Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

LDA density functional study of lithium intercalated compounds in grephite JUAN SALVADOR ARELLANO, Area de Fisica Atomica Molecular Aplicada, UAM Azcapotzalco, 02200, Mexico D.F., PABLO DE LA MORA, Depto. de Fisica, Fac. de Ciencias, UNAM, Mexico, M. J. LOPEZ, L. M. MOLINA, J. A. ALONSO, Departamento de Fisica Teorica, Universidad de Valladolid, 47011, Valladolid, Spain — Local Density Functional (LDA) calculations have been done for different lithium intercalated graphite compounds. We have explored the most common ones namely LiC_6, and LiC_2. Also the LiC_3 has been studied. To explain some details about the structural and electronic properties of the last one, we have used two computer codes, FHI98MD and WIEN2k. This was motivated by a recent work for the LiC_3compound, where it is said that lithium atoms positions are not in the middle plane between the graphene layers formed by the carbon atoms. Discussion of the three mentioned lithium intercalated compounds and somewhat about the superconductivity will be given during the presentation.

Gustavo Tavizon
Depto. de Fis. y Quimica Teorica, Fac. de Quimica, UNAM, Mexico

Date submitted: 30 Nov 2005 Electronic form version 1.4