_2O_3, MgO, CaO, SrO and BaO as glass modifiers are appropriate materials for being designed to meet the applications in the areas of optical communications, laser hosts, optical filters, X- and γ-ray absorbers, photonic devices, etc. [3–9]. Tellurate-borate glasses have been paid much attention due to their ability to host the rare earth elements for the development of fibres and lasers for telecommunication applications [10] and promising materials suitable for optical switching devices [11]. Glasses, containing Bi_2O_3, have been paid attention due to their enormous applications in glass ceramic field as layers for optical and optoelectronic devices, thermal and mechanical sensors, reflecting windows, etc. [12,13]. They are extensively used as lead-free sealing for sensors, solar cells and opto-electronics [14–16]. Bismuthate

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