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Formaldehyde adsorption on Graphane

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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.

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