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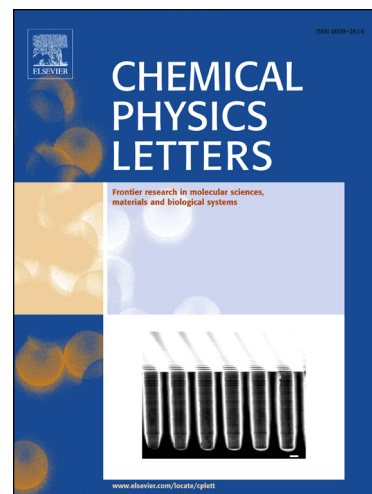
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Enhanced hydrophilic and conductive properties of blue phosphorene doped with Si atom

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Abstract

In this paper, the electronic, magnetic properties and the effect of Si-doped blue phosphorene on the adsorption of a H₂O molecule have been investigated using density functional theory with van der Waals corrections. The results indicate that doping Si into blue phosphorene can facilitate the dissociative adsorption of H₂O molecules. The dissociative energy barrier is reduced from 2.45 eV on pristine blue phosphorene to 0.19 eV on Si-doped blue phosphorene, which indicates a smooth dissociative adsorption. In addition, the dissociative adsorption of H₂O molecules can convert the Si-doped blue phosphorene from hydrophobic to hydrophilic with a semiconductor-to-metal transition.

Keywords: Blue phosphorene; Electronic properties; First principles calculations;

Adsorption

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