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TOP PAPERS 2007 SHOWCASE

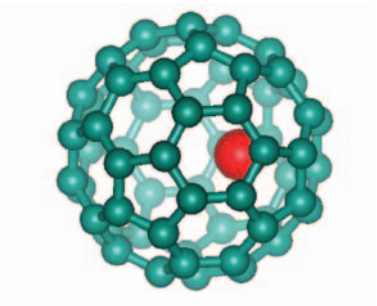
Taming Gd ions in fullerene cages

Encapsulating Gd within C_{60} enhances its correlation energies

Water-soluble Gd-based endohedral metallofullerenes ($Gd@C_{82}(OH)_x$, $Gd@C_{60}(OH)_x$, and $Gd@C_{60}[C(COOH)_{10}]$) are possible new magnetic resonance imaging (MRI) contrast agents. The toxic Gd ions are completely encaged inside the fullerenes, located at an off-centre position within the cage,

A large group headed by R F Sabirianov (University of Nebraska) explored the electronic properties of $Gd@C_{60}$ through a comparison of *ab initio* calculations with photoemission spectroscopy and resonant photoemission (constant initial state spectroscopy).

In comparing their calculations based on the local spin density approximation and the Hubbard model description with the



Optimized structure of $Gd@C_{60}$.

observed photoemission spectra, they observed a strong correlation effect, which manifests itself in the shift of the Gd 4f state to higher binding energy, and correlation energy U of about 7.6 eV, which is larger than normally detected in gadolinium compounds. They attributed that to a lack of screening of the encapsulated Gd. In addition, they noticed prominent resonant intensity features, due to the Gd 5s and 5p cores in the resonant photoemission spectra taken from 6 eV below the Fermi level, which indicate strong hybridization between the Gd valence states and the fullerene cage. All the above phenomena are explained using the LSDA + U calculation.

Correlation effects and electronic structure of $Gd@C_{60}$
R F Sabirianov et al
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