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Ab-initial study of the electronic structure and optical properties of the BaY_2F_8 pure

J. M. Dantas[(1)] and M. V. Lalic[(1)*]

(1) Universidade Federal de Sergipe, Av. Marechal Rondom S/N, São Cristovão, Brasil, e-mail: mlalic@fisica.ufs.br

* Corresponding author.

Abstract – Ab-initio calculations based on density functional theory have been employed to study the electronic and some optical properties of barium yttrium fluoride (BYF). The band gap was calculated to be 7.5 eV. The total electronic density of states (Fig. 1) revealed that the top of the valence band is dominated by the fluoride *p*-states, while the bottom of the conduction band has predominantly yttrium and barium *d*-states. And the optical properties was analyzed in the ultraviolet region up to 40 eV).

Fluorides are an important class of crystals that show atypical physical and chemical characteristics: low phonon energy, low refraction index and wide-in-wavelength transmission region. These features, together with the spectroscopic characteristic of rare earths and transition metals used as doping ions, make these crystals particularly appealing for laser and frequency conversion applications [1]. Barium yttrium fluoride, BaY_2F_8 (BYF), is a very attractive material thanks to its low phonon energy ($\hbar\omega$ ~ 350 – 380 cm^{-1} [2]) and it has been widely investigated as active material for solid-states lasers. Recently, the BaY_2F_8 doped with rare earth has been the subject of numerous studies because of its properties scintillation.

The BYF has a monoclinic crystalline structure with C_{2h}^{3} (C2/m) symmetry group [3]. This work has the objective to study theoretically the electronic structure and optical properties of the pure BYF crystal. The self-consistent band-structure calculations were performed by density-functional theory based, full potential linear augmented plane wave (FP-LAPW) method as embodied in WIEN2k computer code. The crystal structure was calculated and converged with the forces between the atoms very small, maintaining the equilibrium in the structure.

The result shows that the band gap was calculated to be 7.5 eV. The electronic structure calculations revealed that the top of the valence band is dominated by the fluoride *p*-states, while the bottom of the conduction band has predominantly yttrium and barium *d*-states. The optical properties of the BYF pure (absorption spectrum, refractive index, extinction coefficient, reflectivity and electron energy loss spectrum) was analyzed in the ultraviolet region (up to 40 eV). These properties were interpreted in terms of the calculated electronic structure and results discussed and compared with available experimental data.

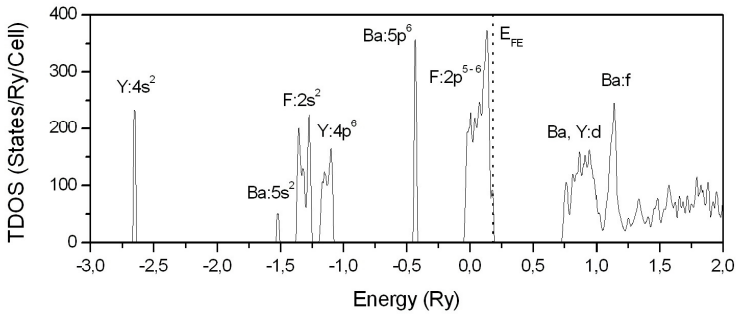

Figure 1: Total density of electronic states of the pure BYF. Dashed lines denote Fermi levels.

References

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