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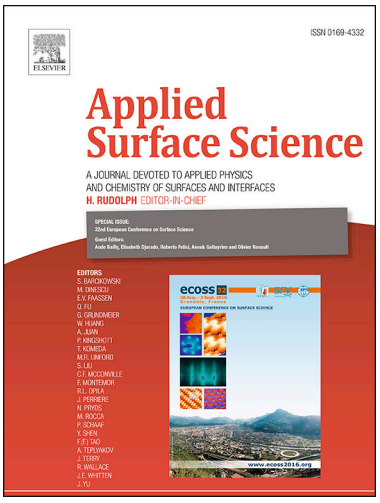

Full Length Article

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Adsorption sensitivity of Fe decorated different graphene supports toward toxic gas molecules (CO and NO)

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Abstract

Sensitivity of Fe-decorated graphene with three different graphene-based supports (single vacancy, double vacancy and four nitrogen decorated) toward toxic gas CO and NO has been investigated by first-principles density functional theory (DFT) calculations. The adsorption configuration, adsorption energy, charge transfer, density of states, competitive behaviors of CO and NO on Fe/GN are thoroughly discussed. Furthermore, Fermi softness is investigated to evaluate the reactivity of the Fe/GN substrates surface. It is found that NO is strongly adsorbed on Fe/GN with considerable adsorption energy of 2.04~2.41eV, while CO is relatively weaker adsorbed on the same substrates with adsorption energy of 1.10~1.53eV. Based on our calculation, when CO and NO exist simultaneously, the possibility of adsorption CO can be neglected on the Fe/GN surface. In addition, Fermi softness is a good descriptor to characterize the reactivity of our Fe/GN surface. Our results could provide crucial information for adsorption sensing of NO on Fe/GN, which may be a useful clue for the design and fabrication of Fe-decorated graphene as NO sensors and adsorbent.

Key words:Fe-decorated graphene, adsorption characteristics, steric effect, Fermi softness

1.Introduction

The demand for high sensitivity, high response, high selectivity, high reliability, fast recovery, and low cost miniaturized sensors has prompted scientists to seek new gas sensing systems based on new nanomaterials. Graphene as a two-demensional carbon sheet is an advanced material, its unique long-range π-conjugated structure brings graphene outstanding mechanical and electrical properties[1-4].