Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Electron density, geometric structure and vibration spectra of endohedral $M_{1-3}C_{60}$ (M = Mn, Co, Fe, Gd) metallofullerenes G. P. LI, R. SABIRIANOV, W. N. MEI, Department of Physics, University of Nebraska at Omaha, Omaha, Nebraska 68182, P. A. DOWBEN, Department of Physics, University of Nebraska, Lincoln, Lincoln NE 68588-0416, X. C. ZENG, Department of Chemistry, University of Nebraska, Lincoln, Lincoln NE 68588-0416 — Endohedrally doped buckminster fullerene C60 with metallic clusters of M_{1-3}, (M = Mn, Co, Fe and Gd) are studied by using density functional theory (DFT), projector augmented wave (PAW) and pseudo-potential (PP) methods. Optimized molecular geometries are obtained from varying the positions of these two/three metal atoms together with the C_{60} cage and finding the energy minimum while considering different multiplicities and magnetic configurations. Subsequently the vibrational frequencies of the cluster, electric and magnetic dipole moments are calculated and compared with experiments. Upon the molecular properties are thoroughly studied, we construct different crystal models utilizing these metallofullerenes and employ the local density approximation (LDA)+U techniques to account for many-body effects.

W. N. Mei
Department of Physics, University of Nebraska at Omaha, Omaha, Nebraska 68182

Date submitted: 30 Nov 2005 Electronic form version 1.4