First-principles study of optical properties of SWCNT/cellulose

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INTRODUCTION

The remarkable optical properties of single-walled carbon nanotubes (SWCNTs) have been one of the area of interest in biosensing. Their near-infrared (NIR) absorbance spectra feature can be covered by semiconducting wavelengths which are currently used in optical communication and in biological optical detection [1-2]. However, its tendency to agglomerate hinders its applicability [3]. There are several investigations on how to functionalize SWCNTs to address the problem of agglomeration [3,4]. The common route is to wrap the SWCNT with a polymer such as cellulose. [4].

Recently, studies on SWCNT/cellulose composites have rapidly increased because their properties can be controlled by just varying the combination of SWCNT and cellulose [3]. In order to determine the appropriate applications for these SWCNT/cellulose composites, it is necessary to understand and investigate their properties.

In this study, we calculate and compare the absorption spectra of pristine SWCNT(7,1) (PSWCNT) and SWCNT(7,1)/cellulose composite.

METHODS

Density Functional Theory

- a computational quantum mechanical modeling method to investigate the electronic structure of many-body systems.
- based on Hohenberg and Kohn theorems.*

* H. Hohenberg, and W. Kohn. (1964). Phys. Rev. 136, B864.

Computational Details

- All calculations are done using the PWscf package of Quantum Espresso [5].
- The optical properties are calculated using the epsilon.x, a post processing code of PWscf.
- Starting from DFT eigenvalues and eigenvectors, the epsilon.x provides the real ($\boldsymbol{\varepsilon_1}$) and imaginary ($\boldsymbol{\varepsilon_2}$) parts of the dielectric function $\boldsymbol{\varepsilon}$.
- Absorption coefficient $\boldsymbol{\alpha}$:

$$\alpha = \frac{2\omega}{c}k$$

where the extinction coefficient $\boldsymbol{k}$ is given by

$$k = \left[\frac{\sqrt{{\varepsilon_1}^2 + {\varepsilon_2}^2} - \varepsilon_1}{2}\right]^{\frac{1}{2}}$$

PROGRAMMING PLATFORM

For DFT calculations:
Quantum Espresso
- Based on plane-waves and pseudopotentials.

For visualization:
XCrySDen
- A crystalline and molecular structure visualization program.

Ref: A. Kokalj, J. Mol. Graphics Modelling, 1999, 17, 176-179

For composite construction:
Virtual Nanolab
- A GUI for different codes that can also build structures easily.

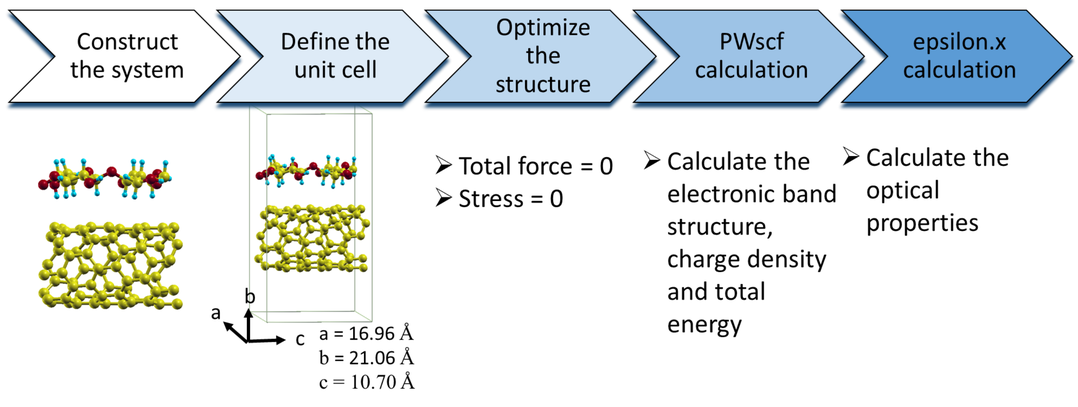
Ref: https://quantumwise.com/

PARAMETERS

XC functional type: Perdew-Burke-Ernzerhof (PBE)[1]
Pseudopotentials type: Norm-conserving
Energy cutoff for wfc: 40 Ry
Energy cutoff for charge density: 200 Ry
k-points: 1 x 1 x 2 Monkhurst-Pack grid

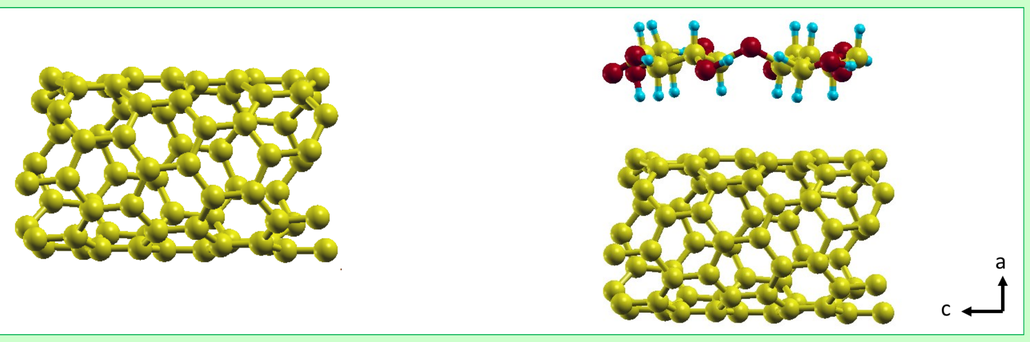
[1] J. P. Perdew, K. Burke, and M. Ernzerhof, Physical Review Letters 77, 3865 (1996).

