Contribution ID: **49** Type: **Poster**

Effects of A-site order on the Mn local structure and polar phases of magnetoelectric REBaMn2O6 (RE: La, Nd, Sm and Y)

Thursday, 8 September 2022 19:35 (20 minutes)

The relationship between Mn local structure and the polar and magnetic phases of A-site ordered REBaMn2O6 [1-3] and disordered RE0.5Ba0.5MnO3 (RE: La, Nd, Sm and Y) manganites has been investigated combining high energy resolution fluorescence and total fluorescence detected X-ray absorption at the Mn K-edge, to overcome the interference of the RE L-edges [4]. The extended k-range EXAFS spectra were measured at the CLAESS beam line of the ALBA synchrotron using the CLEAR spectrometer. An abrupt loss of local distortions of the MnO6 only occurs when the A-site ordered samples develops long-range ferromagnetic non-polar phases (RE=La). With decreasing the A-site ionic size (RE=Nd, Sm), a competition between ferromagnetism and charge localization appears, resulting in the development of a local distortion of the MnO6 octahedron in the low temperature polar phases. For the smallest A-site atom, YBaMn2O6, the local distortion of the MnO6 octahedron already exists at temperatures above the polar charge-ordered phase and vary little with temperature below the transition. This polar local distortion in REBaMn2O6 (RE: Sm, Y) is a bit less than half of the expected for a 1:1 Mn3+-Mn4+ order, i.e. ~0.3-0.5 e-. On the other hand, the A-site disorder weakens the ferromagnetism, favouring the presence of local distortions of the MnO6 octahedron. For the smaller A-site atoms (Sm, Y), a large local distortion of the MnO6 octahedron that is temperature-independent prevents the development of any magnetic order in the A-site disordered RE0.5Ba0.5MnO3 perovskites.
In conclusion, both a large difference in the ionic size of A-site cations and A-site disorder are proven to be detrimental for the development of long-range ferromagnetism in REBaMn2O6 (RE: La, Nd, Sm and Y) by favouring the electronic localization. Moreover, entropy contents in connection with the EXAFS results indicate that the mechanism of the polar structural transitions in ordered REBaMn2O6 (RE: Sm, Y) can be mainly associated with an order–disorder phase transition.

[1] J. Blasco, G. Subías, et al., Phys. Rev. B 103, 064105 (2021)
[2] J. Blasco, G. Subías, et al., Phys. Rev. B 103, 214110 (2021)
[3] J. Blasco, G. Subías, et al., J. Phys. Chem. C 125, 19467 (2021)
[4] G. Subías et al., Phys. Rev. B (2022) submitted

Acknowledgements. We thank the Spanish Ministerio de Ciencia, Innovación y Universidades (Projects No. RTI2018-098537-B-C22 cofunded by ERDF from EU) and Diputación General de Aragón (Project E12-20R) for financial support.

Would you like to participate in the Poster Prize competition?

No

Primary authors: Dr SUBIAS-PERUGA, Gloria (INMA, CSIC-Universidad de Zaragoza); BLASCO, Javier (Instituto de Nanociencia y Materiales de Aragón, CSIC-Universidad de Zaragoza); CUARTERO, Vera (Universidad de Zaragoza); LAFUERZA BIELSA, Sara (Instituto de Nanociencia y Materiales de Aragón (INMA), CSIC-Universidad de Zaragoza); SIMONELLI, Laura (ALBA Synchrotron); GORNI, Giulio; Prof. GARCÍA, Joaquín (INMA, CSIC-Universidad de Zaragoza); Prof. CASTRO, Miguel (Universidad de Zaragoza)

Presenter: Dr SUBIAS-PERUGA, Gloria (INMA, CSIC-Universidad de Zaragoza)

Session Classification: List of posters presented during the conference