ELECTRONIC STRUCTURES AND OPTICAL PROPERTIES OF OPEN AND CAPPED CARBON NANOTUBES

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Electronic structures of a series of carbon nanotubes with different chiralities, ends and bond lengths are studied systematically. Their absorption spectra are calculated with the localized-density-matrix (LDM) method [a]. The PM3 model is employed in the calculation. Nature of optical excitations is investigated by examing their reduced single-electron density matrices and a general understanding is obtained. It is found that the optical excitations may be divided into the end modes and tube modes which have different energies and distinctive features and structural dependence. Finite optical gaps have been confirmed for infinite long CNTs. The densities of states of carbon nanotubes are determined at the self-consistent Hartree-Fock level. The calculated absorption spectra and density of states (DOS) are compared well to the experimental results.

[a] S. Yokojima, and G. H Chen, Chem. Phys. Lett. 292, 379(1998).