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DFT studies of spin-electric effects in single-molecule magnets without inversion symmetry CARLO CANALI, FHOKRUL ISLAM, JAVIER NOSSA MÁRQUEZ, Kalmar University, MARK PEDERSON, NRL, Washington DC, U.S.A. — Recently [1] it has been proposed that in single-molecule magnets (SMMs) lacking inversion symmetry, a mechanism based on the interplay among quantum exchange, spin orbit interaction and chirality of the underlying spin texture, allows for an effective coupling between the spin states and an external electric field. This effect could represent a very efficient and fast way of manipulating the magnetic states of the SMM via a localized electric field generated, e.g., by a nearby STM tip, with possible applications in quantum information processing. In this paper we use DFT encoded in the NRLMOL program to evaluate microscopically the electric dipole moment of a SMM, which is the key quantity controlling the strength of the spin-electric coupling. We present calculations for the triangular antiferromagnetic S= $1/2$ Cu_3 SMM originally considered in Ref. [1], and comment on the case of Mn_{12} acetate SMM, which also lacks inversion symmetry, but has spin S=10 and a large magnetic anisotropy.

[1] M. Trif et al., Phys. Rev. Lett. 101, 217201 (2008).

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