Effect of endohedrally adsorbed molecules on S_{11} electronic transitions of single wall carbon nanotubes

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The optical properties of carbon nanotubes (CNTs) in the near-IR region are of great interest for potential applications as well as for the characterization of the material. For semiconducting single wall CNTs (SWCNTs), photon absorption in the near-IR and visible regions is associated with the excitation of electrons from the valence bands to the conduction bands (van Hove singularities). The resulting electron-hole pair exciton is bound by Coulomb forces. Exciton effects play an important role in the optical transitions in semiconducting SWCNTs. The absorption and emission properties of SWCNTs depend on the properties of surrounding dielectric media as this affects the coulomb interactions that bind the exciton. Theory predicts, and experimental findings reveal, that an increase of dielectric screening around SWCNTs leads to a shift of the S_{11} band to lower frequency.

There is, however, a paucity of experimental characterizations of the effect of endohedrally adsorbed molecules on the electronic properties of SWCNTs. We will report the investigation of a dielectric screening effect on S_{11} optical transition of SWCNTs due to physical endohedral adsorption of simple molecules. Experiments were conducted under high vacuum with a combination of near-infrared and infrared spectroscopy and temperature programmed desorption (TPD). We find an environmental effect on S_{11} electronic transitions caused by molecules adsorbed endohedrally and compare this to the effect due to molecules adsorbed exohedrally.