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A DFT STUDY OF CO GAS ADSORPTION ON METAL DOPED GRAPHENE SHEET

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Abstract: *The interaction of Ni-doped graphene sheet with CO molecule is investigated using density functional theory simulation to analyze the reactivity of doped graphene towards CO molecule. The adsorption energy is calculated for energetically favorable adsorption of CO on doped graphene sheet. Our result indicates that the structural properties of NI-doped graphene sheet are influenced by the adsorption of CO. The electronic band structure result for CO adsorbed on the doped graphene sheet shows the significant changes in the electronic properties of Ni-doped graphene.*

Keywords *– doped graphene, density functional theory, CO, adsorption energies, structural properties,, electronic properties.*

1. INTRODUCTION

CO is one of the pollutant gas in atmosphere .Accurate, adsorption and sensing for CO is required. Graphene as a 2-Dimensional Nanosheet is fascinating nanomaterial in nanoscience. Graphene has vast application in different branches of science and engineering because of fast response time and high sensitivity at room temperature. It can use as a sensor for sensing various gases present in atmosphere. Various research groups around the globe studying changes in structural and electronic properties of doped graphene and its interaction of different gases .Aluminum doped graphene studied by Weidong Wang *et.al,* they found that adsorption energy of Al-doped graphene is -2.69eV. In our research we doped graphene one carbon atom by Nickel and investigated the effect on CO adsorption on Ni-doped graphene sheet. Our result indicate that after adsorption energy of CO on Ni doped graphene is higher , -2.85eV.

1. COMPUTATIONAL METHODE

The density functional theory (DFT) calculations were performed using Quantum ESPRESSO package with the projector augmented wave (PAW) basis sets and periodic boundary conditions. The generalized gradient approximation (GGA) with the perdew-Burke-Ernzerhof (PBE) exchange-correlation functional is used and the plane-wave cutoff energy is set as 50 Ry for all calculations. The single layer of 5X5 graphene supercell is made using Virtual Nano Lab builder. Simulated structure consists of 5x5 graphene unit cells (containing 50 carbon atoms) one carbon atom is doped via substitution by adding an impurity Nickel and single CO molecule adsorbed on it The dopant concentration in 5x5 graphene sheet is 2%. The supercell extended 10 Å in z-axis , to avoid the interference between adjacent periodic images. The geometrical optimization and self-consistency calculation the Brillouin zone is sampled using a 5x5x1 Monkhorst-pack grid and a Gaussian smearing of 0.05 eV. Atomic positions are optimized until the maximum force on each ion is less than 0.001 eV/ Å. For the band structure calculation the high symmetry k-point path was selected as M-T-K-M with the help of XcrysDen.. To evaluate the interaction between a CO molecule and doped graphene sheet, the adsorption energy (E_{ad}) is calculated as given in Eq. (1).

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$$E_{(ad)} = E_{(tot)} - E_{(dg)} - E_{(CO)} \quad (1)$$

In Eq. (1), $E_{(tot)}$ is the total energy of the doped graphene with a bound CO molecule, $E_{(dg)}$ is the energy of doped graphene and $E_{(CO)}$ is the energy of the isolated CO molecule. All energies were calculated for optimized atomic structures.

