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First-Principles Design of Conductance Switching in Functionalized Carbon Nanotubes ELISE LI, NICOLAS POILVERT, NICOLA MARZARI, MIT — Functionalization of SWNT through addition reactions represents an effective method to engineer or manipulate carbon nanotubes. For armchair CNTs,the conductivity is often decreased by orders of magnitude by the introduction of monovalent functional groups which disrupt the conjugated π network, whereas in [1+2] cycloadditions of carbenes or nitrenes, the sp^2 environment and therefore CNT metallicity can be recovered due to the sidewall bond breakage induced by the cyclopropane strain. In real systems, this bond cleavage depends heavily on the chirality and curvature of the tube, and the chemical nature of the addends. Here we explore the underlying mechanism of bond-cleavage chemistry in [1+2] cycloadditions on armchair carbon nanotubes using first-principles calculations. We find the high strain energy in cyclopropane moiety can be compensated by a through space π orbital interaction between the addend and the CNT which lowers the HOMO energy significantly in closed-bond configuration. A bond opening or closing switch marked by large conductance change can therefore be devised by modulating the proximity of the addend π system and the tube surface via optical or electrochemical control, which potentially has extensive applications in nanoscale devices.

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