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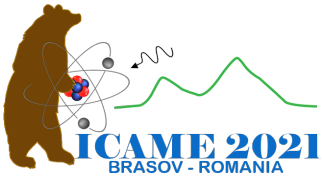

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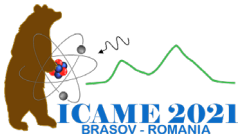

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AB INITIO STUDY OF $FeAl_2O_4$ AND Fe_2AlO_4: ANALISYS OF STRUCTURAL, MAGNETIC AND HIPERFYNE PROPERTIES

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Oxides with the spinel structure are of great interest in different fields. In these oxides the electronic and magnetic properties are very sensitive to structural changes or to the presence of defects such as cation inversion, scale factors, or oxygen vacancies. These defects are at the origin of the incredibly wide variety of behaviours and properties that these oxides present, making it excellent candidates for applications as photovoltaic devices, lithium-ion batteries, photocatalysis, medical applications, etc., [1]. The continuous theoretical and experimental studies of oxides with the spinel structure has allowed in the last decade great advances in the understanding of the relationship between the structural and electronic changes at the nanoscale and the underlying mechanisms which activate the observed properties [2].

As in other systems, the properties of the spinel oxides are strongly related to the synthesis conditions. In the particular case of Al-Fe-O spinels the thermodynamical conditions are an important factor in the final atomic arrangement [3]. Depending on Fe/Al concentration two types of spinel structures can be formed: $FeAl_2O_4$ (Fe aluminate) and Fe_2AlO_4 (aluminium ferrite). The objective of the present work is to study from first principles calculations the structural, electronic and magnetic properties and the hyperfine interactions at the Fe sites in both systems. The main objective is to identify the lowest energy distributions of cations in the two cationic sites of the structures and the spin configuration of each system. The comparison between the calculated hyperfine parameters at the Fe sites and ^{57}Fe Mössbauer experimental result will be used to confirm our structural and magnetic model for each structure. The theoretical study was carried out using the Density Functional Theory (DFT) based first-principles Full-Potential Linearized Plane-Wave (FP-LAPW) method as implemented in the code Wien2k [4], in the framework of the generalized gradient approximation (GGA) + U formalism. To obtain the lowest energy structures for each system different Fe and Al distributions in the cationic sites and different spin configurations were considered. The results obtained allow us an analysis of the degree inversion in both Fe-Al-O compounds, the magnetic moments and the changes in the hyperfine parameters going from the Al-ferrite to the Fe-aluminate. Our results are also compared with different experimental results reported in the literature.

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