



# Effects of Ir and B co-doping on H<sub>2</sub> adsorption properties of armchair carbon nanotubes using Optical Spectra Analysis for energy storage

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Abstract	Article History
<p>In this research, DFT+U approach was used to investigate the performance of Iridium (Ir) and Boron (B) co-doped armchair (8, 8) Single-walled Carbon Nanotube (SWCNT). Calculations of the structural electronic and optical spectra analysis of the system under study were carried out using the <i>ab initio</i> quantum simulations implemented in Quantum ESPRESSO and thermo_pw codes within the popular density functional theory. In the doping process, carbon atoms have been replaced by Ir and B atoms in the SWCNT, the investigations were done on the basis of distance of H<sub>2</sub> (<i>d</i>) from the co-doped SWCNT at intervals of 6.12 Å, 6.45 Å and 6.77Å, variations of temperature, variations of external electric field, band gaps, optical adsorptions and binding energy variations were all taken in to account. It is found that Ir/B co-doping in pristine SWCNT significantly enhanced the H<sub>2</sub> adsorption capacity of the SWCNT. Furthermore, an increase in temperature decrease the performance ability of the co-doped SWCNT, negative adsorptions intensities were recorded by temperature increase by 650, 700 and 750 °C, this can be termed as exothermic adsorption. Therefore it can be demonstrated that H<sub>2</sub> by co-doped SWCNT undergoes endothermic adsorption under ambient temperature and shows exothermic adsorption under higher temperatures.</p>	<p>Received: 18/01/2023 Accepted: 11/03/2023 Published: 10/04/2023</p> <p><b>Keywords</b> Co-doping; Hydrogen adsorption; Energy storage; Iridium; Exothermic adsorption</p> <p><b>License: CC BY 4.0*</b></p>  <p>Open Access Article</p>
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## 1.0 Introduction

In the next 50 years to come, the world may be faced with two most significant problems which are environmental and energy problems (Isabel *et al.*, 2018). Specifically, the energy problem has been reported to be the most significant however, it is too difficult to control. Energy problems related to air pollution were caused by the linear increase in the world population which in turn led to greater demand in energy (Ferdaus *et al.*, 2022). Unfortunately, this has resulted in an exponential increase of global fossil

carbon emissions over the last several decades, and the same trend appears for the global temperature. Furthermore, due to overconsumption of the available fossil fuel, there are high expectations that these fuels may come to their exhaustion very soon (Florinda *et al.*, 2019), to curve this problem; it is necessary to provide replacement with environmentally friendly fuel such as hydrogen.

When hydrogen burns, it ejects only water as the product of combustion. Therefore it has been considered as the best candidate to succeed fossil fuels

for energy demand (Pedro *et al.*, 2021). Additionally, hydrogen has higher energy content per weight unit of all hydrocarbon fuels, it has been reported to have three times more energy per weight than petrol (Véronique *et al.*, 2020). Hydrogen fuel is harmless, it can also be produce anywhere as such it provides an alternative to problem of geopolitical inclination faced with the availability of fossil fuel. Despite all these advantages of hydrogen fuel, there are serious problems regarding its synthesis and storage. It is a gas under ambient conditions, it has a very low density much lesser than air. Although hydrogen has been recognized as very ideal energy carrier which can serve as suitable automobile fuel, it has not been introduced commercially due to lack of storage procedure.

The first synthesis of carbon nanotubes was reported in 1991 (Itas *et al.*, 2020), since then the ability of CNTs to serve as material candidate of hydrogen storage have been widely reported after first report by Dillon *et al.* Although significant progress was made in the experimental fields, there were many conflicting results about the potential of CNTs for hydrogen storage (Xiaohan, 2022). For example it has been reported that CNTs can store large amount of hydrogen even at room temperature, some years later, another report had it that alkali-doping on CNTs demonstrated high hydrogen adsorption. However, the report by Yangs (Yang-huan *et al.*, 2015) revealed that higher adsorption of hydrogen by metal-doped CNT was due to moisture and weight gain in the side of the alkali/metal doped, therefore CNT cannot be used for pure hydrogen storage. Revelations from more experiments reported that hydrogen storage ability of SWCNTs and MWCNTs at ambient conditions cannot be more than 0.43 %. Furthermore; there were also reports that hydrogen storage capacity of different carbon nanostructures give conflicting results at room temperature and higher temperatures. Therefore many of these results seem to be controversial in the sense that they were not confirmed or reproduced by other research groups.

