

Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Exchange constants and second-order magnetic anisotropy in cyanide-bridged Fe₂M₂ single-molecule magnets¹ KYUNGWHA PARK, Virginia Tech, STEPHEN HOLMES, University of Kentucky — Electronic structure and intramolecular exchange constants are calculated for three cyanide-bridged single-molecule magnets, [Tp*Fe^{III}(CN)₃M^{II}(DMF)₄]₂(OTf)₂·2DMF (M^{II}=Mn, Co, Ni) (abbreviated as Fe₂Mn₂, Fe₂Co₂, and Fe₂Ni₂) that have been recently synthesized, within a generalized-gradient approximation in spin-polarized density-functional theory (DFT). Due to strong ligand fields present in the molecules, the Fe ions exhibit a low ground-state spin of $S = 1/2$ in which the orbital angular momentum may not be quenched even without spin-orbit coupling. Based on the calculated electronic structures, the magnetic anisotropy for Fe₂Mn₂, Fe₂Co₂, and Fe₂Ni₂ is computed including single-electron spin-orbit coupling within a DFT formalism. The theoretical values of the induced orbital angular momentum and of the magnetic anisotropy parameters are compared to those for a single-molecule magnet Mn₁₂. The total magnetic anisotropy present in the three single-molecule magnets is due to competition between the magnetic anisotropy of the Fe and of the M ions.

¹This work was supported by the NSF and the Kentucky Science and Engineering Foundation. The computational resources were provided by the TCF at VT and the NCSA.

Kyungwha Park
Virginia Tech

Date submitted: 29 Nov 2006

Electronic form version 1.4