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First-Principles Electronic Structure Calculations of N_2H_4 Adsorbed on Single-Wall Carbon Nanotubes[1] M. YU, W.Q. TIAN, C.S. JAYANTHI, S.Y. WU, University of Louisville — Recent experiments conducted by Desai *et al.* [1] reveal that single-wall carbon nanotube (SWCNT) networks exposed to N_2H_4 vapor at various pressures exhibit considerable drop in resistance with respect to the pristine sample. Experimental findings reveal: (i) n-type behavior for the adsorption of N_2H_4/SWCNT, and (ii) the binding of N_2H_4 on SWCNT as chemisorption. In the present work, we have performed first-principles electronic structure calculations [2] for the N_2H_4 adsorbed on the (14, 0) SWCNT, where several orientations for the N_2H_4 molecule were considered. Calculations for the combined system were performed using 3 unit cells with the DFT/GGA and ultra soft pseudo-potentials. Our calculations reveal: (i) the binding of N_2H_4 on SWCNT as physisorption, and (ii) the electronic structure of SWCNT to be practically unaltered by the adsorption of N_2H_4, suggesting that there will not be a dramatic drop in resistance for N_2H_4/SWCNT. This is in disagreement with the experimental findings. To further understand the experimental observations, we will discuss mechanisms that may alter the binding nature of N_2H_4 on SWCNT. [1] S. Desai, G. Sumanasekera, et al. (APS, March 2008). [2] G. Kresse and J. Furthmuller, Phys. Rev. B **54**, 11169 (1996).

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