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THEORETICAL-EXPERIMENTAL STUDY OF THE STRUCTURAL, MAGNETIC AND ELECTRONIC PROPERTIES OF THE MATERIAL $LaFe_{0.5}V_{0.5}O_3$

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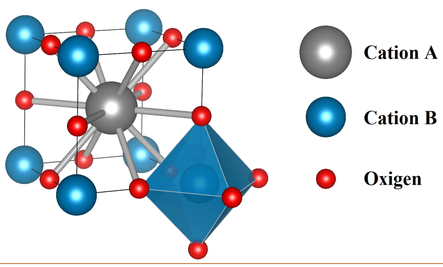
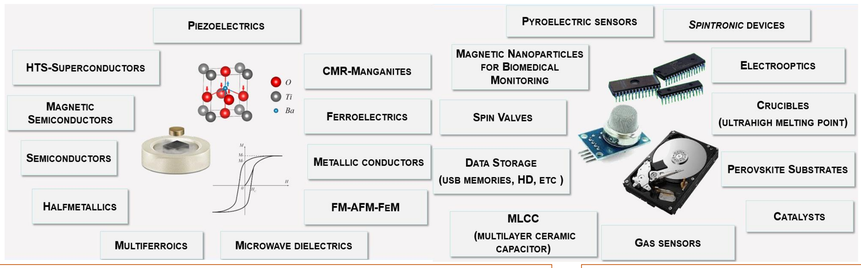
ABSTRACT

The extensive range of applications for materials structured in the perovskite formation (ABO_3) propels an ongoing exploration to alter their properties using varied synthesis techniques and cationic substitutions within the A and B positions. The diversity inherent in these structures emerges from their structural flexibility, a consequence of octahedral rotations and potential cationic displacements. This study involved the synthesis of polycrystalline $LaFe_{0.5}V_{0.5}O_3$ samples through the gel-assisted combustion synthesis method. Structural analysis via X-ray diffraction (XRD) and Rietveld refinement indicated that the material crystallizes within a primitive orthorhombic structure, falling under the Pnma space group (#62). The material's magnetic response was assessed through DC magnetic susceptibility measurements across a temperature range of 50 K to 350 K, as well as magnetization concerning the magnetic field. These analyses revealed an antiferromagnetic behavior, potentially accompanied by a small ferrimagnetic phase, which was attributed to shape anisotropies occurring during the material's synthesis. Furthermore, the electronic properties were explored via Density Functional Theory (DFT). The analysis demonstrated the material's conductive nature and identified the antiferromagnetic phase, specifically in the T-AFM configuration, as the most stable. Finally, the observed coexistence of a minor ferrimagnetic phase aligned with the experimental findings.

