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Effects of NO_2 physisorption and chemisorption on the conduction of graphene nanoribbons[1] AHMED HASSAN, CORY KNICK , AMIR FARAJIAN, Mechanical and Materials Engineering, Wright State University — Graphene nanoribbons have the potential of being used as the functional part of nanoelectronic gas sensors. This study focuses on the changes induced in the conduction of graphene nanoribbons upon adsorption of NO_2. Both chemisorption and physisorption situations, i.e., NO_2 adsorption with and without chemical bond formation, are studied. We use ab initio electronic structure calculations with MP2 correlation energy in order to optimize the structures of graphene nanoribbons, with hydrogen-terminated edges, in presence of NO_2. Subsequently, quantum conductance calculations are performed using Green's function implementation of the Landauer's approach. We explain different conductance modulation patterns in terms of charge transfer and dipole interactions. The results clarify some of the basic functionality issues of nanoelectronic-based gas sensors.

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