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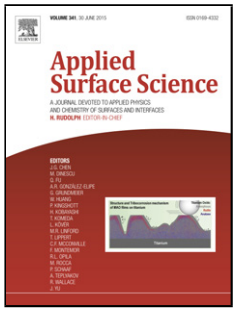

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A first-principles study on adsorption behaviors of pristine and Li-decorated graphene sheets toward hydrazine molecules

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Highlights:

- Pristine graphene sheet was proposed for N_2H_4 molecule adsorption with weak physisorption, suggesting that pristine graphene sheet is insensitive to the presence of N_2H_4 molecule.
- Li-decorated graphene sheet is significantly sensitive to detect N_2H_4 molecule due to high binding energy, implying that Li-decorated graphene sheet could be considered as a potential gas sensor in field of hydrazine molecules.
- The effects of concentrations of N_2H_4 molecules adsorbed on pristine and Li-decorated graphene sheets were studied detailedly.

Abstract

The adsorption behaviors and properties of hydrazine (N_2H_4) molecules on pristine and Li-decorated graphene sheets were investigated by means of first-principles based on density functional theory. We systematically analyzed the optimal geometry, average binding energy, charge transfer, charge density difference and density of states of N_2H_4 molecules adsorbed on pristine and Li-decorated graphene sheets. It is found that the interaction between single N_2H_4 molecule and pristine graphene is weak physisorption with the low binding energy of -0.026 eV, suggesting that the pristine graphene sheet is insensitive to the presence of N_2H_4 molecule. However, it is markedly enhanced after lithium decoration with the high binding energy of -1.004 eV, verifying that the Li-decorated graphene sheet is significantly sensitive to detect N_2H_4 molecule. Meanwhile, the effects of the concentrations of N_2H_4 molecules on two different substrates were studied detailedly. For pristine graphene substrate, the average binding energy augments apparently with increasing the number of N_2H_4 molecules,