DFT investigation of optoelectronic properties of ultra-small C, CN and SiC nanotubes

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Abstract: We investigated the optoelectronic properties of ultra-small armchair (3,3) carbon (C), carbon nitride (CN) and silicon cabride (SiC) nanotubes using the density functional theory (DFT). We performed the calculations for two potentials Perdew-Burke-Ernzerhof Generalized Gradient Approximation (PBE-GGA) and Tran-Blaha modified Becke-Johnson (TB-mBJ) potential. The results show a semiconducting nature with direct and indirect gap for C and SiC nanotubes respectivelly and metallic nature for CN nanotube. The calculated refractive index show an anisotropic bahaviour and decreases for all nanotubes and become less than one providing the photoluminescence phenomenon.

I. Introduction

Single walled carbon nanotube (C-SWNT), carbon nitride nanotube (CN-SWNT) and silicon cabride nanotube (SiC-SWNT) have attracted so much attention due to their unique properties and potential applications and the researchers exploit different techniques to their synthesis [1–3]. These nanotubes with very small sizes less than 1 nm can play a very important role in the minimization of optoelectronic nano-devices, therefore in this article, we study the optoelectronic properties of C, CN and SiC-SWNTs nanotubes with chirality (3.3) 1 and a diameter less than 0.6 nm using DFT. To our knowledge, this study has not yet been done.

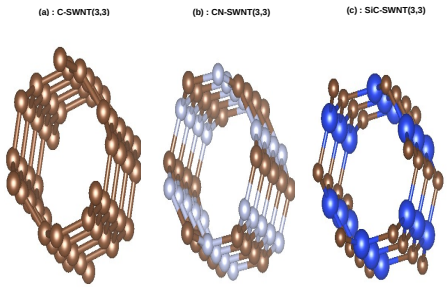

Figure 1: *Relaxed structures of C, CN and SiC-SWNT(3,3) Atom colors: Brown-Carbon, Cyan-Nitrogen and Blue-Silicon*

II. Methods

The electronic band gap and optical refractive index of all nanotubes are calculated using PBE and TB-mBJ potentials as implemented in the WIEN2K code. All the structures are relaxed . The supercells with $1\times\ 1\times 2$ unit cells of all nanotubes are used in this study. For the optical properties, the calculations were performed using 2000 k-points in the first Brillouin zone.

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III. Results and discussion

The band gap is important in order to understand the optoelectronic properties of materials, it is very promising for optoelectronic applications in the case of direct band gap . The band gap values and electronic band structure for C, CN and SiC-SWNT (3,3) are listed in the Table. 1 and Fig. 2 respectivelly. The results show a semiconducting behavior for C and SiC-SWNT(3,3) with direct band gap (0.22 eV (PBE,TB-mBJ) and indirect band gap (2.12 eV (PBE) and 2.74 (TB-mBJ) eV) respectivelly which are in agreement with experimental results [4, 5], while for CN-SWNT(3,3), it has a metallic nature. In the Fig. 3, the refractive index has an anisotropic behavior, it presents various peaks at two directions of polarization and shifted to the positive infinite for CN nanotube confirming the metallic behavior. Moreover, it decreases for all nanotubes and become less than one, providing the photoluminescence phenomenon which serves to use these compounds for optic nanodevices.

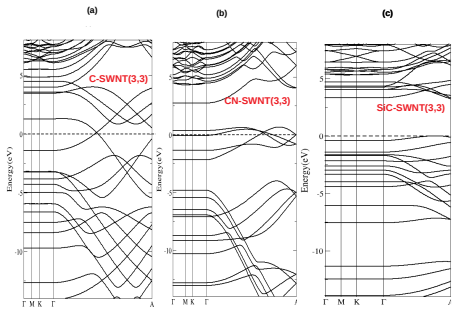

Figure 2: *Electronic band structures of C (a), CN (b) and SiC-SWNT(3,3) (c).*

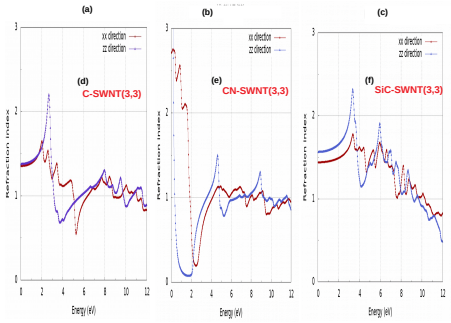

Figure 3: *Refraction index of C (a), CN (b) and SiC-SWNT(3,3) (c).*

Table 1: *Band gap with PBE and TB-mBJ functionals.*

Functional	C (3,3)	CN (3,3)	SiC (3,3)
Eg^{PBE} (eV)	0.22	0	2.12
Eg^{TB-mBJ} (eV)	0.22	0	2.74

Conclusion

The results found in this paper show that the DFT calculations presents a good tool for prediction of the optoelectronic properties of C, CN and SiC-SWNT(3,3) and show also the possibility of application of these materials in optoelectronic fields.

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