Ab-initio approach to interface effects at spinel ferrite heterostructures

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Spinel ferrite heterostructures that combine hard and soft magnetic materials have gained importance in areas as diverse as the search for efficient rare-earth free permanent magnets, or the development of new therapies to treat cancer. The combined system is expected to profit from the individual properties of each component, but the presence of interfaces may add features that are difficult to isolate from experiments. Even restricting to undefective interfaces between isostructural ferrites, such as $CoFe_2O_4/NiFe_2O_4$ or $CoFe_2O_4/MnFe_2O_4$, we need to consider lattice mismatches, bond rearrangement and novel superexchange paths that may affect the global magnetic response. This is particularly relevant for CFO, with a large magneto elastic coefficient highly sensitive to minor strains and modifications of the system symmetry. Here we show how density functional theory simulations are particularly adequate to explore these effects, identifying key aspects that need to be considered to tune the magnetic properties in the presence of multiple interfaces. We evaluate the coexistence of different orientations and crystal terminations to determine the influence of mismatch-induced strains and partial inversion on the net magnetisation, magnetic anisotropy and superexchange paths. We prove the determinant role of the cation distribution and structural inversion on the magnetisation and magnetic anisotropy. Our results provide a useful guide to understand magnetic measurements of hard/soft spinel ferrite heterostructures, and identify the determinant role of even ideal interfaces on the properties of the joint system.

References:

[1] C. Tejera-Centeno, S. Gallego, J. Phys. D **in press**, https://doi.org/10.1088/1361-6463/abf25b (2021)