Consequences of H Doping in the Electronic and Optical Properties of Carbon Nanotubes (CNT)

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Functionalized CNTs show redshifted peaks. Those redshifted peaks are correlated to localized regions in the CNTs.

Pristine

MeO-Dz

The H inclusion splits degenerate bands. The redshifted peaks are due to excitons composed by the impurity band.

Our results are explained by Group Theory analysis. There is a matching in the $\theta$ coordinate for the wavefunctions that couple to each other.