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Adsorption of Nitric Oxide on Carbon Vacancies in Graphene and its Impact on the Conductivity JORGE SOFO, SANGZI LIANG, Physics Department, The Pennsylvania State University, GUGANG CHEN, AVETIK HARUTYUNYAN, Honda Research Institute — The conductance of graphene in FET devices increases when exposed to NO with detection limits down to the part-per-quadrillion level. We explore a possible explanation for this phenomena assuming that NO chemisorbs to vacancies and eventually dissociates. We found that adsorption of NO in graphene vacancies is favorable by 5.3 eV. In order to evaluate the conductivity due to these impurities, we obtain a minimum tight binding model with a Wannier transformation of the Kohn-Sham orbitals obtained by DFT. We evaluate the conductivity using the Kubo-Greenwood formula and the kernel polynomial method. We consider vacancies, NO and N chemisorbed in the vacancies, and O as an adatom on graphene. We found that the conductivity stays the same when NO adsorbs into a vacancy, but it increases when the oxygen atom moves away from the nitrogen atom, either leaving or moving to other parts of the surface, with the former giving a larger increase in conductivity.

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