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Molecular hydrogen adsorption on the boron-doped graphene sheet in presence of magnesium and transition metal ZHAOHUI HUANG, VNICENT CRESPI, Dept. of Physics, Penn State University — Adsorption of hydrogen molecules onto a boron-doped graphene sheet in the simultaneous presence of magnesium and a transition metal has been studied using density functional methods. This setup is inspired by magnesium dihydride. We obersve that there form bonds between metal and boron atoms, which suggest a potential way to prevent metal from aggregating. Macroscopic aggregation of metal atoms makes this structure useless to adsorb hydrogen. We present results for different combination of transition metal and magnesium, and compare the binding energy of hydrogen molecule adorbed onto those structures.

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