Oxygen on Single Wall Carbon Nanotubes : Adsorption Pathways and Effects on Transport Properties

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The interactions of atomic and molecular oxygen on single wall carbon nanotubes (SWCNs) are investigated using ab initio and tight-binding molecular-dynamics (TBMD) schemes. We find that this interaction depends strongly on the spin configuration which, in turn, specifies oxygen's adsorption pathway. Depending on the curvature and the symmetry of the oxygen bonding site, oxygen adsorption can lead to epoxide formation, dissociation of molecular oxygen and/or breaking of a C-C bond of the SWCN. We also report the effect of oxygen adsorption on the transport properties of the SWCNs by calculating the I-V characteristics of oxygen-free and oxygen-adsorbed SWCNs.