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Hyperfine and Density Functional Theory Studies of SrMnGe2O6, SrCoGe2O6 and CaMnGe2O6

Multifunctional materials have been under the spotlight due to their fundamental scientific interest and for potential applications in technology. In particular, the Pyroxene family of materials, with general chemical formula AM(Si,Ge)2O6, has been the subject of of some recent interest due to the discovery of multiferroic and magnetoelectric properties among these materials. More specifically, SrMnGe2O6, SrCoGe2O6 and CaMnGe2O6 are isostructural, crystallizing with monoclinic C2/c symmetry and are characterized by zigzag chains of MnO6 octahedra linked by edgesharing, separated by GeO4 tetrahedra chains along the same axis, linked by corner-sharing. Due to this arrangement these systems present a rich diversity of low-dimensional magnetic properties. The existence and possible interplay of low dimensionality and magnetic frustration results in multiferroic and/or magnetoelectric properties.
Since these properties might arise from local structural features that are not well described by methods based on long-range average structural models, the use of local probe studies is essential. In this context, hyperfine methods, such as perturbed angular correlation (PAC) spectroscopy where the study of the electric field gradient (EFG) in the vicinity of a probe atom, allows reconstructing of the atomic and electronic environment of the probe in the material, helps to clarify the origin of the properties exhibited in these systems. In this work a temperature dependent EFG study will be presented and discussed, guided by Density Functional Theory EFG simulation results, exploring in particular the effect of the *U* correction from the Hubbard Model in an attempt to better explain the experimental results.

[1] Lei Ding et al, J. Mater. Chem C, 2016, 4, 4236 [2] Lei Ding et al, Physical Review B 2016, 93 064423
[2] P Giannozzi, O Andreussi, T Brumme, O Bunau, M Buongiorno Nardelli, M Calandra, R Car, C Cavazzoni, D Ceresoli, M Cococcioni, N Colonna, I Carnimeo, A Dal Corso, S de Gironcoli, P Delugas, R A DiStasio Jr, A Ferretti, A Floris, G Fratesi, G Fugallo, R Gebauer, U Gerstmann, F Giustino, T Gorni, J Jia, M Kawamura, H-Y Ko, A Kokalj, E Küçükbenli, M Lazzeri, M Marsili, N Marzari, F Mauri, N L Nguyen, H-V Nguyen, A Otero-de-la-Roza, L Paulatto, S Poncé, D Rocca, R Sabatini, B Santra, M Schlipf, A P Seitsonen, A Smogunov, I Timrov, T Thonhauser, P Umari, N Vast, X Wu and S Baroni, J.Phys.:Condens.Matter 29, 465901 (2017)
[3] P. Blaha, K. Schwarz, G. K. H. Madsen, D. Kvasnicka, J. Luitz, R. Laskowski, F. Tran and L. D. Marks, WIEN2k, An Augmented Plane Wave + Local Orbitals Program for Calculating Crystal Properties (Karlheinz Schward, Techn. Universität Wien, Austria), 2018. ISBN 3-9501031-1-2

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