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Theory of tunneling spectroscopy in a Mn_{12} single-electron transistor by DFT methods LUKASZ MICHALAK, Lund University and Kalmar University, Sweden, CARLO M. CANALI, Kalmar University, Kalmar, Sweden, MARK R. PEDERSON, Naval Research Lab, Washington DC, USA, VINCENZO G. BENZA, Universita dell Insubria, Como, Italy — We present a theory of single-electron tunneling transport through a Mn_{12} molecular magnet in the Coulomb blockade regime. We employ spin density functional theory to calculate the low-energy spin multiplet states for neutral and charged (anion and cation) Mn_{12}, split by spin-orbit interaction. Tunneling matrix elements between these states are the basic ingredients of a master equation formalism that gives the tunneling conductance as a function of the bias and gate voltage. We compare the results of this formalism with the ones obtained using a phenomenological giant-spin Hamiltonian and highlight the importance of the orbital degree of freedom included in our SDFT approach.

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