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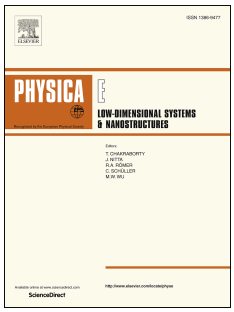

Hydrogenated black phosphorus single layer

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Hydrogenated Black Phosphorus Single Layer

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ABSTRACT

Using the first principles calculations, we investigated the physical properties of hydrogenated black phosphorene layer. For a single H adsorption, the P top site became the most stable adsorption position and this impurity adsorption created a broken P-P bond. Due to this broken bond, the adsorption of a single hydrogen atom on a phosphorene layer induced a total magnetic moment at about 1.0 μ_B and that the spin-polarized state was mainly localized around the dangling phosphorus atom. In the hydrogenated system, the hydrogen atoms preferred the different sublattice adsorption at rather short H-H inter-atomic distance (~ 3.5 Å) while the sublattice dependent formation energy was greatly suppressed at larger than H-H distance of 3.5 Å. We obtained that the hydrogenated phosphorene layer displayed an antiferromagnetic state until the H-H inter-atomic distance became around 8 Å and the energy difference between ferromagnetic (FM) and antiferromagnetic (AFM) states almost vanished beyond this interatomic distance. This result may suggest that the hydrogenated phosphorene layer system shows an antiferromagnetic state at high H concentration while the exchange coupling is greatly suppressed at low H concentration. Thus, it will be possible to manipulate the magnetic property by applying even small magnetic field at low H concentration and this can feature can be utilized for spintronics applications.

Keywords: ab initio, Adsorption, Hydrogen, Black phosphorus, Magnetic properties.