EXECUTIVE SUMMARY

This work explores the long-ranged noncollinear magnetic textures, called spin spirals, in the multiferroic material BiFeO$_3$ as well as the BiFeO$_3$/metal interface. These spin spirals are of prime importance for technological applications owing to their potential for spintronics and low-power magnetoelectric devices. The presence of spin spirals is induced by the Dzyaloshinskii-Moriya interaction (DMI), which originates from spin-orbit coupling. This research investigates the magnetic interaction, and especially the DMI, in multiferroic materials and the interface between multiferroics and metals. With the computational resources of Blue Waters, the research team carried out fully first-principles or ab initio calculations in BiFeO$_3$ to reveal the stability of spin cycloids (the precession of spins along a propagation direction with a perpendicular rotational axis) under various strain conditions and to obtain the accurate magnetic interaction parameters that will be used to construct an effective Hamiltonian for combining Monte–Carlo simulations to study finite-temperature properties.

RESEARCH CHALLENGE

BiFeO$_3$ (BFO) is a multiferroic magnetoelectric material at room temperature. This means that a magnetic field can change its polarization and an electric field can change its magnetization. This property is very rare in nature, which explains the strong interest in BFO and why it is called the “holy grail of multiferroic physics.” BFO is also a noncollinear antiferromagnetic (AFM) material, exhibiting a magnetic cycle at room temperature. Although this spin spiral is well characterized experimentally, several questions remain, such as the stabilization mechanism(s) of the different types of spirals and their interplay with structural distortion. For instance, the type of cycle in bulk BFO in the R3c phase is well characterized as being propagated along one of the [1–10] directions. However, a few recent experimental studies proposed that a type-II cycloid with a propagation along [11–2] may be favored in BFO thin films that are moderately strained, implying that the experimentally observed type-2 cycloid is likely to be a mixture of two type-I domains. In parallel, the team explored the magnetic exchange and the DMI in Fe$_{1-x}$Co$_x$/Pt as shown in Fig. 2. Counterintuitively, the magnetic exchange interaction changes dramatically as a function of the concentration. The magnetic exchange shows a maximum for Co-rich Fe$_{1-x}$Co$_x$/Pt. The value of the magnetic exchange is, however, much smaller than the measurements realized by BLS on Fe$_{60}$Co$_{20}$B$_{20}$/Pt (30 pJ/m). These findings suggest that the hybridization of the Fe$_{1-x}$Co$_x$ with the Pt plays a major role both with the magnetic exchange and the DMI, as shown in Fig. 2(b). Taking into account the presence of the Pt substrate increases the exchange at 30 pJ/m, in agreement with the experimental finding. The calculations of the DMI are now under consideration. In the next period, the team will be able to study the effect of an electric field on Fe$_{1-x}$Co$_x$/Pt created by a ferroelectric layer owing to proximity effect.

WHY BLUE WATERS

A challenge in this study was to obtain the full magnetic phase diagram of the systems with strain, temperature, and electric field. Owing to the very long period of the spin spiral in BFO (approximately 60 nm), an extremely dense k-grid is necessary to resolve the q-point corresponding to the ground-state period. Given the superior stability of the FLEUR code with a large number of cores (beyond 10,000), the study has greatly benefited from using the Blue Waters supercomputer.

PUBLICATIONS & DATA SETS


B. Dupé, “Calculating the magnetic exchange and DMI in Co$_x$/Fe$_{1-x}$/Pt in preparation, 2019.