Abstract Submitted
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Molecular Magnetism in MnTe Clusters[1] JIA CHEN, Department of Applied Physics, Columbia University, ARUN NANDURI, BONNIE CHOI, Department of Chemistry, Columbia University, ANDREW MILLIS, Department of Physics, Columbia University, DAVID REICHMAN, XAVIER ROY, Department of Chemistry, Columbia University — Electron correlation in recently synthesized molecular clusters with Mn_4Te_4 cores in cubane structures and ligand exteriors are studied experimentally and theoretically. We used density functional theory with on-site Coulomb interactions (DFT+U) to construct effective spin Hamiltonians and estimate the dependence of parameters on choice of ligand. The lack of inversion symmetry combined with the heavy tellurium ions leads to a significant Dzyaloshinskii-Moriya (DM) interaction. Comparison of measurements to the magnetic susceptibility calculated from the spin model is used to validate the results. We also extend this work to more complex clusters with more than one cubanes, where interesting high-spin ground state may occur. It has been measured recently, Fe_8Te_8 in dicubane structure has ground state with magnetization of$12\mu_B$, which makes it promising candidate for single molecular magnets.

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Jia Chen
Department of Applied Physics, Columbia University

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