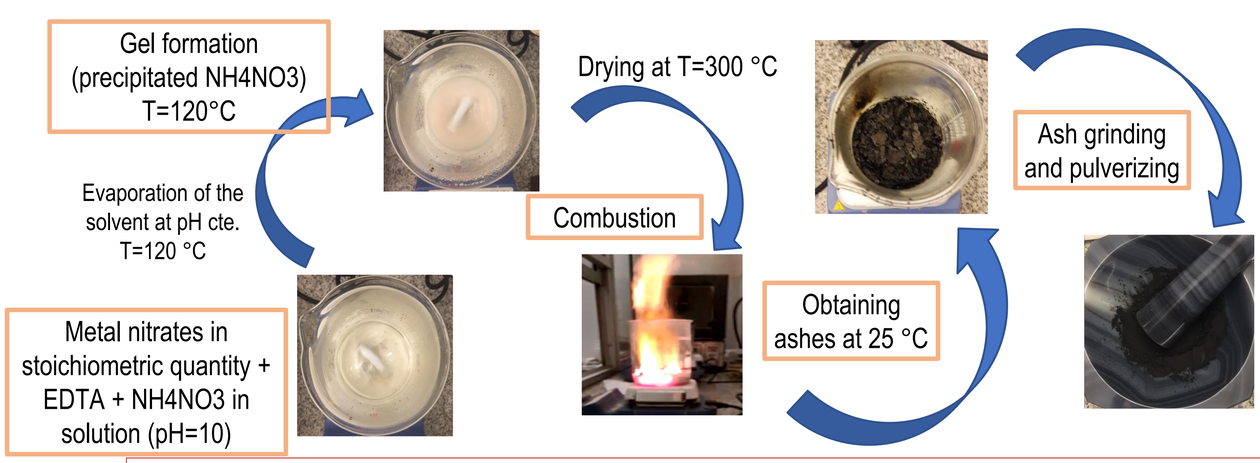
INTRODUCTION



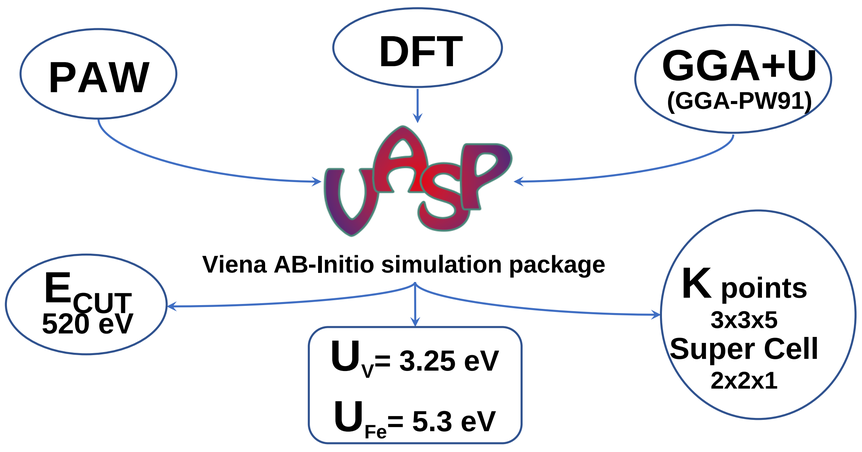


The family of binary oxides with a perovskite-type structure with the general formula ABO_3 has been one of the most studied materials today due to the numerous applications possibly attributed to the structural characteristics and the diversity in magnetic behaviors.

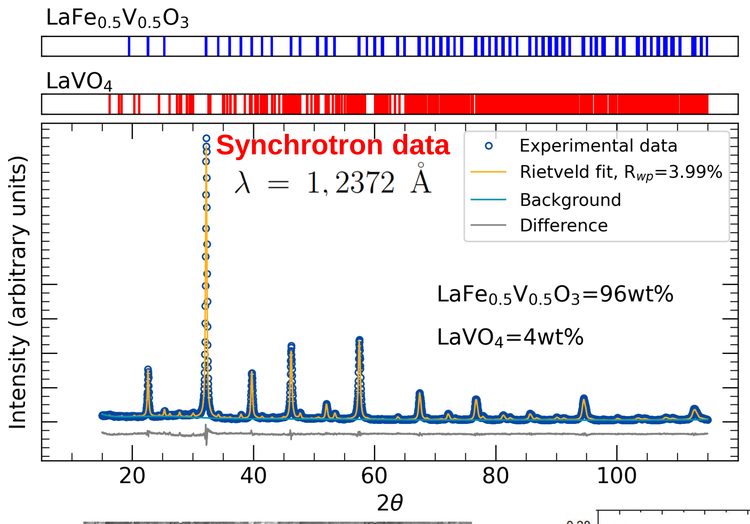
AUTOCOMBUSTION GEL ASSITED METHOD



THEORETICAL CALCULATIONS



DRX, SEM AND MAGNETIC RESPONSE



The $LaFe_{0.5}V_{0.5}O_3$ material crystallizes in a primitive centrosymmetric orthorhombic structure, with a space group Pbnm (#62)

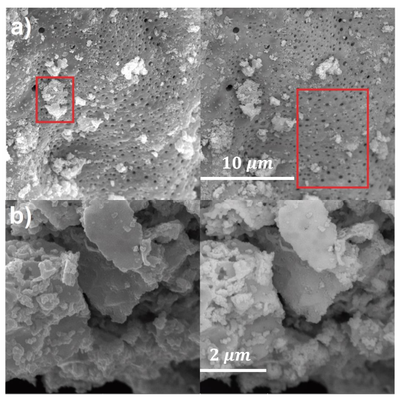
Lattice parameters

a (Å)	b (Å)	c (Å)
5,5598(4)	5,5494(5)	7,8394(6)

