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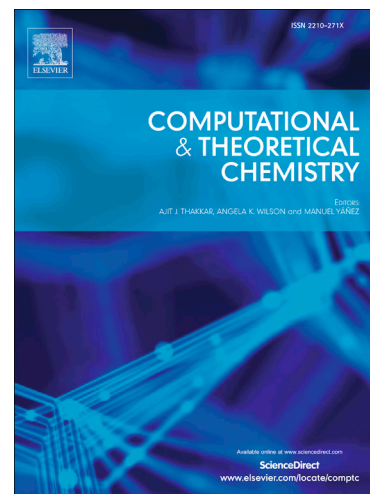
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# Density functional theory investigation of the interactions between the buckled stanene nanosheet and $XO_2$ gases ( $X=N, S, C$ )

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## Abstract

Based on the density functional theory calculations, we examined the adsorption behaviors of triatomic gas molecules (such as  $NO_2$ ,  $SO_2$  and  $CO_2$ ) on the buckled stanene nanosheets. By studying the interactions between stanene and  $XO_2$  gases ( $X=N, S$  and  $C$ ), we exploited the gas sensing capabilities of innovative stanene based sensors. We investigated the electronic properties of the studied systems in terms of the density of states, Mulliken charges and charge density difference calculations. The results indicated that the adsorption of gas molecules on the doped stanene nanosheets is more favorable in energy than that on the pristine ones, implying that the doped stanene acts as an appropriate candidate for sensing materials. The electronic density increases at the middle of the newly formed bonds between stanene and gas molecule. Charge density difference calculations indicated that both  $NO_2$  and  $SO_2$  gases exhibit acceptor characteristics, as evidenced by the charge accumulation on the adsorbed gas molecules. The strong PDOS overlaps between the N, O atoms in the  $NO_2$  molecule and the Sn atoms of the stanene nanosheet, indicated the formation of chemical bonds between them. Also, the PDOS spectra of the O atoms of  $SO_2$  molecule and Sn atoms show significant overlaps, indicating the formation of a double contacting point for  $SO_2$  on the stanene. The band structures diagrams of the gas molecule adsorbed stanene nanosheets show that the VBM and CBM are slightly altered upon gas adsorption. Our theoretical findings show that stanene holds a great potential to be utilized as highly efficient sensor device for detection of triatomic gases like  $NO_2$ ,  $SO_2$  and  $CO_2$  in the atmosphere.

Keywords:  $XO_2$ ; Band structure; Stanene sheet; DFT; charge density difference

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