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# Electronic and Optical Characterization of Doped $Al_2O_3$ Composite: A Study of First Principles.

J. M. Dantas(1), A. F. Lima(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 yttrium (Y), scandium (Sc), zirconium (Zr) and niobium (Nb) doped α-$Al_2O_3$ with corundum structure. The Y and Sc presence preserve the band gap value and increase slightly the dielectric constant of the pure alumina, thus showing a potential to be used in semiconductor industry. Doping with Zr elevates and with Nb decrease the static constant of the pure alumina, but changes significantly its band offset.

Due to the large number of application in science and technology the $Al_2O_3$ (alumina) has been study in yours pure form and also has been doped by various chemical elements. The alumina can crystallize in various structures, depending on the conditions of growth of crystals. The structure more stable (less energy), more common and more important in practice is the structure of corundum, annotated be alpha-$Al_2O_3$. During the last few decades the corundum has been widely studies theoretical and experimentally.

The semiconductor industry in the last years has been searching for a material which could substitute the silicon dioxide ($SiO_2$) in order to construct a new type of dielectric gate in transistors. These transistors could be isolated (dielectric) for stop the passage of the electrical currents in the electromagnetic field. The new material should meet two fundamental criteria: it needs to possess a wide band gap and a high dielectric constant at the same time. Various studies indicate the alumina as one of the most promising candidates for such a substitution [1]: it has a wide band gap, similar band offset as the $SiO_2$ and high dielectric constant ($\kappa$ = 9), which can be elevated even more by appropriate doping of the pure material.

In 2002 the theoretical study of Haverty et al [2] showed that a presence of certain transition metals (Y, Sc) in the alumina with orthorhombic structure (κ-$Al_2O_3$) maintains the gap value and increases the dielectric constant, while the presence of others (Zr, Nb) diminishes the gap. In 2003 these theoretical predictions have been confirmed by Lee et al [3], who studied experimentally the amorphous alumina doped with Y, Sc, Zr and Nb.

The results indicate that the Y and Sc presence preserve the band gap value and increases slightly the dielectric constant of the pure alumina, thus showing a potential to be used in semiconductor industry. Doping with Zr elevates and with Nb decreases the static dielectric constant of the pure alumina, but changes significantly its band offset.

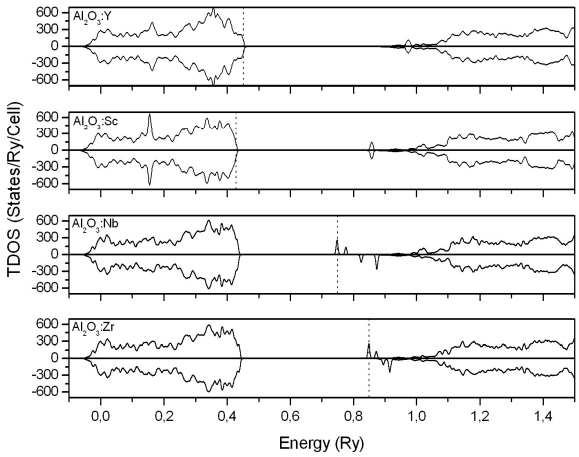


**Figure 1:** Total density of states spin polarized of the alumina doped with Y, Sc, Nb and Zr. Dashed lines denote Fermi levels.

## References

[1] J. Robertson, J. Vac. Sci. Technol. B, 18 (2000) 1785.
[2] M. Haverty et al, Appl. Phys. Lett. 80 (2002) 2669.
[3] J. J. Lee et. al., Appl. Phys. Lett. 83 (2003) 5226.