Unique Spin-orbit Properties of Magnetic Layered Bulk CoTiO₃

Mikel Arruabarrena¹

A. Leonardo^{2,3}, M. Rodriguez-Vega⁴, G. Fiete^{5,6}, A. Ayuela^{1,3}

¹Centro de Física de Materiales, Paseo Manuel Lardizabal 5, Donostia-San Sebastián, Spain ²Department of Applied Physics II, University of the Basque Country UPV/ EHU, Bilbao, Spain ³Donostia International Physics Center (DIPC), Paseo Manuel Lardizabal 4, Donostia-San Sebastián, Spain

⁴Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico, USA

⁵Department of Physics, Northeastern University, Boston, USA

⁶Department of Physics, Massachusetts Institute of Technology, Cambridge, USA

marruabarrena001@ikasle.ehu.es

Cobalt titanate CoTiO₃ has currently attracted a lot of interest in condensed matter physics because of exhibiting unique magnetic and topological properties, like Dirac magnons[1],[2]. We present spin density functional calculations on this cobaltate, including spin-orbit interactions. We analyze the different magnetic configurations. There are two critical temperatures, related to the transition between the magnetic configurations shown in figure 1. We also find that cobalt titanate presents out-of-plane magnetic anisotropy, a finding that seems to be in disagreement with previous experimental reports[3,4]. However, we observe that n-type doping in the form of Ti-Co anti-site ordering can switch the anisotropy in-plane[5].

References

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Figures

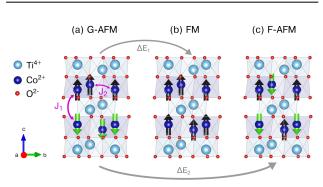


Figure 1: Magnetic configurations of cobalt titanate, presented in ascending energetic order: (a) antiferromagnetic between layers (G-AFM), (b) ferromagnetic (FM), and (c) fully antiferromagnetic (F-AFM).

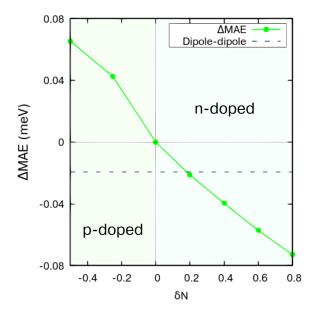


Figure 2: Change of the magnetocrystalline anisotropy energy (Δ MAE) with respect to the variation of the number of electrons in the unit cell (δ N). In the n-doped region, for δ N values larger than 0.2, the magnetocrystalline anisotropy energy becomes smaller than the magnetic dipole-dipole interaction, which switches the anisotropy in-plane.