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Combined Density Functional Theory and Perturbed Angular Correlation Study of SrMnGe2O6 and CaMnGe2O6

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Multiferroic materials have been under the spotlight due to their fundamental scientific interest and for potential applications in technology. Among these interesting materials are the group of compounds belonging to the Pyroxene family with general chemical formula AM(Si,Ge)2O6. More specifically, SrMnGe2O6 [1] and CaMnGe2O6[2] are isostructural, crystallizing with monoclinic C2/c symmetry and are characterized by zigzag chains of MnO6 octahedra linked by edge-sharing, 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 EFG simulation results using ab-initio and WIEN2k [3] and Quantum ESPRESSO [4], attempting to clarify the nature of the two distinct local environments that are experimentally observed in these compounds.

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