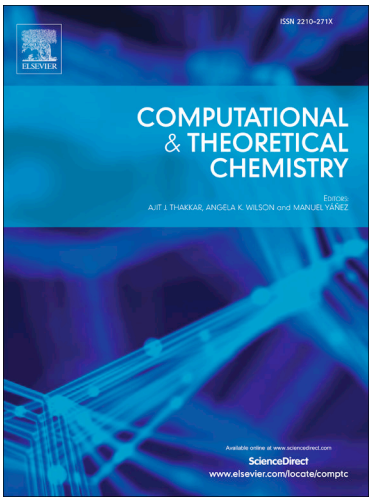

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Density functional theory investigation of the interactions between the buckled stanene nanosheet and XO_2 gases (X=N, S, C)

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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 bad 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