First-Principles Electronic Structure Calculations of N\textsubscript{2}H\textsubscript{4} Adsorbed on Single-Wall Carbon Nanotubes\textsuperscript{1} M. YU, W.Q. TIAN, C.S. JAYAN-THI, S.Y. WU, University of Louisville — Recent experiments conducted by Desai et al. \cite{1} reveal that single-wall carbon nanotube (SWCNT) networks exposed to N\textsubscript{2}H\textsubscript{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\textsubscript{2}H\textsubscript{4}/SWCNT, and (ii) the binding of N\textsubscript{2}H\textsubscript{4} on SWCNT as chemisorption. In the present work, we have performed first-principles electronic structure calculations \cite{2} for the N\textsubscript{2}H\textsubscript{4} adsorbed on the (14, 0) SWCNT, where several orientations for the N\textsubscript{2}H\textsubscript{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\textsubscript{2}H\textsubscript{4} on SWCNT as physisorption, and (ii) the electronic structure of SWCNT to be practically unaltered by the adsorption of N\textsubscript{2}H\textsubscript{4}, suggesting that there will not be a dramatic drop in resistance for N\textsubscript{2}H\textsubscript{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\textsubscript{2}H\textsubscript{4} on SWCNT. \cite{1} S. Desai, G. Sumanasekera, et al. (APS, March 2008). \cite{2} G. Kresse and J. Furthmuller, Phys. Rev. B \textbf{54}, 11169 (1996).

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