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Heavy metals and some gases adsorption on Graphene surfaces

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Abstract
Graphene applications are known worldwide in field of adsorption. The heavy and toxic metals absorptions, and as a catalyst and removal of toxic by-products are major fields of research. Unique structural properties of graphene make it a useful material as adsorbent. Different electronic properties, like partial density of states (PDOS), reveal that on doping with a cluster, the band gap of the surface decreases and the substrates start showing magnetic character. The adsorption properties of graphene make it a commendable material in surface chemistry. Electron density difference plots give insights into the adsorption behavior of heavy metals and some poisonous gases.

Keywords: Graphene, heavy metals, gases, doped graphene

Introduction
A variety of organic pollutants which are the source of environmental pollution, like drugs formed by organic compounds are not absorbed by the animals. These pollutants enter the environment by different means, such as by human excreta and waste materials. A large variety of pesticides include carbamates, organophosphates, and organochlorines are used worldwide to kill the agricultural pests. Some of the pesticides, if used in excess, remain inside the vegetables and other agriculture food products. (Wang *et al.,* 2013) [1] Some of the organic pesticides are the major water pollutants, as they are discharged by the sewage water. As the carbamates are the major inhibitors for acetylcholinesterase, their deposition may affect nerve transmission. Some of the carbamates and their metabolites may also be carcinogenic (Santalad *et al.*, 2010) [2]. A large number of techniques have been employed for the removal of these pollutants from the environment. Some of the methods are effective and some have side effects, so we need to develop a method which can serve as a better substitute for the removal of organic as well as inorganic pollutants.
Adsorption of the pollutants is one of the most effective ways for their removal, which does not cause the release of any secondary pollutants (Dubey *et al.,* 2009) [3]. So we need to find a chemical compound having good as well as exploitable adsorption properties. Because of the excellent adsorption properties of graphene, it can be useful for the removal of a variety of hazardous organic and inorganic chemicals. Graphene is one of the carbonaceous materials like activated carbon. A common sorbent sheet, randomly substituted with heteroatoms, is an effective sorbent for removal of metal ions, their complexes and other chemical species. Graphene is a densely packed two dimentional sp^2 carbon sheet with one-atom thickness arranged in a hexagonal pattern. Recent developments about graphene suggest how important it is in the present era for removing hazardous and carcinogenic substances from various contaminated materials (Novoselov *et al.*, 2012) [4]. In addition, graphene is a zero gap semiconductor. The robust and flexible structure of graphene provides a unique matter for surface chemistry. All the forms of graphite are made of graphene i.e. zero dimensional fullerene, one-dimensional graphene and three-dimensional graphite. In terms of properties, graphene is unique as it has a soft membrane and at the same time possesses a high Young's modulus, and good thermal and electrical conductivities (Abergel *et al.*, 2010; Georgakilas *et al.* 2012) [5, 6]. In addition, a single-layer graphene is a zero band gap material and highly transparent, exhibiting optical transmittance of 97.7%. With its high theoretical specific surface area of 2600 $m^2\ g^{-1}$, graphene provides a rich platform for surface chemistry (Huang *et al*., 2012; Wei *et al.*, 2012) [7, 8].

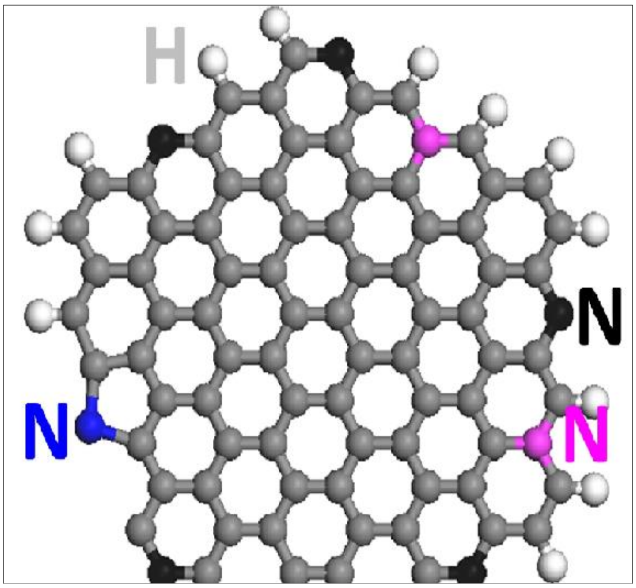

Fig 1: Doped Graphene with Nitrogen atom

The combined extraordinary physical and chemical properties of graphene, in turn, have ignited extensive research in nanoelectronics, super capacitors, fuel-cells, batteries, photovoltaic, catalysis, gas sorption, separation and storage, and sensing (Xiang *et al*., 2012; Zhang *et al*., 2012) [10, 9]. So based on these properties of grapheme, various graphene-based materials can be prepared. By exploiting the properties of graphene, various purposes could be served, like in surface chemistry as absorbents for extracting various hazardous and carcinogen substances, in fuel cells and in semiconductors.

