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Hydrogen adsorption at graphene layers doped with transition metals: Insight from DFT simulations.

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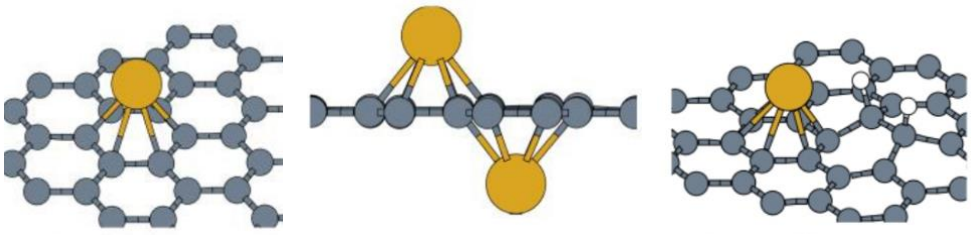
The interaction of hydrogen with graphitic systems has been extensively studied, searching for novel materials capable of adsorbing high quantities of hydrogen. In this study, we have employed DFT simulations to analyze the dissociation of hydrogen at graphene layers doped with various types of metal atoms, such as Li, Mg, Al, Cu, Zr and Ru. Also, we have studied the tendency of these metal atoms to form clusters in the surface of graphene. Depending on the element, strong differences are found in the trends for clustering, with dispersion on the graphene layer strongly favoured for s-p metals such as Li or Al. Then, we have investigated the energetics of the dissociative adsorption of H2 in the neighbourhood of adsorbed metal atoms. While reactive d-electron metals easily break the H-H bond, transfer of the dissociated hydrogen atoms to the graphene layer is hampered by large barriers. Finally, we have also studied the interaction between dissociating hydrogen with metal atoms adsorbed at the other side of a graphene layer. The presence of the metal induces sizable variations in the H-C binding strenght.



Adsorption of Zr atoms at graphene

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