Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Hydrogen, methane and water adsorption on a carbon-silicon surface[1] FERNANDO MAGAÑA, GERARDO VAZQUEZ, Instituto de Fisica, Universidad Nacional Autonoma de Mexico, Apartado. Postal 20-364, C.P. 01000, Mexico, D. F., Mexico — Density functional theory and molecular dynamics were used at 300 K to study the adsorption of several molecules on a graphene layer modified with silicon, with the Si atoms located substitutionally. We studied the adsorption of H_2, CH_4, H_2O.

[1]We acknowledge partial financial support by grant DGAPA-UNAM number IN111807 and the technical assistance of Kanbalam supercomputer center, UNAM.

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Date submitted: 27 Nov 2009 Electronic form version 1.4