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Spin-orbit interactionsand magnetic field in antiferromagnetic triangular molecular magnets J.F. NOSSA, M.F. ISLAM, C.M. CANALI, Linnaeus University, M.R. PEDERSON, Naval Research Laboratory — Frustrated triangular molecular magnets such as Cu_3 are characterized by a doubly generate S=1/2 ground-state (GS) with opposite chirality. Recently it has been proposed theoretically [1] and verified by ab-initio calculations [2] that an external electric field can efficiently couple these two chiral spin states, even in the absence of spin-orbit interaction (SOI). SOIs are nevertheless important, since they introduce a splitting in the GS manifold. In this talk we will discuss different schemes on how to evaluate within spin density functional theory the effect of the SOIs on the chiral states. The connection between SOI and the Dzyalozhinsky-Moriya interaction will be discussed. We will also present calculations of the energy dependence on an external magnetic field, whose presence is important to achieve full control of the spin-electric coupling within the manifold of the GS chiral doublets.

[1] M. Trif et. al. Phys. Rev. B 82, 045429 (2010) and M. Trif et. al. Phys. Rev. Lett. 101, 217201 (2008)
[2] F. Islam et. al. Phys. Rev. B 82, 155446 (2010)

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