First-principles study of spin decoherence in VOPc-graphene nanoribbon complexes

Xiao Chen, James N. Fry and Hai-Ping Cheng

Department of Physics, University of Florida, Gainesville, FL

Nanographene qubit arrays facilitate quantum-to-quantum transduction between light, charge, and spin, making them an excellent testbed for fundamental science in quantum coherent systems and for the construction of higher-level qubit circuits. In this work we study decoherence of an electronic spin due to coupling with a surrounding spin bath in a system of multiple vanadyl phthalocyanines (VOPc), a candidate of spin-1/2 molecular qubit, on armchair-edged graphene nanoribbons (GNR). Density functional theory (DFT) is used to obtain low energy isomeric atomic structures at different spacings between VOPcs. Decay of spin coherence in Hahn echo experiments was simulated using the cluster correlation expansion (CCE) method with a spin Hamiltonian involving hyperfine and electric field gradient tensors calculated from DFT. We found that GNR induced a significant decrease of the decoherence time T_2 compared with isolated single VOPc. Quadrupole interactions cause a large electron spin echo envelope modulation (ESEEM), which is harmful to spin decoherence, at small magnetic field. However, this ESEEM is suppressed upon increase of the field.

This work is supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award No. DE-SC0022089. Computations were done using the utilities of the National Energy Research Scientific Computing Center and University of Florida Research Computing.