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Adsorption of water on a carbon-gold surface[1] FERNANDO MAGAÑA, GERARDO J. VAZQUEZ, Instituto de Física, Universidad Nacional Autónoma de México — Density functional theory and molecular dynamics were used at 300 K to study first the interaction of a gold atom (Au) with a graphene layer with a vacancy. The Au Atom is adsorbed on the vacancy then we studied the adsorption of H_2O on the Au anchored on the vacancy of graphene. We found that the water molecule is adsorbed on such configuration and it is not even dissociated at high temperatures like 1000 K.

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