Stability of spin-electric coupling in triangular single-molecule magnets under external contacts

FHOKRUL ISLAM, Linnaeus University, Sweden, JAVIER NOSSA, Carnegie Institution of Washington, USA, CARLO CANALI, Linnaeus University, Sweden, MARK PEDERSON, Department of Energy, USA — Triangular single molecule magnets (SMMs) with antiferromagnetic exchange coupling exhibit Kramer degenerate chiral spin-doublets ground states, which can be efficiently coupled by an electric field, even in the absence of spin-orbit interaction. Recent first-principles calculations [1] show that unsupported V$_3$ SMM has giant spin-electric coupling corresponding to dipole moment of about one tenth of the water-molecule dipole moment. The corresponding Rabi time for electric switching between two chiral states can be on the order of one nano-second for reasonable electric fields, which makes these molecules very attractive candidates for storing and manipulating pairs of coupled spin-chiral qbits. However, for device applications of the spin-electric coupling, these frustrated SMMs need to be supported on a surface or between metallic leads. Preserving this effect in an external environment is a challenging problem requiring appropriate functionalization. In this talk we will discuss the stability of the spin-electric coupling in V$_3$ SMM when coupled to gold leads or deposited on a graphene surface. [1] J. F. Nossa et al., Electric control of spin states in frustrated triangular molecular magnets (unpublished)