Applications of Graphene and Modified Graphene
Metals

Carpio *et al.* (2014) evaluated graphene oxide–EDTA's adsorption capacity for two heavy metals, Cu^{2+} and Pb^{2+}, at different concentrations, varying pH and contact time. It was found that a 5% increase of EDTA content in graphene oxide–EDTA made it possible to achieve removal with a shorter contact time than previous studies for both lead and copper. Ellis *et al.* (2013) reported the adsorption performance of calcium alginate and calcium alginate with encapsulated graphene oxide gel bead adsorbents for the removal of Cu^{2+} ions from aqueous solution. The adsorption isotherm data was fitted by Langmuir isotherms. Chella *et al*. (2014) [11] prepared the graphene manganese ferrite composite by a solvothermal process. It was used as an adsorbent for Pb^{+2} and Cd^{+2} ions. It was found that with respect to contact time measurements, the adsorption of Pb^{+2} and Cd^{+2} ions increased. The experimental data was well fitted and presented through the Langmuir isotherm model. Thermodynamic properties showed that the adsorption of Pb^{+2} and Cd^{+2} ions on to graphene manganese ferrite composite was spontaneous and exothermic. Results showed that the prepared composite possesses good adsorption efficiency and thus could be considered as an excellent material for removal of toxic heavy metal ions. Hence, the graphene manganese ferrite composite can be used as an adsorbent as well as an antimicrobial agent. Magnetic cobalt ferrite-reduced graphene oxide nanocomposites (Zhang *et al.*, 2013) [12] were developed as adsorbents to remove Pb^{+2} and Hg^{+2} from aqueous solution. It was found that the data fitted well to pseudo-second order kinetics and Langmuir isotherm models. The synthesis of magnetic cobalt ferrite-reduced graphene oxide nanocomposites is sample. cost effective and safe.

Gas adsorption on Graphene surfaces

On the basis of first-principles of density-functional theory (DFT), Tang *et al.* (2015) investigated the effects of gas adsorption on the change in geometric stability, electronic structure and magnetic properties of graphene with anchored Co (Co-graphene) systems. The adsorbed NO, SO_2, CO or HCN on Co/pristine-graphene show semiconducting property and the relatively weak adsorption of NH_3 on Co/pristine-graphene exhibits semimetal property. Meng *et al.* (2014) synthesized Cu_2O nanorods modified by reduced graphene oxide. They were used for the sensing of NH_3 at room temperature. The sensor also showed excellent repeatability and selectivity to NH_3. The remarkably enhanced NH_3-sensing performances could be attributed to the improved conductivity, catalytic activity for the oxygen reduction reaction and increased gas adsorption in the unique hybrid composites. Results showed that such a low power, sensitive, and selective sensor could be useful for the development of a new generation of ammonia sensors. Hegde *et al.* (2013) investigated the chemical activity of the carbon site of pristine graphene, Stone–Wales (SW) defect site, and BN-site of BN-doped graphene towards adsorption of a toxic gas, H_2S. The analysis was based on first-principles density functional theoretical calculations incorporating van der Waals interactions. It was found that in the cases of pristine graphene and BN-doped graphene, the charge density of the HOMO and LUMO states was uniformly distributed throughout the graphene sublattice. In this, van der Waals interaction was found with a weak binding energy. In the case of graphene with Stone–Wales defect, the HOMO and LUMO states were confined to the alternating sites of the SW defect. In this case, the van der Waals interaction between the molecule and the surface was stronger compared to that of pristine and BN-doped graphene. Zhu *et al.* (2014) prepared the reduced graphene oxide/ Si Schottky diode by a simple drop-casting/ annealing process that was explored for the possibility of selective gas detection. Results indicated that the reduced graphene oxide/ Si-based device was selective to gases like NO_2 and NO. Two types of unprecedented effects could be attributed to the presence of oxygen functional groups, including the selective binding interactions (strong or weak) to different gas molecules, as well as the impendence to charge interaction between gas molecules and sp^2 hybridized carbon areas in reduced graphene oxide. Hong *et al.* (2014) synthesized graphene-supported carbon-coating cobalt and carbon nanoshells (Co/C-GNS and CNS-GNS) and used them for the absorption of toxic gases and smoke. The resultant Co/C-GNS and CNS-GNS hybrids exhibit an extraordinary adsorption performance for toxic CO and heavy smoke during the combustion of acrylonitrile-butadiene styrene. Kumar *et al.* (2015) synthesized zinc oxide-reduced graphene oxide nanocomposites and used them for NO_2 gas sensing. The results showed that the zinc oxide-reduced graphene oxide composite possesses better electrical conductivity and NO_2 gas sensing properties than those of the reduced graphene oxide sample. Additionally, the effects of the relative humidity on the resistances of the zinc oxide, reduced graphene oxide, and zinc oxide-reduced graphene oxide composite samples were investigated and the results showed that the resistance of zinc oxide-reduced graphene oxide nanocomposites depends very little on the relative humidity.

Conclusion

After studying the adsorption of heavy metals and gases, it has been concluded that the adsorbent properties of graphene can be modified by doping of a metal or crystal of metals. Unique structural properties of graphene make it a useful material as adsorbent. Different electronic properties, like partial density of states (PDOS), reveal that on doping with a cluster, the band gap of the surface decreases and the substrates start showing magnetic character.

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