The general inefficiency by CNTs to provide good storage capacity for hydrogen is due to weak interactions between C and H atoms (Itas *et al.*, 2021), so there is need to develop a high standard way to improve this interactions so that high efficiency will be achieved. Generally, this can be achieved by either doping with heteroatoms or by incorporating light metal atoms. Through these processes, the binding energy of the hydrogen molecules would be enhanced due to charge induced dipole interactions. To achieve this aim, this work developed a new method of improving the hydrogen adsorption efficiency of CNTs through co-doping with Iridium (Ir) and Boron (B) atoms. The former is a transition metal with atomic number 77, it is brittle, silvery-white and very hard. It

is regarded as the second heaviest metal after Osmium. Iridium is an ideal catalyst for the electrolytic production of hydrogen from water (Miklos *et al.*, 2016). The ultimate aim of this research is to develop a low-cost hydrogen storage avenue with capacity greater than 5.5 %wt.

## 2.0 Materials and methods

Ab initio quantum simulations were performed to calculate the electronic and optical properties of the system under study via Quantum ESPRESSO and thermo-pw codes. Structural optimizations were done with codes implemented in VESTA, BURAI and nanotube builder (Itas *et al.*, 2022). Computations of the density functional theory were done with GGA-PBE parameterized exchange functional (Itas *et al.*, 2022). The energy cut-off value for the construction of the plane-wave basis set for SWCNT was achieved at 50 Ry, and the k-point value which correlates to the  $\epsilon_{cut}$  value was  $1 \times 1 \times 28$  k-mesh (Yahaya *et al.*, 2023). The H<sub>2</sub> adsorption potentials of the Ir/B co-doped SWCNT were investigated based on electronic, thermal and optical dielectric constants in terms of the random phase approximation and based on the electron-electron interactions. Moreover H<sub>2</sub> adsorption were also investigated by varying the guest molecule distance to the Ir/B co-doped SWCNT. Studies of the Density of State (DOS) were conducted for selected systems in order to detect the influence of adsorption of small H<sub>2</sub> molecules on Ir/B co-doped SWCNT. The Ir/B co-doped SWCNT has been optimized by replacing carbon atom with Ir and B atoms sequentially. The effects of temperature on the optical adsorptions of the co-doped SWCNT were done by increasing the temperature at intervals of 650, 700 and 750 °C while keeping H<sub>2</sub>-co-doped system distance fixed at 6.45 Å.

## 3.0 Results and discussion

### 3.1 Structural properties and optimization

In order to have a good thermodynamically stable surface for hydrogen storage in terms of the Ir/B co-doped SWCNT system. It is necessary to build a well optimized structure that is stable to both the segments of the SWCNT and the doping impurities. This is to ensure that adverse effects are minimized along the axial directions of the nanotube. In this work, the pristine form of the armchair SWCNT was built ensuring the C-C bond length of 1.42 Å. this is in good agreement with the standard bond length used in the theoretical calculations for modeling CNT structures (Budyka *et al.*, 2005). To ensure structural stability in the doping process, C atoms in SWCNT were replaced by Ir and B atoms on the same face along the nanotube length maintaining the same 1.42 Å. Figure 1 (a) presents the pristine form of the (8, 8) SWCNT as the representative model of the armchair CNT. Ir and B

