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Comparative study and first principle calculations of the halide perovskite CsSnBr3

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Perovskites are very interesting for applications such as optoelectronic devices emitting light, such as OLEDs and lasers. On the other hand, one can consider using these perovskites in a very special architecture: the tandem cells. The principle of these tandem cells is to put in series two types of absorbers to optimize the absorption of the solar spectrum and thus increase the efficiency of the cells: the perovskites could make it possible collection to increase the UV part of the solar spectrum. Many perovskite crystals (ABX3) have been discovered to present second order properties for NLO, they undergo phase transitions in which they transform into slightly disordered original crystals. Perovskite crystal $CsSnBr_3$ undergoes three successive phase transitions at T=19.1 and 26°C respectively. The crystal symmetry is sequentially transformed from rhombohedral to monoclinic then to cubic with a decreasing temperature, and this phase transition influences the structural properties and consequently the electronic and optical properties of this material. The results found for the perovskite cubic structure has been compared with experimental values and other theoretical works and they are in good agreement, but concerning the monoclinic structure, our results consist of a prediction. The calculation of the electronic properties shows the semi-conductor character of this material since there is a small spacing of the valence electron (Br-4p5) and conduction (Sn- 5p2) bands which is estimated at Eg=0.5375 eV in the cubic structure. This gap energy plays a key role in evaluating the use and yield of this material in solar cells.

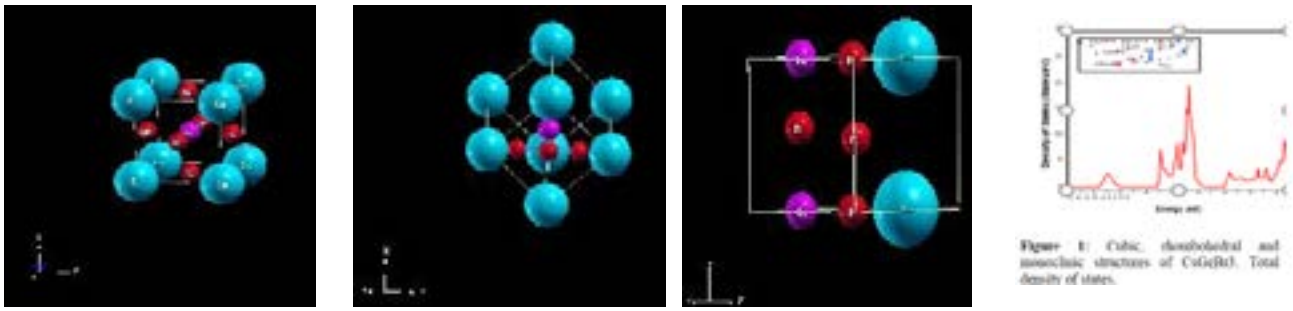

Figure 1: Cubic, rhombohedral and monoclinic structures of CsGeBr3. Total density of states.

Recent Publications:

1. L C Tang et al. (2005) New infrared nonlinear optical crystal synthesis, structure and powder second-harmonic generation properties. J. Phys.: Condens. Matter. 17(46):7275.
2. P Ren, J Qin and C Chen (2003) A novel nonlinear optical crystal for the IR region: noncentrosymetrically crystalline CsCdBr3 and its properties. Inorg. Chem. 42:(1)8-10.
3. U Schwarz et al. (1996) Effect of pressure on the optical-absorption edges of CsGeBr3 and CsGeCl3 Phys. Rev. B 53(19):12545.
4. D K Seo et al. (1998) Pressure-induced changes in the structure and band gap of CsGeX3 (X=Cl, Br) studied by electronic band structure calculations. Inorg. Chem. 37(3):407-410.
5. M Mori and H Saito (1986) An X-ray study of succesive phase transitions in CsSnBr3. J. Phys. C 19(14):2391-2401.

Biography

Karima Benyahia pursued her PhD from the University of Sidi Bel Abbes, Algeria and postdoctoral studies in the Department of Physics at the Galileo Gallile University of Padova, Italy and in the Chemistry Department, SINTEF, Oslo. Norway. She is mainlly interested in materials for solar cells.

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