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Application of DFT+U for calculating magnetic parameters for manganese based molecular magnets SHRUBA GANGOPADHYAY, NanoScience Technology Center, Department of Chemistry, University of Central Florida, Orlando, FL, 32826, ARTEM MASUNOV, NanoScience Technology Center, Department of Chemistry, Department of Physics, University of Central Florida, Orlando, FL, 32826 — Single-molecule magnets are promising materials for molecular spintronics and quantum computing applications. Two methods feasible to predict the exchange coupling parameters of molecular magnets, broken symmetry Density Functional Theory and DFT with empirical Hubbard U parameter (DFT+U). In this contribution we apply DFT+U to study magnetic coupling for two Mn12-based molecular magnetic wheel using Vanderbilt Ultrasoft Pseudopotential plane wave DFT method implemented in Quantum ESPRESSO. Unlike most previous studies, we adjust U parameters for both metal and ligand atoms using five dineuclear organometallics as the benchmarks. Our study finds antiparallel spin alignment of the weakly interacting fragments of Mn_{12}, while the magnetic coupling inside the fragments are much stronger, both are in agreement with experimental observations.

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