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Adsorption of CO and CO_2 molecules on nitrogen-doped armchair silicene/graphene nanoribbons as a gas sensor

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Abstract: The adsorption of CO and CO_2 molecules on pristine and nitrogen-doped silicene/graphene nanoribbons (N-doped SiGNR) has been studied using density functional theory (DFT). The electronic structure, energy gap, density of states and adsorption energies are obtained. The adsorption energies of CO molecules on pristine and N-doped SiGNR is a strong chemisorption with adsorption energies being larger than 1.0 eV, therefore, SiGNR could catalyse or activate this adsorbate due to the strong interaction, suggesting the possibility of N-doped SiGNR as a metal-free catalyst. Also, our results show that the adsorption energy of CO_2 on N-doped SiGNR is between −2.17and -3.23eV, indicating that SiGNR could be a good CO_2 sensor and more sensitive to the adsorption of CO_2 than pristine and N-doped SiGNR. Thus, the sensitivity of gases on SiGNR can be significantly improved by introducing nitrogen as dopants. Moreover, the energy gap of pristine and N-doped SiGNR is opened upon adsorption of CO and CO_2 in various ways. In general, the energy gap for CO molecule on SiGNR are larger than those of CO_2 molecules on SiGNR.
Key word: giardiasis, Najaf, P-selectin, ferritin, IL-8.

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