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Hydrogen Molecule Adsorption on a Borophene-Titanium System GREGORIO RUIZ-CHAVARRIA, Universidad Autonoma Chapingo — From the synthesis of graphene have developed a wide range of researchs on their use, both theoretical and experimental. So there have been research on graphene-based electronics, but also on issues of energy, particularly hydrogen adsorption on graphene-based systems. Given the potential represented by these structures is very natural to wonder about similar structures, but based in elements near carbon. One of the lines developed very recently consider the boron as the element to build graphene-like structures. Different studies, both theoretical and experimental have been made where the studied structures are graphene type or fullerene, where boron is used in place of carbon. We will use as a starting point the proposed structures by Xiaobao[1] and Tang.[2] This structure is known as the borophene, which in first place will be decorated with titanium and then, this system interact with hydrogen molecule. In our calculation we use functional density theory, atomic pseudopotentials, Born approximation and molecular dynamic.

[1]Xiaobao Y, et al, Phys Rev B, **77**, 041402 (2008)
[2]Tang H. and Ismail-Beigi S., PRL, **99**, 115501 (2007)

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