

Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Electronic structure and bonding properties of potassium (K) on graphite under external electric field. ALEJANDRO TAPIA, ROMEO DE COSS, Department of Applied Physics, Cinvestav-Merida, Mexico., GABRIEL CANTO, Centro de Ciencias de la Materia Condensada, UNAM, Mexico. — The effect of an external electric field on the potassium (K) adsorption on the graphite surface, are studied by means of first-principles total-energy calculations. The results were obtained with the pseudopotentials LCAO method (SIESTA code) and the Generalized Gradient Approximation (GGA) for the exchange-correlation potential. The structural parameters, bonding properties, and electronic structure of the K-graphite system are studied in the triangular (2×2) overlayer phase as a function of the external electric field magnitude. We find an important change in the K-graphite bonding as a consequence of the charge transfer from the adatom towards the substrate induced by the electric field. The results are discussed in the light of the experimental observed diffusion of K into graphite induced by external electric fields. This work was supported by Consejo Nacional de Ciencia y Tecnología (CONACYT, México) under Grants No. 43830-F and No. 44831-F.

Romeo de Coss
Department of Applied Physics, Cinvestav-Merida, Mexico.

Date submitted: 06 Dec 2004

Electronic form version 1.4