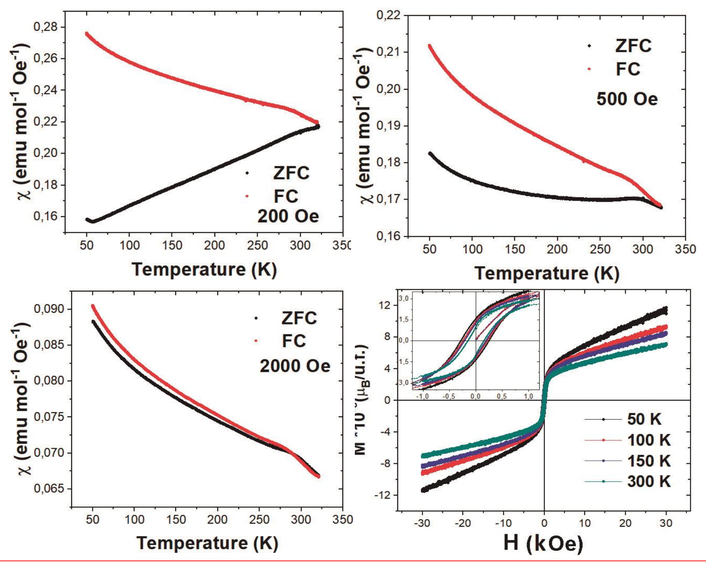
Refinements parameters

χ^2	R_{wp}	R_E
1,31	9,43 %	7,02 %

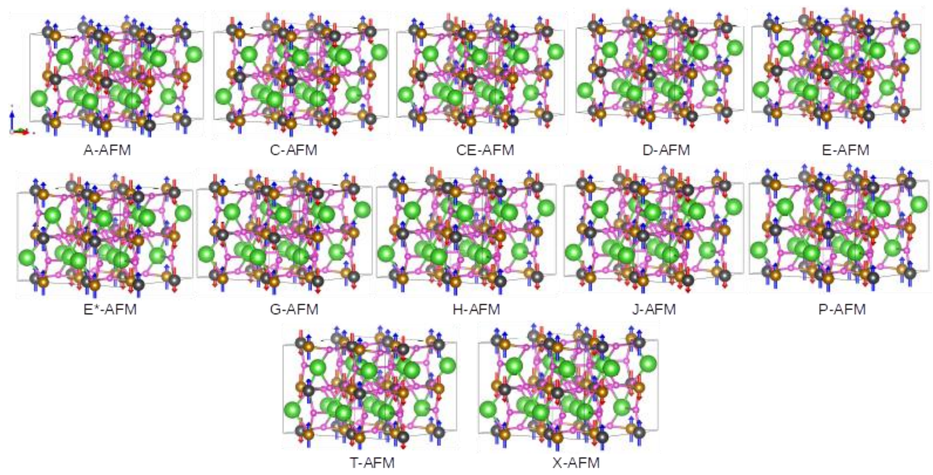
R_E	$R(BS)$	$R_{wp}(BS)$	GOF
7,02 %	5,53 %	9,43 %	1,81

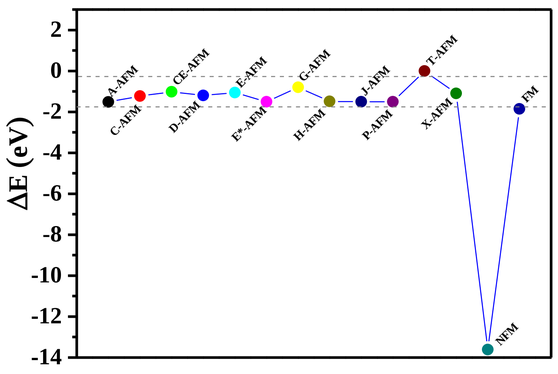


Granular and solidified regions coexist in the material, so it is not possible to establish an average grain size.

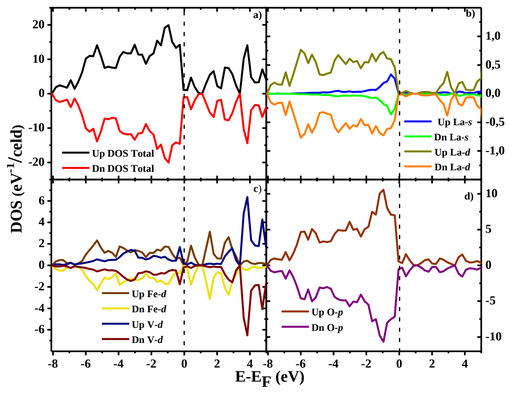


DISCUSSION AND THEORETICAL RESULTS





The present graph shows that the AFM phase is the stable phase with respect to the FM and NM. In addition, among AFM configuration, the T-AFM is the most stable.



The results of the electronic properties show that the material has a conductive behavior, due to the contributions of the p-O, d-Fe and d-V orbitals at the Fermi level.

CONCLUSION

The assisted gel combustion method used for the synthesis of the $LaFe_{0,5}V_{0,5}O_3$ material substantially reduces the synthesis time and the need to apply thermal treatments with inert atmospheres to obtain it. The morphological characterization showed that the material presents a porous structure where there is the simultaneous presence of granular regions and regions where a high density of conglomerates is present, which can be seen as an anisotropy of shape in the material. The magnetic characterization showed that antiferromagnetic interactions predominate in the material with a small ferromagnetic phase for low temperatures possibly attributed to the anisotropies present in the material.

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