Strongly Correlated Electrons in the $[Ni(hmp)(ROH)X]_4$ Single Molecule Magnet: A DFT+U Study

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The single molecule magnet $[Ni(hmp)(MeOH)Cl]_4$ is studied using both density functional theory and the DFT+U method, and the results are compared. By incorporating a Hubbard-U like term for both of the nickel and oxygen atoms, the experimental ground state is successfully recovered, and the exchange coupling constants derived from the DFT+U calculation fit the experimental results very well. The results show that the nickel 3d electrons and oxygen 2p electrons in this molecule are strongly correlated, and thus the inclusion of on-site Coulomb energies is crucial to obtain correct results.

This work is supported by DOE DE-FG02-02ER45995 (H.-P. Cheng and C. Cao), NSF/DMR/ITR-0218957 (H.-P. Cheng and C. Cao), NSF DMR0239481 (S. Hill), and NSF DMR0506946 (S. Hill). The authors want to thank NERSC CNMS/ORNL and the University of Florida High Performance Computing Center for providing computational resources and support that have contributed to the research results reported here.