Modelling Fe-Mo Double Perovskite Nanowires for Spintronics Applications

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From the well-known half-metallic Sr_2FeMoO_6 (SFMO) double perovskite were excised nanowires (NWs) with axes parallel to the [001] direction in a Sr-Fe-Mo-O monocrystalline perovskite used as reference. Because the bulk SFMO compound is colossally magnetoresistive, has a high Curie temperature and is very sensitive to the Fe/Mo content ratio or antisite occupation, we expected to found modifications on the electronic properties of the NWs; specifically, the energy band gap could change the kind and magnitude, as a function of the chemical elements distribution on the NWs' surface. The changes on the electronic states occupation could be different for each spin channel, turning these nanowires into promising systems to be incorporated in the design and development of spintronic or sensing devices. All calculations were made in the Density Functional Theory scheme, using the Generalized Gradient Approximation and the Perdew-Burke-Ernzerhof functional. Some NWs, uncharged or positive charged, have direct energy band gaps smaller than the corresponding to the crystalline material, generating the possibility to use these for optoelectronic applications. Contrasting, the negatively charged NWs are conductors without any spin polarization. Finally, the numerical results show that the lateral chains of metallic atoms are trivalent and those atoms bond to oxygen mostly in an ionic way, contrasting to the metal atoms along the central chain, which are hexavalent; the application area of these nanowires would be linked, naturally, to their relevant physical behaviour, but could be used in the development of optoelectronic or photovoltaic devices or even as conducting electrodes.

Acknowledgments: This work was supported by the IPN–SIP projects 20170885 and multidisciplinary 2016–1770 and 2016–1771. D. P. Fernández and A. Torres want to acknowledge the graduate fellowship from CONACYT and support from BEIFI.

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