2. RESULTS AND DISCUSSION

We first optimized a pristine graphene sheet. The lattice constant and C-C bond length of pristine graphene is 1.42 Å (Fig. 1.a), which is same as reported results [3]. Substitution of a single C atom by Ni atom in Ni-G results in distortion of the structure due to higher vande wall radius of the dopant atom compared to the host carbon atoms. The obtained relaxed structure of NiG is shown in Fig. (1.b), where the dopant atom forms bond with neighboring carbon atoms. The bonds around the dopant atom expands to 1.68 Å (Ni-C). After determine the most stable structure of doped graphene, we next discuss the adsorption of CO on Ni-G. CO molecule is initially placed on-top site of the doping atoms. The system is allowed to relax as per the parameters described above, and for these optimized system the adsorption energy and the binding distance (equilibrium graphene-gas molecule distance) are calculated. After CO adsorption, we find that there is significant change in the structure of Ni-G as shown in Fig. 1.c, where it demonstrates the fully relaxed structures of CO adsorbed-NiG. After relaxation, the most stable adsorption configuration is found to be the one in which carbon atom of CO is oriented downwards with C-atom of molecule close to the nickel atom. The CO molecule is located at a distance 1.86Å above the doped graphene sheet i.e. is the distance between the Ni atom and C atom of CO-molecule. The energetic behavior of CO adsorptions on NiG studied by calculating the adsorption energies as in equation 1. The negative $E_{(ad)}$ values indicate that CO adsorption is energetically favorable. The high values of adsorption energy (-2.85 eV) and small binding distance (1.86Å) show that the interactions of CO with NiG is strong and CO adsorbed-NiG system via very strong physisorption bond.

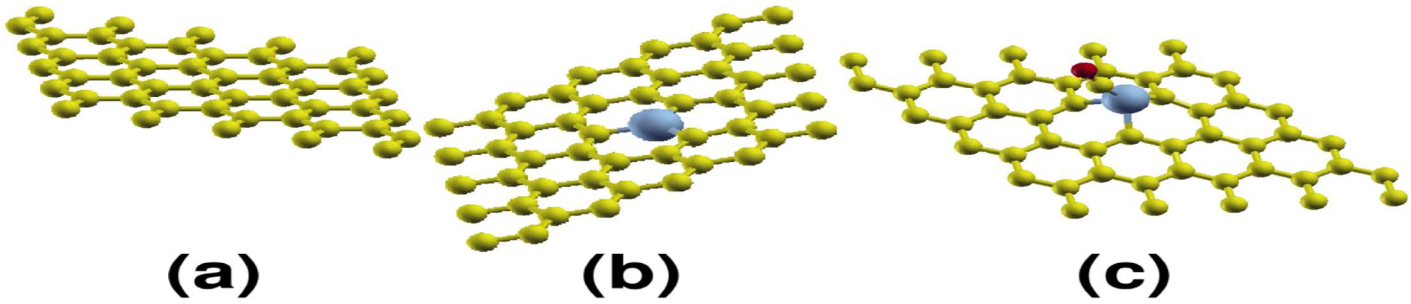

Fig 1

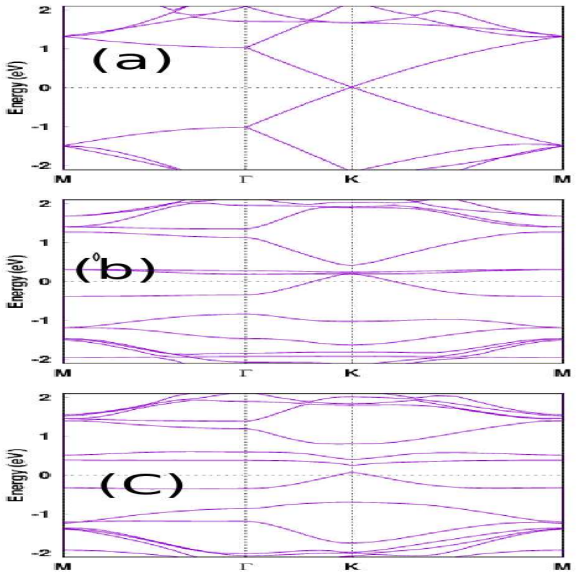

Fig 2

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2. CONCLUSION

The application of Ni doped graphene for CO adsorption have been investigated using first principles DFT method to analyze the gas sensing properties of nickel doped graphene towards CO molecule. The structural and electronic properties of NiG found to be highly sensitive to the adsorption of CO. The electronic band structure of NiG before and after CO adsorption indicate that CO adsorption should result in significant change in the electrical conductance of NiG. Nickel doped graphene is highly reactive to CO molecule and can be used as an effective gas sensor for sensing CO gas.

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