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Water adsorption on a titanium-graphene surface with high metal density GERARDO J. VAZQUEZ, EDUARDO RANGEL, GREGORIO RUIZ-CHAVARRIA, FERNANDO MAGAÑA, Instituto de Física, Universidad Nacional Autónoma de México — Density functional theory and molecular dynamics were used to study the adsorption of a water molecule on a graphene layer modified with titanium at high metal coverage, with the Ti atoms located above the centers of the carbon hexagons. Two stable configurations for the titanium-graphene sheet were considered. One with one titanium atom per eight carbon atoms and the other with one Ti atom per two C atoms. We found that the water molecule is adsorbed on both configurations, but it is dissociated in two different ways forming H, O and HO when the interaction is with the second configuration.

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