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Optical and structural characterization of (Mn, Fe) codoped lead chalcogenides for optoelectronics applications

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Abstract

Lead chalcogenides (LCs) exhibit non-stability and lower device efficiency due to smaller bandgap (Eg) leading to poor optical properties for photovoltaic (PV) applications. In this work, optical properties of transition metals (TMs) such as (Mn and Fe) co-doped with LCs especially PbS in the framework of

DFT+U (8 eV) and L/APW+lo method are theoretically investigated to predict new optical material for photovoltaic and other optoelectronics applications. The XAFS spectroscopy technique was used to analyze electronic structures and optical properties of (Mn, Fe) co-doped LCs. Midgap states of co-doped PbS reveal to improve the absorption of infrared light mainly due to slight doping with TMs. Compared to pure PbS, Mn doping in PbS induces Eg widening, blue-shift, and improve the light absorption edge. Due to co-doping, the magnetic order is translated that can lead to forming a charge compensated system which is beneficial to minimize vacancies related to defects formation.

Author keywords

(Mn; Fe) co-doping; Lead chalcogenides; Light absorption edge; Optical property

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