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Ab initio study of H2S adsorption on graphene doped with P and S

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Graphene, the two-dimensional carbon allotrope with large specific surface area, has shown to be less sensitive to most of the gases, in its pure form. Doping of graphene with other elements has proved to be very efficient in improving the sensitivity of graphene-based gas sensors. Density functional theory (DFT) calculations have reported that O_2, NO, NO_2 and SO_2 are strongly chemisorbed onto phosphorus doped graphene (abbreviated as PG) through the formation of P-X (X=O, N, S) bonds. Similarly, sulphur doped graphene (abbreviated as SG) has shown high selectivity sensing of NO_2 compared with NH_3, CO, SO_2, CH4. Graphene doped with phosphorus and sulphur has been experimentally synthesized. Motivated by the enhanced sensing behavior and successful synthesis of PG and SG, we analyze the suitability of employing them for H2S sensing, which has not been reported earlier. The adsorption property of H_2S on PG and SG sheets are theoretically studied using first-principles DFT calculations. We found that in both PG and SG, the dopant atom protrude out of the graphene layer and there is no significant change in their atomic structures after H2S adsorption.The calculations showed weak physisorption of H_2S on both SG and PG with small adsorption energies of -0.01eV and -0.03eV and large molecule-doping atom distances of around 3.5Å.The results from the Hirshfeld charge distribution analysis of the structuresindicate negligible effect of H_2S on the electrical conductance of the doped graphenes. It was observed that the local curvature induced by P and S doping resulting from the bigger size of the dopant than carbon, does not enhance the reactivity of graphene to H_2S.The observed weak interactions between doped graphene and H_2S indicate that graphene sheets doped with P or S are not suitablefor the detection of H_2S.

Biography

Seba Sara Varghese received her Master's degree (ME) in Microelectronics from Birla Institute of Technology and Science (BITS), Pilani in 2012. She is currently pursuing her PhD in the area of graphene based gas sensors at BITS, Pilani Dubai Campus. Since September 2014, she has been working as a Visiting Graduate Research Assistant in the Department of Chemical Engineering at the Petroleum Institute, Abu Dhabi. Her research interests include microelectro-mechanical systems (MEMS) and nanotechnology, carbon nanotubes and graphene.

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