Band Structure Modification in Carbon Nanotubes Due to Crystal Encapsulation

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We report the modification of the band structure of single-walled carbon nanotubes (SWNTs) through encapsulation of the inorganic material manganese ditelluride (MnTe2). Using photoluminescence excitation mapping we show that this leads to a global reduction of the E11 and E22 band gap energies by a similar percentage (up to 3.8%). Beyond a threshold diameter for filling of ~1 nm the shifts increase with tube diameter due to the increased quantity of filled material. The direct relationship between the E11 and E22 shifts leads us to interpret this as due to a lowering of the carbon-carbon transfer integrals within the tubes. The radial breathing mode frequencies are also found to increase due to the tube filling, which is consistent with idea that the interaction between the tubes and the MnTe2 filling becomes stronger with increasing tube diameter. The measurements suggest that crystal-filling enables a permanent, air-stable and large band gap modulation for carbon nanotubes. The development of local or modulated filling along length of the nanotubes therefore offers the opportunity for the development of longitudinal modulation of the band structure to produce one dimensional heterostructures.