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Does Moisture Influence the Chemical Detection of Gas Molecules Adsorbed on Single-Wall Carbon Nanotubes? MING YU, University of Louisville, W.Q. TIAN, Jilin University, China, C.S. JAYANTHI, S.Y. WU, University of Louisville — In this work, the role of water in the detection of hydrazine (N_2H_4) by a single-wall carbon nanotube (SWCNT) is investigated using first principles electronic structure calculations (DFT/GGA–USPP)[1]. This calculation is undertaken to interpret the experimental resistivity measurements for N_2H_4 adsorbed on SWCNT that reveal an n-type behavior [2]. Our preliminary theoretical studies of the adsorption of N_2H_4 on SWCNT revealed physisorption for N_2H_4 and an unaltered band structure for the SWCNT [3]. This prompted us to look into the role of water on the bonding of N_2H_4 to the SWCNT. We found that, by introducing a monolayer of water film on the (8,0) SWCNT, the adsorption of N_2H_4 can introduce occupied states near the Fermi level, exhibiting an n-type behavior. However, the introduction of just few water molecules was not sufficient to influence the electronic structure of N_2H_4/SWCNT. Presently, we are studying the influence of water films on the chemical detection of a variety of other gas molecules (N_2, NH_3, *etc.*) by SWCNTs, and the results from such studies will also be reported. [1]. G. Kresse *et al.* Phys. Rev. B **54**, 11169 (1996). [2]. S. Desai, *et al.* (APS, March 2008). [3]. M. Yu, *et al.* (APS, March 2008).

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