CHARGE TRANSFER EFFECTS ON (ZIG-ZAG) SINGLE-WALLED BORON NITRIDE NANOTUBES (SWBNNTs)

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One of the most important applications in Nanotechnology is to capture solar energy involving charge transfer (CT) processes. Many of these processes are being developed through modified fullerenes or nanotubes.

A boron nitride (BN) nanotube (NT) is a structural analogue of a carbon nanotube (CNT) in nature wich alternates B and N atoms and so entirely substitutes C atoms in a graphitic-like sheet. BNNTs were theoretically predicted and then successfully synthesized in 1995. Primarily, the interest in BNNTs has been due to the undisputed fact that in contrast to metallic or semiconducting CNTs a BNNT is a wide-gap semiconductor. We note that while CNT research is growing exponentially year by year, BNNT research follows a linear-like dependence, in recent years the amount of BNNT-related papers has begun to increase notably.

The group of Q. Huang et al. [1] have studied the properties of Zinc-Phthalocyanine (Zn-Pc) doped SWBNNTs detecting the absorbed photons in the visible region with the possibility of charge separation. These kind of NTs don't absorb in this spectral region but when they are modified with Zn-Pc they exhibit new charge transfer bands in this region which is a very remarkable fact.

In order to detect and confirm the charge transfer character of these new electronic transitions, we have simulated the theoretical Resonance Raman (RR) spectra for a series of models such as the afore mentioned SWBNNTs. These theoretical models have been made by increasing the length and the diameter of the BNNTs (see Figure 1 (a-d)) with the aim of analyzing the effect of these parameters in the RR spectra. The RR intensities have been calculated according to the equations given by Wolde et al. [2],

$$I_j = \Re B_j^2 \omega_j^2$$

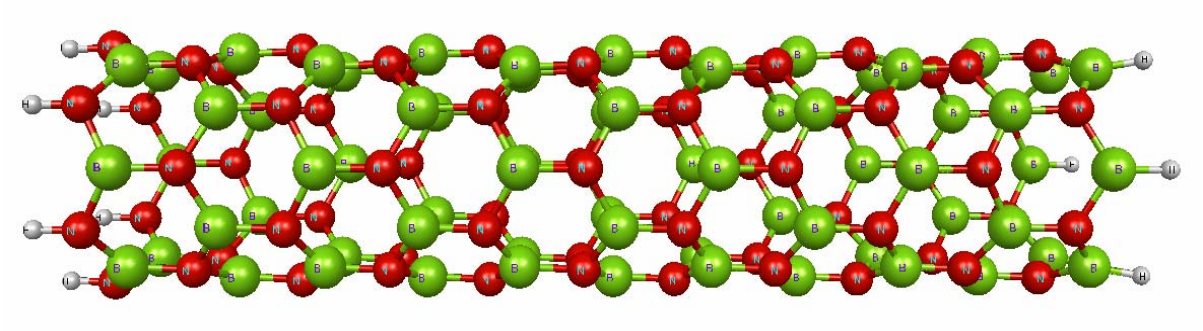
where Bj is given by

$$B_j = (2.41 \times 10^6) f \sqrt{M} L_j \omega_j^{-3/2}$$

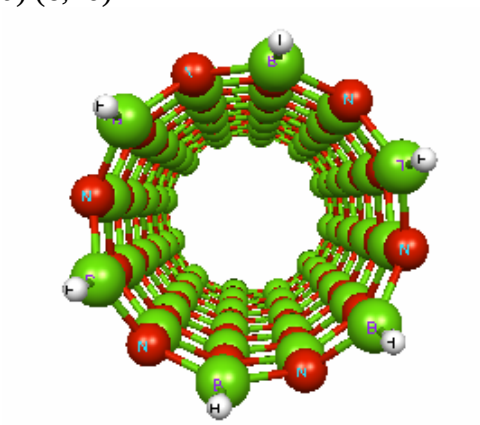
The intensities are determined by the forces (f) calculated at the Franck-Condon point of the excited states and, therefore, they are related to the respective bands by using the normal modes matrix (L) corresponding to the ground electronic state.

