Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Electron Transfer and Localization in Endohederal Metallofullerenes[1] SHENYUAN YANG, ICQS and Institute of Physics, Chinese Academy of Sciences; U of Tennessee; ORNL, MINA YOON, ORNL; U of Tennessee, CHRISTIAN HICKE, Michigan State U, ZHENYU ZHANG, ORNL; U of Tennessee, ENGE WANG, ICQS and Institute of Physics, Chinese Academy of Sciences — Endohedral metallofullerenes constitute an appealing class of nanoscale building blocks for fabrication of a wide range of noval materials. One open question of fundamental importance is the precise nature of charge redistribution with the carbon cages (C_n) upon metal encapsulation. Using ab initio density functional theory, we systematically study the electronic structure of metallofullerenes, focusing on the spatial charge redistribution. For all large metallofullerenes ($n >$32), the valence electrons of the metal atoms are all transferred to the fullerene states. Surprisingly, the transferred charge is found to be highly localized inside the cage near the metal cations, rather than uniformly distributed on the surfaces of the carbon cage as traditionally belied. This counterintuitive charge localization picture is attributed to the strong metal-cage interactions within the systems. These findings may prove to be instrumental in the design of novel fullerene-based functional nanomaterials.

[1] Supported by the DMSE program and grant no. DE-FG02-05ER46209 of USDOE, grant no. DMR-0606485 of USNSF, and NSF of China.

Shenyuan Yang
ICQS and Institute of Physics,
Chinese Academy of Sciences; U of Tennessee; ORNL

Date submitted: 26 Nov 2007 Electronic form version 1.4