PROGRAM FLOW IN QUANTUM ESPRESSO



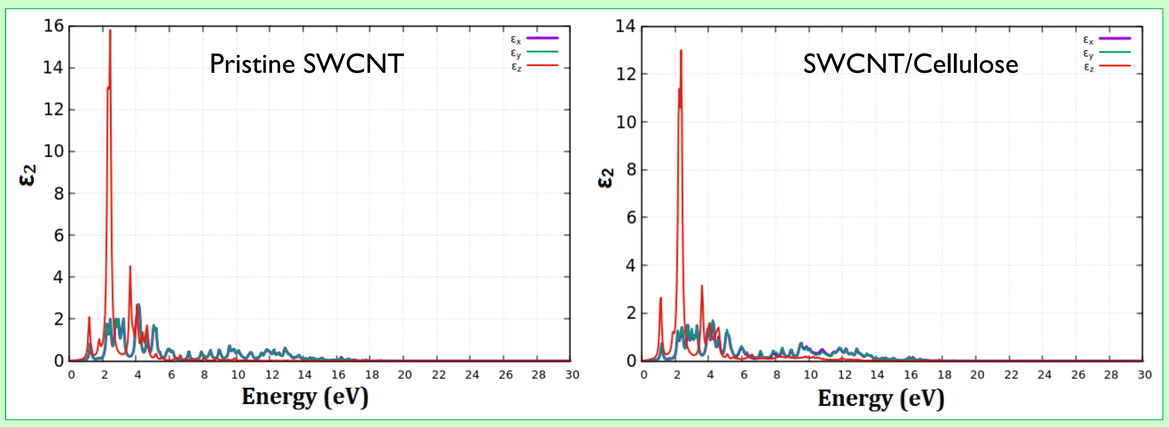
RESULTS

Crystal structure



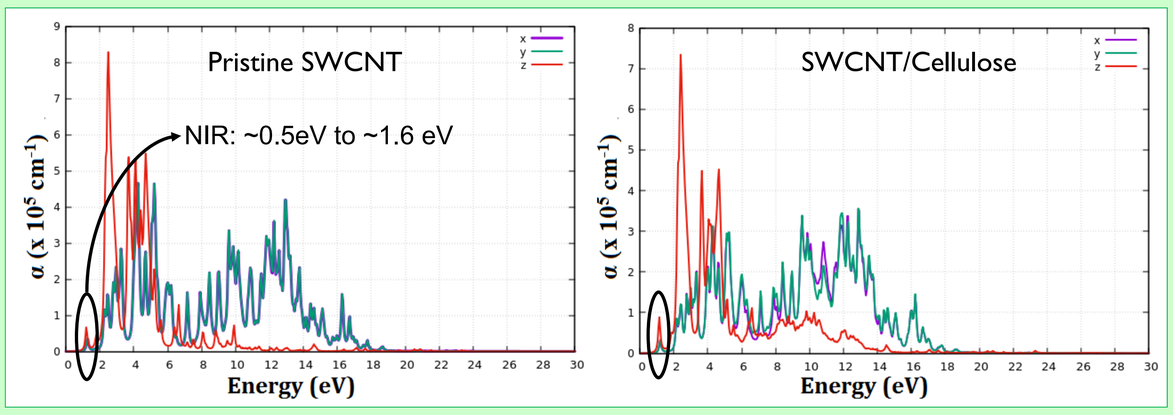
Pristine SWCNT SWCNT/Cellulose

Imaginary part of the dielectric function



- The imaginary part of the dielectric function is associated with the dielectric losses and thus it is responsible for the absorption.

Absorption spectra



- The peak found in the 0.5 eV to 1.6 eV energy range is enhanced in SWCNT/Cellulose as compared to the pristine SWCNT.
- SWCNT/cellulose composite is a better candidate for NIR sensing applications.

SUMMARY

- The absorption spectra of pristine SWCNT(7,1) and SWCNT(7,1)/cellulose composite were calculated.
- The peak found in the near-infrared (NIR) energy range, i.e. 0.5 eV to 1.6 eV, is enhanced in the SWCNT/cellulose system.
- Since higher absorption provides higher sensitivity and larger signal to noise ratio, the SWCNT/cellulose system is a better candidate for NIR sensing applications.

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[5] P. Giannozzi, et al, J. Phys.: Condens. Matter, 21(39):395502, 2009

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