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First-principles characterization of carbon nanotubes functionalized with [2+1] cycloadditions YOUNG-SU LEE, NICOLA BONINI, NICOLA MARZARI, Massachusetts Institute of Technology — First-principles calculations predict that [2+1] cycloadditions of carbenes or nitrenes on single-wall carbon nanotubes can induce bond cleaving between adjacent sidewall carbons, recovering in the process the sp^2 hybridization of the pristine tubes [1]. Electrical conductance is strongly affected by the local bonding environment, and the sp^2 re-hybridization induced by cycloadditions restores the conductance of the pristine tubes even in the presence of significant chemical or structural disorder. Phonon dispersions, Born effective charges, and polarizabilities of functionalized carbon nanotubes have been also studied, to provide a link between the local bonding structure and experimental Raman and infrared spectra.

[1]Y.-S. Lee and N. Marzari, Phys. Rev. Lett. 97, 116801 (2006)

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