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Localized Excitons in Carbon Nanotubes. LYUDMYLA ADAMSKA, STEPHEN K. DOORN, SERGEI TRETIAK, Los Alamos National Lab — It has been historically known that unintentional defects in carbon nanotubes (CNTs) may fully quench the fluorescence. However, some dopants may enhance the fluorescence by one order of magnitude thus turning the CNTs, which are excellent light absorbers, in good emitters. We have correlated the experimentally observed photoluminescence spectra to the electronic structure simulations. Our experiment reveals multiple sharp asymmetric emission peaks at energies 50-300 meV red-shifted from that of the lowest bright exciton peak. Our simulations suggest an association of these peaks with deep trap states tied to different specific chemical adducts. While the wave functions of excitons in undoped CNTs are delocalized, those of the deep-trap states are strongly localized and pinned to the dopants. These findings are consistent with the experimental observation of asymmetric broadening of the deep trap emission peaks, which can result from scattering of acoustic phonons on localized excitons. Our work lays the foundation to utilize doping as a generalized route for wave function engineering and direct control of carrier dynamics in SWCNTs toward enhanced light emission properties for photonic applications.

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