Structural and Magnetic Properties of Gd$_3$N@C$_{80}$

JING LU, Mesoscopic Physics Laboratory, Department of Physics, Peking University, Beijing 100871, P. R. China, RENAT SABIRIANOV, W.N. MEI, Department of Physics, University of Nebraska at Omaha, Omaha, Nebraska 68182-0266, Nebraska, YI GAO, X.C. ZENG, Department of Chemistry, University of Nebraska at Lincoln, Lincoln, Nebraska 68588, CHUNGANG DUAN, Department of Physics, University of Nebraska at Lincoln, Lincoln, Nebraska 68588 — Using relativistic and on-site correlation corrected density functional theory, we have investigated the structural and magnetic properties of recently synthesized Gd$_3$N@C$_{80}$. The most stable structure of Gd$_3$N@C$_{80}$ has the three magnetic Gd ions pointing to the centers of hexagons in C$_{80}$. The magnetic ground state of this structure has the three coplanar spins ($S = 7/2$) offset by $120^\circ$ angles. At the same time, the state with the highest multiplicity, where all the spins are parallel aligned, is found only about 4.5 meV higher in energy. Therefore, at room temperature, we expect Gd$_3$N@C$_{80}$ to be paramagnetic with spin fluctuating between different multiplicities.

$^1$This work was supported by Nebraska Research Initiative (No. 4132050400) of the USA

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Date submitted: 13 Dec 2006
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