First-Principles study of an S=1 quasi-1D quantum molecular magnetic material

Maher Yazback

Department of Physics, Quantum Theory Project, University of Florida, Gainesville, Florida 32611

We use density functional theory to study the structural, magnetic and electronic structure of the organo-metallic quantum magnet $NiCl_2$ 4SC $(NH_2)_2$ (DTN). Recent work has demonstrated the quasi-1D nature of the molecular crystal and its quantum phase transitions at low temperatures. This includes a magneto-electric coupling and, when doped with Br, the presence of an exotic Bose-glass state. We systematically show that, by using the generalized gradient approximation (GGA) with inclusion of a van der Waals term to account for weak inter-molecular forces and by introducing a Hubbard U term to the total energy, our calculations reproduce the magnetic anisotropy, the inter-molecular exchange coupling strength and the magnetoelectric effect in DTN, which were observed in previous experiments. Further analysis into the electronic structure gives insight into the underlying magnetic interactions, including what mechanisms may be causing We use density functional theory to study the structural, magnetic and electronic structure the ME effect. Using this computationally efficient model, we predict what effect applying an electric field might have on the magnetic properties of this quantum magnet.