Structural, thermodynamic and transport properties of functionalized carbon nanotubes from first-principles

YOUNG-SU LEE, NICOLA MARZARI, Department of Materials Science and Engineering and Institute for Soldier Nanotechnologies, Massachusetts Institute of Technology — We have studied the structural, thermodynamic and transport properties of carbon nanotubes functionalized via cycloaddition of nitrenes and carbenes, using our recently-developed band-structure and quantum conductance method based on maximally-localized Wannier functions. This approach allows us to study the effects of chemical functionalization on the transport properties of nanostructures containing thousands of atoms, while maintaining full ab-initio accuracy. We find that the stability of the two distinct sites of attachment on the sidewalls of achiral CNTs is strongly affected by diameter, due to the competition between elastic and chemical forces. A subtle interplay of electronic effects between $sp^2$ and $sp^3$ hybridization results in very significant differences for the transport properties of metallic nanotubes.

Young-Su Lee
Massachusetts Institute of Technology

Date submitted: 14 Dec 2004