Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Electronic structure and bonding properties of K and K $^+$ on graphite under external electric field[1] ALEJANDRO TAPIA, ROMEO DE COSS, Department of Applied Physics, CINVESTAV-Merida, Mexico., GABRIEL CANTO, CCMC-UNAM, Ensenada, Mexico. — The effect of an external electric field on the adsorption of K and K^+ on the graphite (0001) 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 and K^+-graphite system are studied in the triangular (2x2) overlayer phase as a function of the external electric field magnitude. We find an important change in the K and K^+-graphite bonding as a consequence of the charge transfer from the adatom towards the substrate induced by the electric field. However, we find that none of the investigated systems show diffusion of K or K^+ into graphite even with a strong electric field. The results are discussed in the light of the experimental observed diffusion of K into graphite, presumably induced by external electric fields.

[1]This work was supported by Consejo Nacional de Ciencia y Tecnologia (CONACYT, Mexico) under Grants No. 43830-F and No. 44831-F.

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Date submitted: 07 Dec 2005 Electronic form version 1.4