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**Amphoteric Doping of Carbon Nanotubes by Encapsulation of Organic Molecules:** VINCENT MEUNIER, BOBBY G. SUMPTER, ROBERT J. HARRISON, Oak Ridge National Laboratory, COMPUTATIONAL CHEMICAL SCIENCES GROUP TEAM — The unique structural and electronic properties of carbon nanotubes provide a tremendous potential for applications in the field of molecular electronics. Practical realizations of new nanotube-based devices hinge on a number of outstanding problems, such as the capability in achieving large-scale air-stable and controlled doping. Recent experimental evidence [Nature Materials 2, 683,2003] suggests that amphoteric doping of single-walled carbon nanotubes is possible by using simple organic molecules possessing different electron affinities and ionization energies. In order to optimize and investigate the electronic transport processes in carbon nanotubes doped with organic molecules we have performed large-scale quantum electronic structure calculations coupled with a Green's function formulation for determining the quantum conductance. Our results suggest that the electronic structure of a carbon nanotube can be easily manipulated by encapsulating appropriate organic molecules.

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