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.