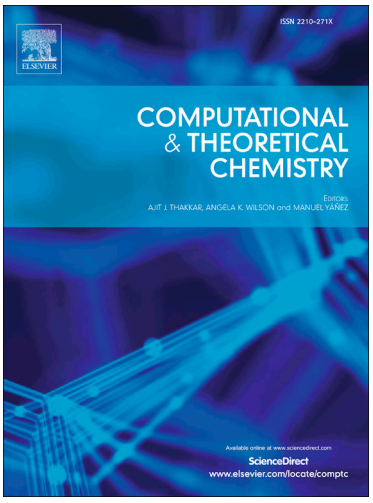

Formaldehyde adsorption on Graphane

Emiliano Ventura-Macias, J. Guerrero-Sánchez, Noboru Takeuchi

PII: S2210-271X(17)30365-1
DOI: http://dx.doi.org/10.1016/j.comptc.2017.08.010
Reference: COMPTC 2591

To appear in: *Computational & Theoretical Chemistry*

Received Date: 10 July 2017
Revised Date: 7 August 2017
Accepted Date: 8 August 2017

Please cite this article as: E. Ventura-Macias, J. Guerrero-Sánchez, N. Takeuchi, Formaldehyde adsorption on Graphane, *Computational & Theoretical Chemistry* (2017), doi: http://dx.doi.org/10.1016/j.comptc.2017.08.010

Formaldehyde adsorption on Graphane

Emiliano Ventura-Macias, J. Guerrero-Sánchez, and Noboru Takeuchi

Centro de Nanociencias y Nanotecnología, Universidad Nacional Autónoma de México, Apartado Postal 14, Ensenada Baja California, Código Postal 22800, México.

Using first principles calculations, we have studied the adsorption of a formaldehyde molecule on a hydrogenated graphene substrate, by a free radical initiated reaction. This kind of reaction begins at a hydrogen vacancy on the graphane layer, in which, the oxygen atom of the formaldehyde molecule attaches. Then, the nearest hydrogen atom is abstracted by the carbon atom of the formaldehyde, forming a stable molecule, and leaving behind a new dangling bond on the graphane substrate. Our calculations show that the reaction has an energy barrier of the order of 0.56 eV, larger than in the case of silicane, indicating that graphane is not a very good substrate for formaldehyde adsorption. Analysis of the electronic structure and spin density distributions help us to understand the proposed reaction.

Keywords: graphane, formaldehyde, hydrogen abstraction, chain reaction.