Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Simultaneous Adsorption of Water and Carbon Dioxide on Graphene-Titanium-Silicon Carbide System GREGORIO RUIZ-CHAVARRIA, Universidad Autonoma Chapingo — The adsorption of water and carbon dioxide has been studied separately in several works in recent times. These processes are important for the transcendence that would imply perform them in a simple and stable way. Controlling these processes we could fix carbon from the atmosphere and possibly obtain hydrocarbons. In a previous work [1], with colleagues, we performed a numerical calculation of the adsorption of water on a sheet of graphene. In this work I present a theoretical numerical calculation of the simultaneous adsorption of water and carbon dioxide on a titanium-graphene system that relies on silicon carbide as substrate support. In this calculation we consider the interaction of water and carbon dioxide with the graphene-titanium system and the substrate, but also the interaction between water and carbon dioxide. In development of this calculation I used density functional theory, atomic pseudo-potentials and molecular dynamics. I compare the results obtained with the reports of previuos works.

[1] Carbon, 47, 2 (2009), pp531-533

Gregorio Ruiz-Chavarria
Universidad Autonoma Chapingo

Date submitted: 14 Nov 2013 Electronic form version 1.4