DFT study on electronic properties of gas- and metal-adsorbed divacancy-defected SWCNTs

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ABSTRACT

We have calculated the electronic properties of gas- and metal-adsorbed divacancy (DV)-defected single-walled carbon nanotubes (SWCNTs) using density functional theory (DFT). Hydrogen (H) atom is adsorbed on (6,0) DV-SWCNT while silver (Ag) and gold (Au) atoms are adsorbed on (7,0) DV-SWCNT. Our results have shown that the divacancy-induced semiconducting behaviour of the (6,0) nanotube changes into metallic upon adsorption of H atom. Additionally, the metallic DV-defected (7,0) SWCNT retains its metallicity after adsorption of Ag and Au atoms.

INTRODUCTION

Single-walled carbon nanotube [1] (SWCNT)
- → subject of intensive research due to its unique properties
- → can either be metallic or semiconducting depending on its chirality

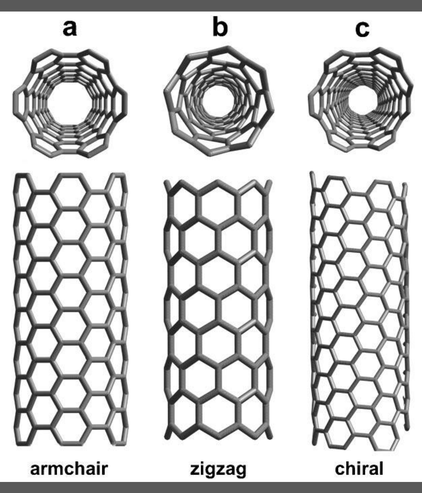


Fig. 1: SWCNT models with different chiralities [2].

Nanotubes usually have defects and the most commonly observed ones are monovacancy and divacancy in which the latter has been found more stable relative to isolated monovacancy [3].

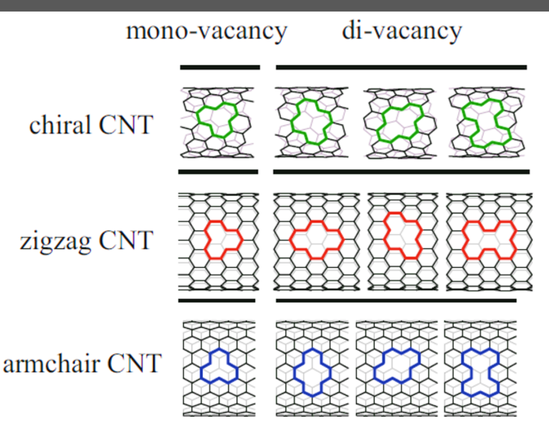


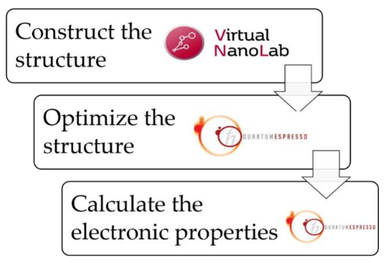
Fig. 2: SWCNT structures with mono- and di-vacancies [4].

In our study, we investigate the effect of gas (H) and metal (Ag and Au) atoms adsorption on electronic properties of divacancy-defected zigzag SWCNTs.

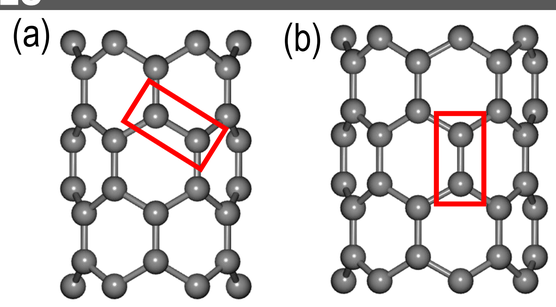
COMPUTATIONAL DETAILS

Electronic properties calculations were performed using Density Functional Theory (DFT) based on plane wave pseudopotential method with GGA [5,6] implemented on QUANTUM ESPRESSO [7,8].

Nanotubes were constructed using Virtual NanoLab (VNL) [9].



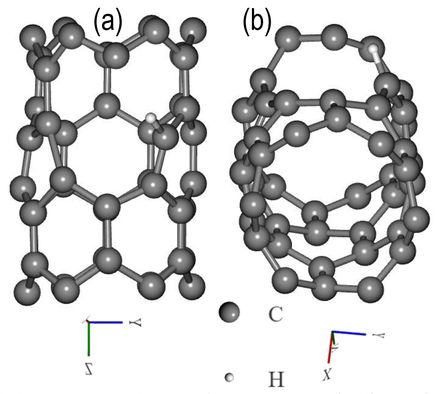
Simulation process in DFT calculations.



