

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Electronic structure and bonding properties of hydrogen on K(2x2)/Graphene.¹ CÉSAR ACOSTA, JORGE ALEJANDRO TAPIA, Facultad de Ingeniería, Universidad Autónoma de Yucatán, ROMEO DE COSS, Departamento de Física Aplicada, Cinvestav-Mérida — The effect of the adsorption of hydrogen atom on the electronic properties of K(2x2)/graphene system, are studied by means of first-principles 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 H atoms on K/graphene system are calculated by molecular dynamics. We find an important charge transfer from the substrate towards the H atoms. The strong H-C chemical bond produced a considerable deformation in the graphene layer. The bonding energy of hydrogen is larger for the K/graphene system than for the single layer of graphene. The present results suggest that the hydrogen adsorption on layered carbon systems could be stimulated by the pre-adsorption of simple metals.

¹This research was supported by PRIORI-UADY under Grant No. FING-05-004 and Consejo Nacional de Ciencia y Tecnología (CONACYT-México) under Grant No. 43830-F.

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Date submitted: 23 Nov 2007

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