References:

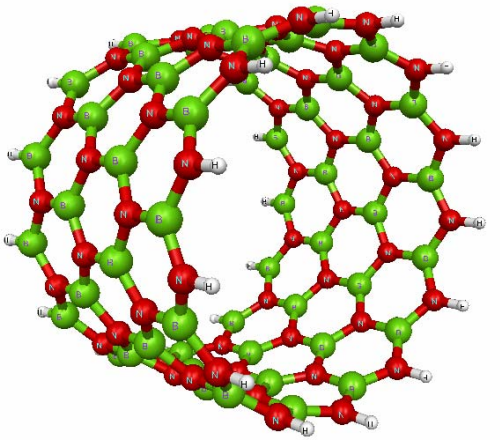
[1] Q. Huang, A.S.D. Sandanayaka, Y. Bando, C. Zhi, R. Ma, G. Shen, D. Golberg, J. Zhao, Y. Araki, O. Ito, L. Gao, Adv. Mater, 19 (2007) 934.
[2] A. Wolde, H.J.C. Jacobs, F.W. Langkilde, K. Bajdor, R. Wilbradt, F. Negri, F. Zerbetto, G. Orlandi, J. Phys. Chem. 98 (1994) 9437.



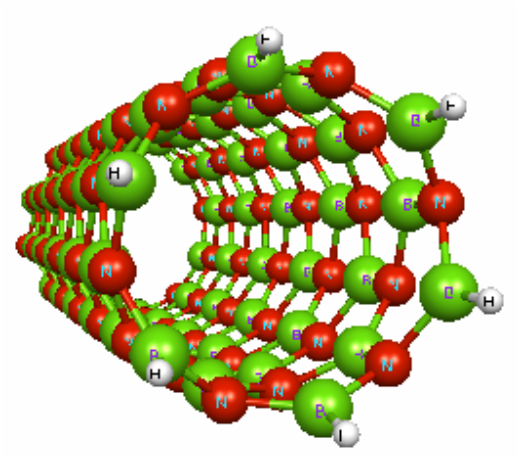
a) (6,10)



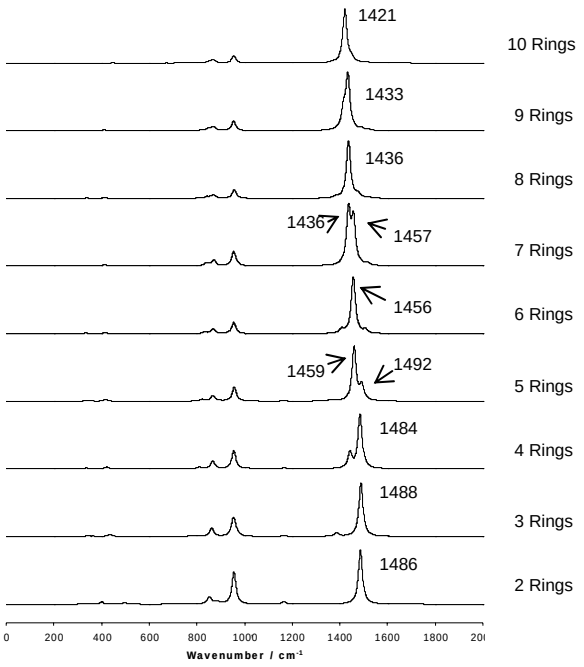
b) (6,10)



c) (13,3)



d) (6,10)



e)

Figure 1: (a-d) Differents sizes and views of zig-zag SWBNNT, (n,m)=(diameter, length). (e) Theoretical Resonance Raman (RR) spectra of zig zag SWBNNT increasing the length up to 10 rings.