

Abstract Submitted  
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**Role of OH Adsorption on the Properties of MRI contrast agent  $\text{Gd}_3\text{N@C}_{80}$**  VINCE ONG, SHIV KHANNA, PANOS FATOUROS, Virginia Commonwealth University, SHIV KHANNA RESEARCH GROUP COLLABORATION, PANOS FATOUROS COLLABORATION — Endohedral metallofullerenes  $\text{Gd}_3\text{N@C}_{80}$  decorated with hydroxyl groups are now known to be excellent contrast enhancement agents for Magnetic Resonance Imaging (MRI) leading to strong relaxivity enhancements. One of the outstanding issues is the nature of OH adsorption and its effect on the properties of endohedral  $\text{Gd}_3\text{N}$  motif. We have carried out theoretical studies on the electronic structure and magnetic properties of the endohedral metallofullerenes functionalized with hydroxyl groups to demonstrate that the nature of OH can have significant effect on the magnetic spin density. The new findings may provide physical insight into the observed strong relaxivity enhancements.

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