Diameter Dependence of the Effect of Light Polarization on Interband Transitions in Zigzag Carbon Nanotubes

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Due to the one-dimensional nature of carbon nanotubes (CNTs), their optical spectra are expected to be highly dependent on the polarization of the incident light. For light polarized perpendicular to the nanotube axis, the absorption spectrum is known to be suppressed due the depolarization effect, also referred to as antenna effect in the CNT literature. However, photoluminescence experiments have shown the existence of distinct peaks with significant magnitude in the absorption spectra of single-walled nanotubes under the perpendicular polarization of light.[1] Therefore, studying the effect of light polarization on the absorption spectra beyond the depolarization effect is important in gaining a better understanding of the absorption behavior of CNTs.

We employ the density functional theory (DFT) to calculate the optical absorption spectra of infinitely-long zigzag CNTs for parallel and perpendicular polarizations of light. We study the interband transition spectra without including the local-field effects in order to explore the effect of light polarization on the orbital overlaps and dipole moments independently of the depolarization effect. To investigate the diameter dependence of this effect, we have chosen (4,0), (8,0), and (16,0) nanotubes with diameters of ~ 0.34, ~ 0.63, and ~ 1.27 nm, respectively.

According to our calculations, for an (8,0) nanotube the overall transition rate spectrum for perpendicular polarization is sparse compared to the one with parallel polarization (Figure 1). However, at certain photon energies (1.2 eV, 1.8 eV and 10.6 eV) the transition probability can be quite significant for perpendicular polarization. We observe that the overall transition rate in the infra-red/visible range (0-3 eV) is in general stronger for parallel polarization of light (Table 1), but R_W (the ratio of the transition rates with parallel to those with perpendicular polarizations) decreases as the diameter of the nanotube increases. On the other hand, in the ultra-violet range (3-11 eV), the strength and the number of peaks for parallel and perpendicular polarizations become comparable for (4,0) and (8,0) nanotubes, and R_W increases with diameter (Table 1).

[1] Y. Miyauchi, M. Oba and S. Maruyama, Phys. Rev. **B** 74, 205440 (2006)

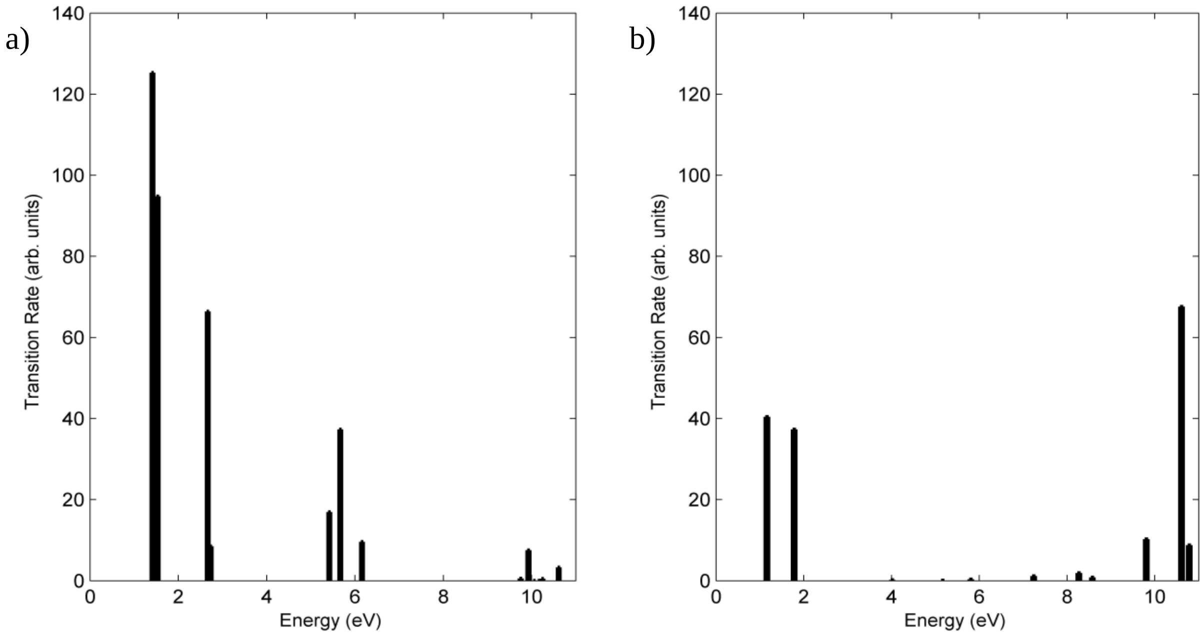

Figure 1: Transition rate vs. transition energy for an (8,0) nanotube for (a) parallel polarization and (b) perpendicular polarization of light.

Range	(4,0)	(8,0)	(16,0)
Infra-red/Visible (0-3 eV)	11.07	3.79	2.11
Ultra-violet (3-11 eV)	0.49	0.83	127.01

Table 1: Ratio of the transition rates for parallel and perpendicular polarizations of light (R_W) in different energy ranges.