Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Water adsorption on a titanium-graphene surface with high metal density

GERARDO J. VAZQUEZ, EDUARDO RANGEL, GREGORIO RUIZ-CHAVARRIA, FERNANDO MAGAÑA, Instituto de Física, Universidad Nacional Autónoma de México — Density functional theory and molecular dynamics were used to study the adsorption of a water molecule on a graphene layer modified with titanium at high metal coverage, with the $\text{Ti}$ atoms located above the centers of the carbon hexagons. Two stable configurations for the titanium-graphene sheet were considered. One with one titanium atom per eight carbon atoms and the other with one $\text{Ti}$ atom per two $\text{C}$ atoms. We found that the water molecule is adsorbed on both configurations, but it is dissociated in two different ways forming $\text{H}_2\text{O}$ and $\text{HO}$ when the interaction is with the second configuration.

Fernando Magaña
Instituto de Física, Universidad Nacional Autónoma de México

Date submitted: 20 Nov 2008     Electronic form version 1.4