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Interaction of Water Molecule with FE-Graphene System GREGORIO RUIZ-CHAVARRIA, Universidad Autonoma Chapingo — In this work I made a numerical simulation of the interaction between the water molecule with a Fe-graphene system. The graphene system used in this calculation is no planar, unlike the graphene widely used, but this system is a buckling system, quasi-two-dimensional system. This system has been studying previously experimental and theoretically [1]. One way to obtain graphene is from silicon carbide [2] which is subjected to thermal treatement, obtaining graphene with silicon carbide as substratum. I first obtain the stability for the graphene buckling, then add a Fe molecule, studying the stability of the system graphene buckling with Fe molecule. Finally add a water molecule, studying the evolution of the total system. I compare the obtained results with other results. To make our calculations I use Density Functional Theory, atomic pseudopotentials, Born-Openheimer approximation and Molecular Dynamic. [1] Hibino, H, et al, NTT Technical Review, Vol. 8, No 8,2010. [2] Ruan, M, et al, MRS Bulletin,Vol. 37, p. 1138 , 2012.

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