Experimental and theoretical studies of structural and electronic properties of perovskite Sr_2SbMnO_6

O. Ortiz-Diaz[1,2], C. A. Parra Vargas[1,2], F. Gonzalez[1], J. Otálora Acevedo[2,3], W. O. Sosa[1], Rafael Julian González Hernández[3], J. Arbey Rodriguez[3]

1. Grupo de Física de Nuevos Materiales, Departamento de Física, Universidad Nacional de Colombia, Bogotá DC
2. Grupo de Física de Materiales, Escuela de Física, UPTC, Tunja
3. Grupo de Estudio de Materiales

In this work, a first principles study of structural and electronic properties for the cubic perovskite material Sr_2MnSbO_6 is reported. We used the full-potential linearized augmented plane wave plus local orbitals method (L/APW+lo) within the non-collinear spin density functional theory as implemented in the WIEN2k code [1]. Lattice constants were computed by fitting the total energy versus volume data according to the Murnaghan equation of state. The results obtained were in agreement with the experimental values. The Generalized Gradien Aproximation (GGA) proposed by Perdew, Burke and Ernzerhof (PBE) scheme are used for the exchange-correlation energy functional. A detail study of the density of states and band structures carried out considering the two spin polarizations is presented. Furthermore, we prepared the material by means of solid state reaction method and we recorded X Ray Diffraction (XRD) pattern, at room temperature, and we was performed Rietveld refinement. Based on this study we found the *I4mm* space group, with lattice parameter values *a=b=5,54 Å, c=8.10 Å.* *A*greement between experimental and calculated values is discussed.

This work was partially supported by División de Investigaciones (DIN), Universidad Pedagógica y Tecnológica de Colombia, UPTC.

[1] P. Blaha, K. Schwarz, G. Madsen, D. Kvasnicka, J. Luitz, WIEN2k, An Augmented Plane Wave Plus Local Orbitals Program for Calculating Crystal Properties (Vienna University of Technology) 2001. ISBN 3-9501031-1-2.