Abstract Submitted
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Ab initio energetics, kinetics, and quantum transport characteristics of graphene nanoribbons as nanosensors for detecting nitrogen dioxide[1] AMIR A. FARAJIAN, KIRTI K. PAULLA, AHMED J. HASSAN, CORY R. KNICK, Wright State University — Molecules adsorption on graphene nanoribbons (GNRs) can be used to engineer and make use of their properties for applications such as energy storage and sensors. We investigate adsorption characteristics by considering nitrogen dioxide as a sample molecule for assessing nanosensor functionality of GNRs. Using ab initio modeling, energetics of various adsorption possibilities are determined and their rate constants are calculated and compared. Nonbonding and weak sp3 adsorptions at the hydrogen-terminated edges are shown to be more feasible than center adsorptions. This shows increased reactivity compared to graphene. Calculated quantum transport responses upon molecules adsorption indicate possibility of sensing extremely low nitrogen dioxide concentrations. Possible approaches for improving gas nanosensor functionality of GNRs are discussed. Reference: RSC Advances, 2013, DOI: 10.1039/c3ra46372a.

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