

Abstract Submitted  
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**The effects of adsorption orientations on transport through a nanotube gas sensor**<sup>1</sup> AMIR A. FARAJIAN, Department of Mechanical and Materials Engineering, Wright State University, ARTA SADRZADEH, OLGA V. PUPYSHEVA, BORIS I. YAKOBSON, Department of Mechanical Engineering and Materials Science, Rice University — We calculate the quantum transport of a nanoelectronic gas sensor for various adsorption orientations of the gas molecules. The nanosensor employs electronic transport properties of a carbon nanotube exposed to NO<sub>2</sub> molecules. The calculations are based on ab initio electronic structures, combined with the Green's function formulation of Landauer's transport theory. Our results show that different energetically equivalent orientations of the NO<sub>2</sub> molecules result in different details of transport characteristics. The main features of transport modulation, however, are the same for all the orientations. Implications for nanotube-based gas sensors are discussed.

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