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Quantum control of molecular antiferromagnets: an approach based on electric fields MIRCEA TRIF, DIMITRIJE STEPANENKO, University of Basel, FILIPPO TROIANI, CNR-INFM National Research Center, Modena, DANIEL LOSS, University of Basel — Single molecule magnets show clear signatures of coherent behavior, and have a wide variety of effective low-energy spin Hamiltonian suitable for encoding qubits and spin-based quantum information processing. At the nanoscale, the prefered mechanism for control of quantum systems involves application of electric fields, which can be locally applied, and rapidly switched. In this work, we provide the tools for the search for single molecule magnets suitable for electric control. We analyze the mechanisms that leads to spin-electric coupling in the molecules with the shape of regular polygons. We find that the spin-electric coupling in triangular molecules is governed by the modification of the exchange interaction, while in pentagonal molecules the spin-electric coupling proceeds via spin-orbit interaction. We apply a Hubbard model to single-molecule magnet to find a connection between the spin-electric coupling and the properties of the chemical bonds in a molecule. We study the experimental signatures of spin-electric coupling in nuclear magnetic resonance, electron spin resonance, magnetization, electric polarization, and specific heat of the molecules.

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