Hydrogen, methane and water adsorption on a carbon-silicon surface\textsuperscript{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\textsubscript{2}, CH\textsubscript{4}, H\textsubscript{2}O.

\textsuperscript{1}We acknowledge partial financial support by grant DGAPA-UNAM number IN111807 and the technical assistance of Kanbalam supercomputer center, UNAM.