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Spin-electric coupling in Cu_3, V_{15} and other frustrated molecular magnet rings: a first principle study M.F. ISLAM, J.F. NOSSA, C.M. CANALI, Linnaeus University, M.R. PEDERSON, Naval Research Laboratory — Frustrated triangular single-molecule magnets (SMMs) without inversion symmetry, such as Cu_3 and V_{15}, are characterized by a doubly degenerate 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 couple these two chiral spin states, even in the absence of spin-orbit interaction (SOI). The efficiency of these coupling depends on the electric dipole moment between chiral states. In this talk we report on first-principle calculations of the coupling strength for the triangular SMMs Cu_3 and V_{15}. The spin-electric coupling is found to be considerably stronger in V_{15} than in Cu_3. We discuss the mechanism leading to an enhanced spin-electric coupling, which can be used as a convenient guide to synthesize SMMs that can respond more efficiently to an external electric field.

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

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