Solid State and Electronic Structure of Rare Earth Metal Intercalated Graphite from First-principles Theory

Chang-Ming Fang, Joseph Bauer, Jean-Yves Saillard, and Jean-Francois Halet

Laboratoire des Sciences Chimiques de Rennes, UMR 6226 CNRS-Université de Rennes 1, Avenue du Général Leclerc, 35042 Rennes Cedex, France

Reprint requests to Dr. C.-M. Fang. E-mail: cm.fang@orange.nl
or Prof. Dr. J.-F. Halet. Fax: +33 2 23 23 68 40. E-mail: halet@univ-rennes1.fr

Z. Naturforsch. **2007**, *62b,* 971 – 976; received April 27, 2007

Dedicated to Dr. Bernard Chevalier on the occasion of his 60th birthday

The structural arrangements of the graphite intercalates LnC$_6$ (Ln = La, Ce, Nd and Yb) were investigated using Density Functional Theory (DFT) within the Generalized Gradient Approximation (GGA). The EuC$_6$-type structure ($A\alpha A\beta A\alpha A\beta A\alpha A$ stacking) is slightly energetically preferred for La and Ce, whereas with the other rare earth metals almost the same cohesive energies are found for the three different atomic arrangements $A\alpha A\alpha A\alpha A\alpha A\alpha A\ldots$, $A\alpha A\beta A\alpha A\beta A\alpha A\ldots$, and $A\alpha A\beta A\gamma A\alpha A\beta A\ldots$ A rather important charge transfer occurs from the metals to the carbon sheets, with the electrons partially occupying the bottom of the carbon π^* band. As a consequence, a lengthening of the C–C bond lengths of *ca.* 0.02 Å is computed with respect to the C–C bonds in graphite. Two-dimensional metallic character is expected for LaC$_6$ according to its band structure.

Key words: Intercalated Graphite, Density Functional Calculations, Electronic Structure, Rare Earth Metals, GIC's