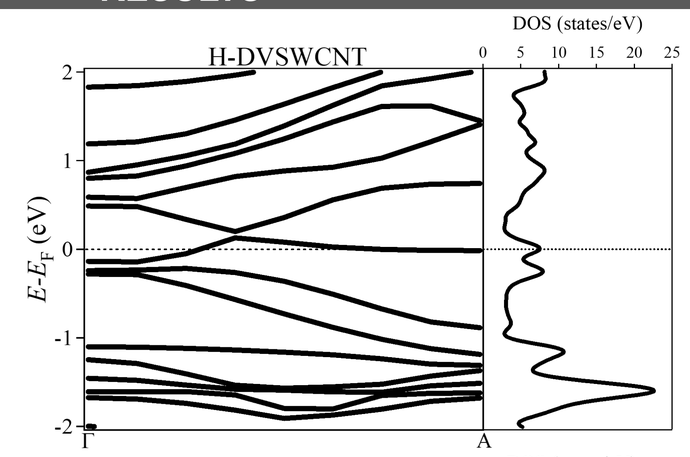
Constructed structural models of (a) (6,0) SWCNT and (b) (7,0) SWCNT with 48 and 56 C atoms, respectively. Two atoms are then removed to produce DV-defected tube with 46 and 54 C atoms, respectively.

RESULTS

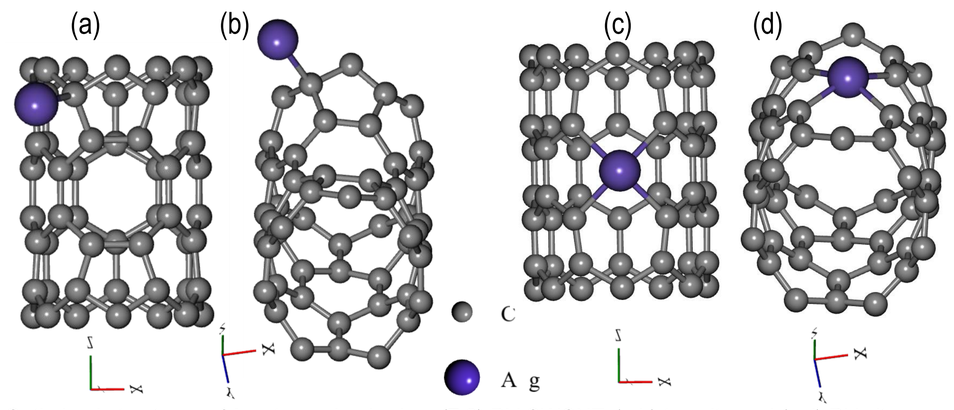
- The H atom adsorbed on defected (6,0) tube settled on top (T) of carbon atom.
- Ag and Au atoms adsorbed on defected (7,0) tube settled on top of C atom and on the divacanct (DV) site.



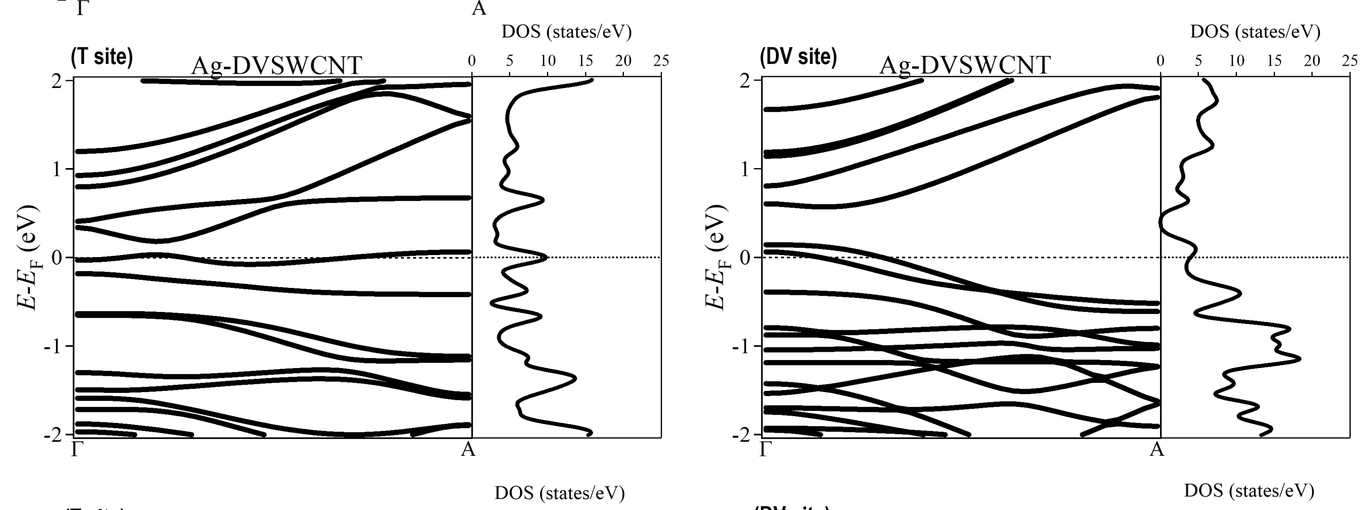
Optimized structures of H-adsorbed (6,0) DV-SWCNT.

