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Electronic transport, structure, and energetics of endohedral Gd@C82 metallofullerene and nanopeapods L. SENAPATI, J. SCHRIER, K. B. WHALEY, Department of Chemistry and Pitzer Center for Theoretical Chemistry, University of California, Berkeley, CA 94720 — Electronic structure and transport properties of the fullerene $C_{82}$and the metallofullerene Gd@C_{82} are investigated with density functional theory and the Landauer-Buttiker formalism for transport. The metal binding site for Gd is found to differ from that in Sc, Y, and La metallofullerenes, and is located on the C_2 symmetry axis, adjacent to the C-C double bond. Insertion of Gd into C_{82}causes a slight deformation of the carbon structure in the vicinity of the Gd atoms. Significant overlap of the electron distribution is found between Gd and the C_{82} cage, with the transferred Gd electron density localized mainly on the nearest carbon atoms. This charge localization reduces some of the conducting channels for the transport, resulting in a reduction in the conductivity of the Gd@C_{82} species relative to the empty C_{82} molecule. The electron transport across the metallofullerene is found to be relatively insensitive to the spin of the transported electrons relative to that of the Gd atom. In addition, we present results of transport calculations when the optimized Gd@$C_{82}$is inserted into a carbon nanotube to form a nanopeapod structure.

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