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Electronic Structure, Magnetic Interactions, and the Role of Ligands in Mn_n(n=4, 12) Single-Molecule Magnets MYUNG JOON HAN, School of Physics, Seoul National University, Korea, TAISUKE OZAKI, RICS-AIST, Japan, JAEJUN YU, School of Physics, Seoul National University, Korea — We report our first-principles calculation studies of electronic structure and magnetic properties of Mn_n (n=4,12) single-molecule magnets. For the calculations, we used the linear combination of localized pseudo-atomic orbital (LCPAO) method based on the density functional theory within local density approximation (LDA) and LDA+U. To investigate the role of ligands and its contribution to the determination of magnetic properties, we calculated the electronic structures of Mn_n clusters with different ligand configurations. Detailed analysis reveals an important contribution of the bridging carbon atoms, connecting the Mn-O core and the outer ligand complex, to the magnetic ground states of the magnetic molecules. In addition, we calculated the effective exchange-coupling constants among Mn-ions by applying the rigid spin approximation in the non-collinear magnetic perturbation theory within the non-orthogonal LCPAO basis set. The results are in reasonable agreement with the experimental values and the former theoretical ones. We also consider the effect of on-site Coulomb interactions in determination of the magnetic properties of single-moloecule magnets.

Myung Joon Han
School of Physics, Seoul National University

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