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Static refractive index engineering of a singlewalled carbon nanotube through co-doping: A theoretical study

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ABSTRACT

This paper presents a theoretical study of pristine single walled carbon nanotube (SWCNT) and SWCNT co- doped with combinations of Aluminum (Al), Phosphorous (P) and Nitrogen (N) along with their dielectric function spectra and calculated refractive indices. Dielectric function spectra of a pristine SWCNT and the SWCNT co-doped with Aluminum (Al) & Phosphorus (P) and another one co-doped with Al, P and Nitrogen (N) have been calculated using density functional theory implemented through the Cambridge sequential total energy package (CASTEP). The spectra show the variation of real and imaginary part of the dielectric function with frequency of the incident light. Polarized and unpolarized light as well as light through polycrystalline media has been considered. The value of static refractive index has been calculated using these curves. A substantial increase in the value of the static refractive index is observed when a pristine SWCNT is co-doped with Al and P but if in addition N atom is also introduced, a reduction in the value of static refractive index is observed though it does not fall lower than that of the pristine SWCNT. Thus, we propose that co-doping with atoms of different combinations of elements can be used as a novel and effective tool to manipulate the dielectric function and refractive index of SWCNTs and can pave the way to effective designing of various sensitive optical devices using SWCNTs for a variety of technological applications.

1. Introduction

Because of the incredible mechanical, electrical and thermal properties and chemical stability of single-walled carbon nanotubes (SWCNTs), these have been the subject of extensive research in the previous decades. Extensive work carried out on these in the recent years has revealed intriguing physical properties of these molecular scale wires. At present, CNTs have been successfully integrated into miniaturized electronic, electromechanical, and chemical devices, scanning probes, and into nano-composite materials [1,2]. Over the past few years, optical nanomaterials research has also uncovered intriguing optical attributes of their physical properties, lending themselves to a variety of device applications [3–13]. Experimentally, optical properties of CNT's have been studied by the optical ellipsometry [14], by the electron energy loss spectroscopy [15], by the reflectivity measurements [16], and also by the absorption experiments [17]. The great breadth and depth of optical phenomena in carbon nanotubes are exemplified by the number of reports investigating how photophysical and photo-chemical properties are affected by defects [18], exciton–phonon interactions [19], biexciton formation

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Table 1
Exchange correlation optimization.

LDA	GGA			
CA-PZ	RPBE	PBESOL	WC	PW91
0.190 eV	**0.097 eV**	0.161 eV	**0.063 eV**	0.003 eV

Closest to the experimental value is in bold.

[20,21], exciton–plasmon coupling [22], external magnetic [23] and electric fields [22,24]. Even in the solar energy field, it is conceivable to use CNT films as transparent electronic materials and to use nanotube composites for solar cell printed solar cells. Many researchers are working on projects related to solar cells and solar energy methods incorporating CNTs [25–33]. The extraordinary properties of CNTs, such as their light weight, excellent mechanical strength, three-dimensional flexibility and outstanding electro-catalytic properties can be used to improve the performance of solar cells. In addition, SWCNTs are also being incorporated in optical systems as anti-reflection coatings (ARCs). These transparent surface coatings with suitable optical path differences can suppress the reflection of substrates. In addition to these excellent optical properties, these SWCNT ARCs also exhibit self-cleaning ability because of the high fraction of air trapped between arrays [32,33]. Hybrid carbon nanotube systems – nanotubes containing extrinsic atomic type species such as semiconductor quantum dots, extrinsic atoms or ions, are shown to be promising candidates to extend the potential of CNTs for the development of new nano-optoelectronic devices with customized properties – both application oriented (e.g. photovoltaic devices of improved light-harvesting efficiency) [9] and for fundamental research (nanophotonics, nanoplasmonics, and quantum information processing) [34,35]. Such doping has already been achieved by a variety of techniques, including arc discharge [36], pyrolysis [37] and chemical vapor deposition [38]. Their strong potential for the future generation of the optoelectronic device applications, however, lies in the ability to tune their physical properties in a controllable, predictable way.

The present work aims at harvesting the idea of tuning the dielectric functions and refractive indices of SWCNTs using simultaneous doping of two or more elements into the pristine structure. A pristine (8,0) SWCNT, an (8,0) SWCNT co-doped with Al and P and an (8,0) SWCNT co-doped with Al, N & P were modeled using the software material studio (version 7.0) and dielectric function spectra for each of the simulated structure were calculated using density functional theory for polarized light, unpolarized light and light through polycrystalline media. The analysis of the dielectric function spectra obtained and static refractive indices thus calculated establishes co-doping as a novel and effective tool for manipulating these optical properties of SWCNTs. The study is of utmost importance as it will lead to the development of novel hybrid SWCNT systems with specific optical properties suitable for specific optical devices for various technological applications.

2. Computational details

In this theoretical work, all the calculations were implemented using Cambridge Sequential Total Energy Package (CASTEP) based on density functional theory [39]. CASTEP is available as a userfriendly module with the material studio software [40]. We performed the geometry optimizations and band structure calculations on a pristine (8, 0) zigzag type SWCNT, an Al-P co-doped SWCNT and an Al-N-P co-doped SWCNT. Like any ab initio calculation, the self-consistent Kohn Sham (KS) equation has been used to compute the eigen functions here. For the exchange and correlation terms, we used the generalized gradient approximation (GGA) functional with the Revised Perdew–Burke–Ernzerhof (RPBE) sub-functional [41]. The choice of the functional sub-functional combination is based on the optimization of the parameters in a previous study which was done on a (9, 0) SWCNT [42]. The norm-conserving pseudo-potential in reciprocal space was selected for the optical properties calculations. The electronic wavefunctions were expanded in plane wave basis set with finite basis set correction. A cutoff energy of 500 eV for the grid integration was used for computing the charge density. 3D triclinic super-cells were generated for BZ calculations (Fig. 1).

The Brillouin zone integration was performed using the monkhorst–pack scheme. Self-consistent field (SCF) calculations were conducted using the convergence criteria detailed in the Table 2. Optical properties calculations were performed on the simulated structures of the pristine (8, 0) SWCNT, Al-P co-doped (8, 0) SWCNT and Al-N-P co-doped SWCNT to determine the dielectric function spectra. The results obtained were analyzed to deduce the affect of co-doping on the dielectric functions and refractive indices of the SWCNTs.

3. Results and discussions

3.1. Exchange correlation optimization

Band gap study was performed on a1 (9, 0) SWCNT during a previous work by the authors to determine which exchange correlation functional is the most suitable for DFT studies on a SWCNT [42]. The results obtained are tabulated in Table 1.

Comparing these results with the measurements made by Leiber et al. (E_g = 0.080 eV) [43], it can be seen that GGA-RPBE/GGA-WC exchange correlation approximation is the most effective theoretical tool for DFT studies on SWCNTs. That is why; GGA functional in combination with RPBE sub-functional has been used for the DFT calculations in the current study.