First-Principles Electronic Structure Calculations of N$_2$H$_4$ Adsorbed on Single-Wall Carbon Nanotubes

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$_2$H$_4$ 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$_2$H$_4$/SWCNT, and (ii) the binding of N$_2$H$_4$ on SWCNT as chemisorption. In the present work, we have performed first-principles electronic structure calculations [2] for the N$_2$H$_4$ adsorbed on the (14, 0) SWCNT, where several orientations for the N$_2$H$_4$ 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$_2$H$_4$ on SWCNT as physisorption, and (ii) the electronic structure of SWCNT to be practically unaltered by the adsorption of N$_2$H$_4$, suggesting that there will not be a dramatic drop in resistance for N$_2$H$_4$/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$_2$H$_4$ on SWCNT. [1] S. Desai, G. Sumanasekera, et al. (APS, March 2008). [2] G. Kresse and J. Furthmuller, Phys. Rev. B 54, 11169 (1996).

1This work is supported by the US Army (SMDC).