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Structural, electronic, mechanical and thermodynamical properties of some double Perovskite oxides: A DFT calculation

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Recently, perovskites have been investigated with great attention both theoretically as well as experimentally in physics, chemistry, and material science because of their variety of applications in science and technology. The double perovskites are very important members of this diverse perovskite family having different structures, composition and physical properties in the fields of spintronics, multiferroics, half metallic, ferromagnetic, magneto-dielectric, and magneto-optics [1,2]. Magnetically, double perovskite family exhibits a wide range of magnetic behaviours[3]. Full-potential linearized augmented plane wave (FP-LAPW) method based upon density functional theory (DFT) as employed in WIEN2K has been used to calculate structure, electronic, magnetic and thermodynamical properties. Structural investigation has been carried within GGA scheme of PBE. For electronic (Fig.1a), magnetic and mechanical investigations GGA, GGA+U, mBJ approximations have been employed. These perovskites occupy cubic structure with space group Fm-3m (225). Most of the double peroveskites show ferromagnetic nature and if spins are plotted, interestingly, they show half-metallicity, which make these materials application in spintronic devices. Further, electronic band profile of these materials depicted another feature used in indirect band gap semiconductors. The mechanical properties like Young's modulus (Y), Poisson's ratio (n), Bulk modulus (B) and Shear modulus (G) have been also calculated from the value of elastic constants. Furthermore, temperature and pressure dependent thermodynamic properties have also been calculated within quasi-harmonic Debye approximation. We have plotted specific heat at constant volume (Cv) in Fig1b, thermal expansion (a), Grüneisen parameter and Debye temperature. The Debye temperature can be used in describing the excitation of phonons and to designate various lattice thermal phenomena while the Grüneisen parameter explains the phonons contribution to specific heat.

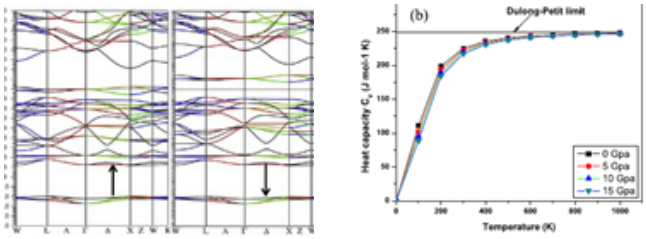

Fig.1 (a) Band structure along high symmetry directions showing half-metallic nature (b) variation of Cv under temperature reaching to Dulong-Petit limit Ba2CdOsO3