Abstract Submitted
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Charge transfer and adsorption-desorption kinetics in carbon nanotube and graphene gas sensing[1] SANG-ZI LIANG, Department of Physics, Pennsylvania State University, GUGANG CHEN, AVETIK HARUTYUNYAN, Honda Research Institute USA, Inc., MILTON COLE, JORGE SOFO, Department of Physics, Pennsylvania State University — Detection of molecules in the gas phase by carbon nanotube and graphene has great application potentials due to the high sensitivity and surface-to-volume ratio [1, 2]. In chemiresistor, the conductance of the materials has been proposed to change as a result of charge transfer from the adsorbed molecules. Due to self-interaction errors, calculations using LDA or GGA density functionals have an innate disadvantage in dealing with charge transfer situations. A model which takes into consideration the dielectric interaction between the graphene surface and the molecule is employed to estimate the distance where charge transfer becomes favorable. Adsorption-desorption kinetics is studied with a modified Langmuir model, including sites from which the molecules do not desorb within the experimental time. Assuming a constant mobility, the model reproduces existing experimental conductance data [1, 2]. Its parameters provide information about the microscopic process during the detection and varying them allows optimization of aspects of sensor performance, including sensitivity, detection limit and response time. [1] G. Chen et al., Sci. Rep. 2, 343 (2012). [2] G. Chen et al., Appl. Phys. Lett. 101, 053119 (2012).

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