



Real
Sociedad
Española de
Física

ID de la contribución : 161

Tipo : Oral parallel contribution

Theoretical evaluation of $[V(\alpha\text{-C}_3\text{S}_5)_3]^{2-}$ as a nuclear-spin sensitive single-molecule spin transistor.

lunes, 17 de julio de 2017 16:40 (25)

In a straightforward application of molecular nanospintronics to quantum computing, single-molecule spin transistors can be used to measure and control nuclear spin qubits, since a conductance jump occurs when the electronic spin inverts its polarization, and this happens at a specific magnetic field determined by the nuclear spin state. So far, this procedure has only been studied using TbPc2, the first known Single Ion Magnet. Here we theoretically explore the adequacy for this procedure of the highly stable molecular spin qubit $[V(\alpha\text{-C}_3\text{S}_5)_3]^{2-}$. We determine the spin-dependent conductance and verify that, at the Fermi energy, the intrinsic electronic spin does not share spatial density distribution with the polarized current electrons, indicating that the spin states may survive in the conduction regime. We estimate some physical parameters to guide the experiments, and verify the robustness of the theoretical methodology by applying it to two chemically related vanadium complexes.

Primary author(s) : Dr. CARDONA-SERRA, Salvador (Instituto de Ciencia Molecular)

Co-author(s) : Dr. GAITA-ARIÑO, Alejandro (Instituto de Ciencia Molecular); Dr. STAMENOVA, Maria (School of Physics / CRANN); Prof. SANVITO, Stefano (School of Physics / CRANN)

Presenter(s) : Dr. CARDONA-SERRA, Salvador (Instituto de Ciencia Molecular)

Clasificación de la sesión : Molecular Electronics

Clasificación de temáticas : Molecular Electronics