

Abstract Submitted  
for the MAR08 Meeting of  
The American Physical Society

**An Investigation of Magnetic, Electronic and Structural Properties of Metallofullerenes**<sup>1</sup> S. VINCENT ONG, MEICHUN QIAN, SHIV KHANNA, Dept. of Physics, Virginia Commonwealth Univ., Richmond, VA 23284 — Gadolinium based endohedral metallofullerenes  $\text{Gd}_3\text{N@C}_{80}$  functionalized with OH radicals have been found to enhance the relaxivity by orders of magnitude over conventional agents and are being sought as new contrast agents in magnetic resonance imaging (MRI). Using state of the art density functional theory (DFT) in the regime of the local density approximation with the on-site Coulomb interaction (LSDA+U), we have carried out theoretical studies to determine the electronic and magnetic properties of gadolinium-based and lutetium-based nitride fullerenes, namely  $\text{Lu}_{3-x}\text{Gd}_x\text{N@C}_{80}$  ( $x = 1-2$ ). While  $\text{Gd}_3\text{N@C}_{80}$  has previously shown promising features as a contrast agent, the idea of replacing gadolinium atoms by lutetium has been proposed to result in a mixed-metal species for multi-modal imaging. Our results indicate that  $\text{Lu}_2\text{GdN@C}_{80}$  is the most stable of all possible configurations with a binding energy 16.57 eV, can be considered for use as both an MRI contrast agent, due to gadolinium's high magnetic moment, and as a potential radioactive therapeutic or diagnostic agent, by neutron activation of a lutetium radioisotope. These results along with details of electronic structure will be presented.

<sup>1</sup>We gratefully acknowledge funding by NIH Grant No. R01-CA119371

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Date submitted: 26 Nov 2007

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