

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Adsorption of Water Molecule on Silicene-Fe System GREGORIO RUIZ CHAVARRIA, UNIVERSIDAD AUTONOMA CHAPINGO — After graphene synthesis[1], there have been numerous studies on similar systems in two dimensions so, we have the borophene [2], germanene [3], silicene [4,5], phosphorene [6], etc. Following this line, I do a study that takes the silicene system at its starting point, system to which it add Fe atom. At first, the stability of SILICENE-Fe system is studied, which is stable. Then a water molecule is added to the SILICENE-Fe system, which is captured, as is bounded to the Fe atom. To make this study I used Functional Density Theory, Born-Openheimer Approximation, Atomic Pseudopotentials and Molecular Dynamics.

- [1] Novoselov, K.S.;Geim, A.K. et al, Science, **306** , 666 (2004).
- [2] Yang, X., et al, PRB,**77**, 041402(R) (2008).
- [3] Bianco, E., et al, ACS Nano, **7**, 4414 (2013).
- [4] Kamal, C, et al, J.Phys.: Condens. Matter, **25**, 085508 (2013).
- [5] Drummond, N.P., et al, PRB,**85**, 075423 (2012).
- [6] Liang, L., et al, Nanolett., **14**, 6400 (2014).

GREGORIO RUIZ CHAVARRIA
UNIVERSIDAD AUTONOMA CHAPINGO

Date submitted: 28 Jan 2016

Electronic form version 1.4