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GGA+U study of exchange interactions in a Mn5 single-molecule magnet EMALEE POPOFF, Virginia Tech, Blacksburg, VA, SALVADOR BARRAZA-LOPEZ, Georgia Tech, Atlanta, KYUNGWHA PARK, Virginia Tech, Blacksburg, VA, HUI-LIEN TSAI, Department of Chemistry, National Cheng Kung University, Taiwan — Electronic structure of a single-molecule magnet (SMM) Mn5 is investigated using GGA+U formalism. There are two types of Mn ions in the SMM Mn5: Mn3+ (S=2) and Mn2+ (S=5/2). In a prototype single-molecule magnet Mn12, superexchange interactions between Mn ions through oxygen anions are known to be antiferromagnetic. Our calculation on Mn5, however, showed that the Mn ions are all ferromagnetically coupled to each through various ligands. This results in the ground state spin of S=11, which is in good agreement with experiment. We discuss the nature of the ferromagnetic coupling between the Mn ions by analyzing calculated projected density of states. We also present calculated exchange coupling constants considering various broken symmetry states.

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