Título:

Density Functional Theory for the study of the physical properties of Fe_3O_4 and $CoFe_2O_4$

Abstract:

We present a computational study based on the Density Functional Theory (DFT) on the optical, magnetic and density of states (DoS) properties of Fe_3O_4 and $CoFe_2O_4$. Using ab initio calculations, we analyze the electronic structure, the optical transitions and obtain the structural and magnetic ground states. Furthermore, we investigate the DoS to understand the distribution of electronic states in the valence range energy and describe the orbital hybridization between the atoms.