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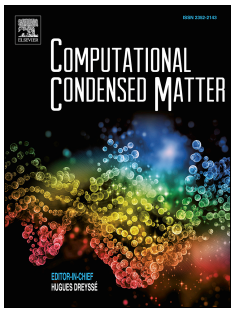

Cation modified A_2(Ba, Sr and Ca) $ZnWO_6$ cubic double perovskites: A theoretical study

Rajneesh Chaurasiya, Sushil Auluck, Ambesh Dixit

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Cation modified A_2(Ba, Sr and Ca)$ZnWO_6$ cubic double perovskites: A theoretical study

Rajneesh Chaurasiya[1], Sushil Auluck[2], Ambesh Dixit[1,#]
[1]Department of Physics & Center for Solar Energy, Indian Institute of Technology Jodhpur, 342037, India
[2]National Physical Laboratory, Delhi, India
[#]ambesh@iitj.ac.in

Abstract:

The cubic double perovskites A_2ZnWO_6 (A = Ba, Sr and Ca) are studied to understand the effect of A cation site, using the density functional theory (DFT) based full potential augmented plane wave method (FP-LAPW) with GGA and mBJ exchange correlation potentials. The structural robustness and stability are investigated using the bond lengths and the total energy. The band structure and density of states suggest that all these cubic double perovskites are indirect wide band gap semiconductors. The band gap varies from 3.90 eV (2.97 eV) for Ba_2ZnWO_6 system to 3.40 eV (2.8 eV) for Ca_2ZnWO_6 system using mBJ (GGA) exchange correlation potentials. Our studies suggest that cation site modification has a strong effect on physical and electronic properties, in contrast to the structural robustness. The lattice parameter decreases from 8.19 Angstrom to 7.9 Angstrom from Ba to Ca at alkali cation site and the electronic band gap variation follows the common cation rule. The charge densities show enhanced localization of charges near the zinc and oxygen sites with increasing alkali cation atomic radii. In addition, we discuss the impact of A site cation modification on the dielectric and optical properties for A_2ZnWO_6 double perovskites.

Keywords: Density Functional Theory, Double perovskite, Band structure, Density of states, Dielectric constant, Reflectivity, and Optical spectra.