Theoretical study of formaldehyde interaction with pristine and Si-doped phosphorene

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Formaldehyde ($H_2CO$) is a toxic gas present in the smoke generated by several industries, chronic exposure to this gas can cause respiratory diseases, being associated with the development of cancer in organs of the respiratory system [1]. Therefore, to guarantee the environment security, it is important to monitor formaldehyde presence. Researchers theoretically studied the use of Si-doped graphene as formaldehyde sensor [2]; however, phosphorene discovery has been increasing studies relative to the use of pristine and metal doped phosphorene as CO, $CO_2$, $NH_3$, NO and $NO_2$ sensor [3][4]. Despite that, the study of pristine and Si-doped phosphorene as formaldehyde sensor is new. Therefore, the aim of this study is to evaluate electronic and structural properties of formaldehyde interaction with pristine and Si-doped phosphorene, to analyze the use of phosphorene as formaldehyde sensor. This study was based on the Density Functional Theory, implemented in SIESTA code [5]. Formaldehyde interaction with pristine and Si-doped phosphorene was studied considering eight configurations. Binding energies found for formaldehyde interaction with pristine phosphorene range from $-0.03$ eV to $-0.05$ eV and no significant change in the electronic properties after the interactions was observed, indicating an extremely weak interaction. Binding energies found formaldehyde interaction with Si-doped phosphorene range from $-0.01$ eV to $-1.00$ eV. The most stable configuration was the one in which C is the closest atom of the nanostructure, with bonding energy of $-1.00$ eV and the smallest C-Si bond distance of 1.89 Å, characterizing as chemical interaction. The electronic properties indicate variation of the gap from 0.20 eV to 0.67 eV after the interaction. These results indicate that Si-doped phosphorene could be a potential formaldehyde sensor.