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Encapsulated Organic Molecules in Carbon Nanotubes: Novel p-n junctions YI LIU, NICHOLAS KIOUSSIS, Department of Physics, California State University, Northridge, CA 91330-8268 — Recently Lu et al [1] have shown that both p- and n-type doping can be realized on single-walled carbon nanotubes (SWCNTs) by encapsulating various organic or organometallic molecules, such as TCNQ, F_4TCNQ, TTF, and TDAE, with different electron affinities or ionization potentials. Using a method that combines density functional theory and Keldysh nonequilibrium Green's functions, we have investigated the charge transport properties of such encapsulated SWCNTs. We have found that the current-voltage characteristics of p-type and n-type doped SWCNTs are very different, which can be explained in terms of their individual band structures. More importantly, if these p-type and n-type doped SWCNTs are joined together, p-n junctions can be achieved. Current-voltage curves for such p-n junctions will be presented.

1. J. Lu, S. Nagase, D. Yu, H. Ye, R. Han, Z. Gao, S. Zhang, and L. Peng, Phys. Rev. Lett. **93,** 116804 (2004).

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