Abstract Submitted
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Ab-initio study of NH3 and NH adsorption over graphene[1] CESAR CAB, FI-UADY, FELIPE CAB, CICY, ALEJANDRO TAPIA, FI-UADY, SIMULACION DE NANOMATERIALES TEAM — Currently, solid state sensors for detecting chemicals are an intensive area of research and development. Solid state sensors have advantages over conventional systems such as decrease the size and cost, broadening the range of applications. In this work we study the possibility of using graphene for the detection of NH3 and NH, through structural and electronic changes induced in graphene by adsorption of both molecules. The results are obtained with the seudopotential LCAO and GGA approximation for the exchange correlation potential. Study reveals that nitrogen in the NH and NH3 molecules have affinity for the surface of graphene. Analysis of charge transfer is performed to analyze the adsorption process. The molecules have preferential sites of adsorption for NH3, which are the interstitial sites of the hexagonal lattice, the links between carbon atoms, and over the carbon atoms. In the case of NH (nitrene) these sites correspond to the spaces between links, and over carbon atoms. Also, adsorption of both molecules produces major distortions in the network of graphene, which are analyzed.

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