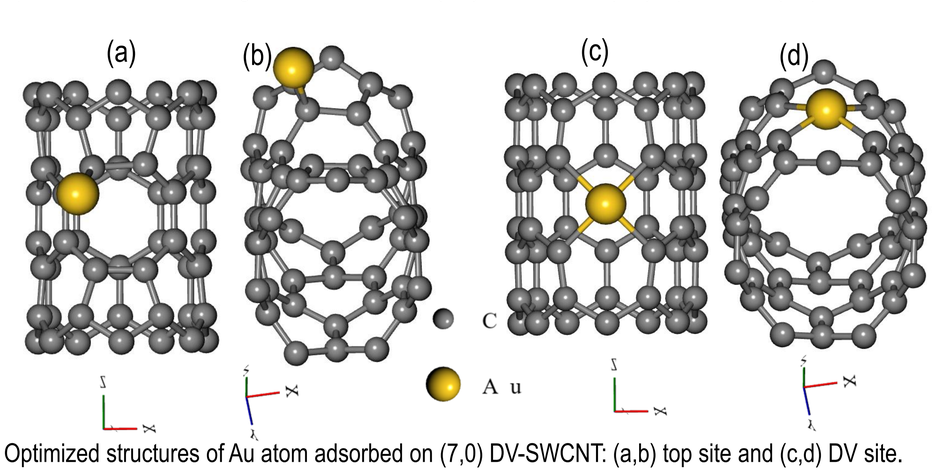


- A semiconducting DV-defected (6,0) SWCNT becomes metallic after adsorption of H atom.
- Meanwhile, the metallic behaviour of DV-defected (7,0) SWCNT is retained upon adsorption of Ag and Au atoms on various sites.

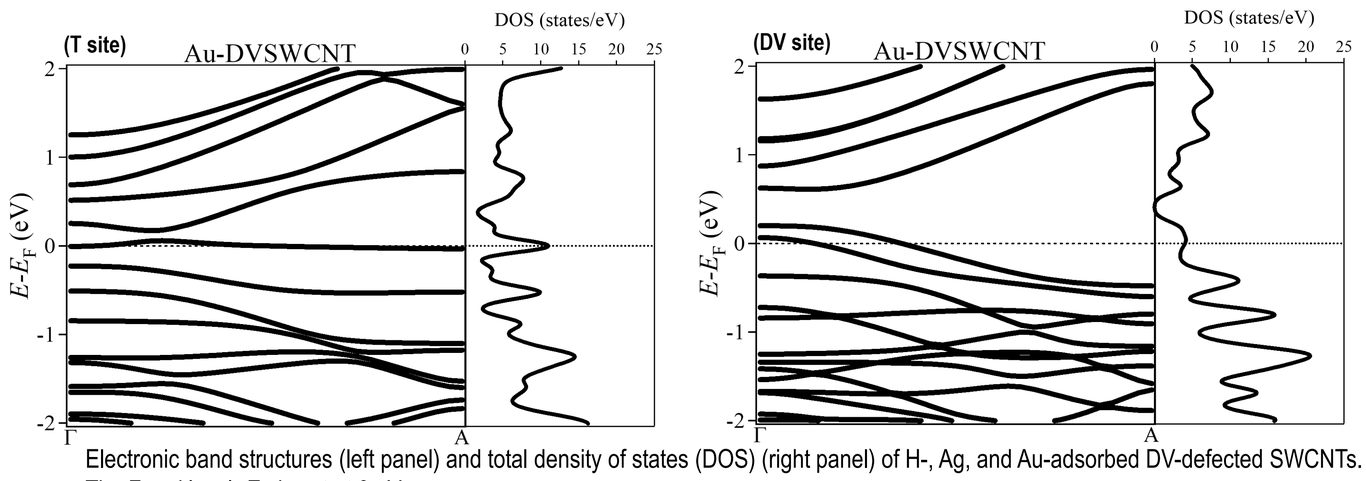


Optimized structures of Ag atom adsorbed on (7,0) DV-SWCNT: (a,b) top site and (c,d) DV site.





Optimized structures of Au atom adsorbed on (7,0) DV-SWCNT: (a,b) top site and (c,d) DV site.



Electronic band structures (left panel) and total density of states (DOS) (right panel) of H-, Ag, and Au-adsorbed DV-defected SWCNTs. The Fermi level, E_F, is set at 0 eV.

SUMMARY

- Electronic properties of gas- and metal-adsorbed divacancy-defected SWCNTs were calculated using DFT implemented in QUANTUM ESPRESSO.
- H atom is adsorbed on semiconducting divacancy-defected (6,0) SWCNT. Band structure showing band at the Fermi level, E_F, and nonzero DOS at E_F indicate metallic behaviour.
- Ag and Au atoms are adsorbed on metallic divacancy-defected (7,0) SWCNT. Bands at E_F, and high DOS at E_F confirms retained metallicity of the material.

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