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Fluxional handles for direct control of conductance in functionalized carbon nanotubes YOUNG-SU LEE, NICOLA MARZARI, Department of Materials Science and Engineering, Massachusetts Institute of Technology — A class of covalent functionalizations for single-wall carbon nanotubes is identified — from extensive first-principles calculations — that preserves the conduction channels of metallic nanotubes. Cycloaddition of carbenes or nitrenes can induce bond cleaving between two adjacent sidewall carbons, restoring their original sp^2 hybridization and recovering in the process a transparent π manifold, radically at variance with the strong scattering permanently induced by other common covalent functionalizations. The chirality and curvature of the nanotube and the chemistry of the addends can force or inhibit this bond cleavage, that in turn controls very distinctly the transport properties of the functionalized conductor. A well-defined range of diameters can be found for which certain addends - such as dicyanocarbene - exhibit a bistable switchable state, where the opening or closing of the sidewall bonds, and the accompanying on/off switch in the conductance, can be directed with chemical, electrochemical or optical means.

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