Electromechanical Effects in Carbon Nanotubes

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We perform ab initio calculations of charged graphene and single-wall carbon nanotubes (CNTs). A wealth of electromechanical behaviors is obtained: (1) Both nanotubes and graphene expand upon electron injection. (2) Upon hole injection, metallic nanotubes and graphene display a non-monotonic behavior: Upon increasing hole densities, the lattice constant initially contracts, reaches a minimum, and then starts to expand. The hole densities at minimum lattice constants are 0.3 |e|/atom for graphene and between 0.1 and 0.3 |e|/atom for the metallic nanotubes studied. (3) Semiconducting CNTs with small diameters ($d < 20$ Å) always expand upon hole injection; (4) Semiconducting CNTs with large diameters ($d > 20$ Å) display a behavior intermediate between those of metallic and large-gap CNTs. (5) The strain versus extra charge displays a linear plus power-law behavior, with characteristic exponents for graphene, metallic, and semiconducting CNTs. All these features are physically understood within a simple tight-binding total-energy model.