atoms are shown in blue and yellow color in Figure 1 (b). In terms of H<sub>2</sub> adsorption, Figure 1 (c) demonstrates the positions of the H<sub>2</sub> molecules relative to the Ir/B co-doped SWCNT. The H-H bonding length was set to the standard value of 74 pm. The adsorption potentials of the Ir/B co-doped SWCNT were examined by varying the H<sub>2</sub> distance to the co-doped SWCNT which is set as  $d = 6.12, 6.45$  and  $6.77$  measured in Å. Although all the optimized structures were found to be stable (Itas *et al.*, 2020), the heat of

formation of all the systems was endothermic at ambient temperature and exothermic at temperatures above 600 °C. Furthermore, comparison of the heat of formation energies suggests that the doped structures are obtainable from nanotubes by chemical exothermic reactions. Results from our DFT calculations revealed that the carbon electrons have the residence in energetically lower orbitals after co-doping (Shuangsheng *et al.*, 2021).

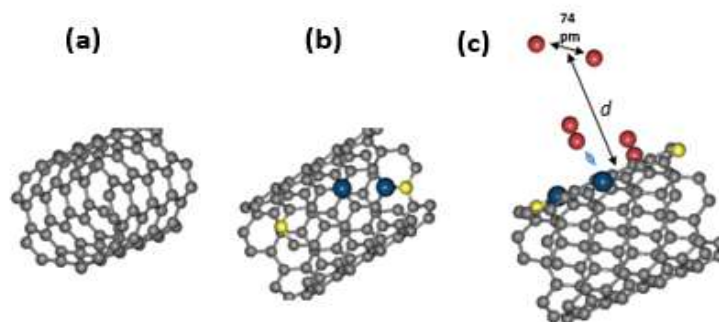


Figure 1. Optimized structures of (a) pristine SWCNT, (b) Ir/B co-doped SWCNT and (c) H<sub>2</sub> adsorbed Ir/B co-doped SWCNT

Table 1. Calculated energies of formation for systems under study

Parameter	SWCNT	B-doped SWCNT	Ir/B co-doped SWCNT
<b>Total energy</b>	-143202.17	-150213.04	-151743.90
<b>Binding energy</b>	-7366.32	-7256.29	-70112.59
<b>Heat of formation</b>	569.44	330.42	215.21
<b>Isolated atomic energy</b>	136831.87	140113.22	159671.54

### 3.2 Binding energies

The adsorption of the single molecule of H<sub>2</sub> gas was studied in the Ir/B co-doped SWCNT system. From the results calculated, H<sub>2</sub> molecule prefers to stay at the interface of Ir/B-SWCNT rather than staying in to the SWCNT tube. Upon adsorption, it was found that the metallic behavior of the co-doped SWCNT significantly increased. Also H<sub>2</sub> adsorption is independent on the tube orientation with respect to the doping elements. Table 1 present the calculated energies in kcal/mol of the SWCNT, B-doped SWCNT and Ir/B co-doped SWCNT.

As presented in Table 1, it has been found that addition of Ir and B atoms significantly increase the binding energy for H<sub>2</sub> adsorption. Analytically, the binding energies of all the three systems are endothermic reaction. However, the surface adsorption of the guest H<sub>2</sub> molecule is endothermic below 600 °C and exothermic above 600 °C, claim to this report are presented in Figure 7. This behavior can be connected

to the small size of the SWCNT and the repulsion behaviors of electrons due to electron density of the SWCNT (Sarah *et al.*, 2021). By comparing the binding energies, we can conclude that Ir/B co-doped SWCNT has the highest binding energy as such can serve as best surface for H<sub>2</sub> energy storage. After adsorption, Ir/B co-doped SWCNT demonstrates fully active adsorption edges with fast ion-electron transfer structure. This provides abundant electrochemical active adsorption sites and extends interlayer spacing. Based on this, the capacity-controlled adsorption mechanism of H<sub>2</sub> storage is achieved in Ir/B co-doped SWCNT.

### 3.3 Electronic properties

To get more details about the electronic transport behaviors of the pristine SWCNT, Ir/B-doped SWCNT and H<sub>2</sub> adsorbed co-doped SWCNT systems, we have conducted our calculations with respect to the electronic band structures. Furthermore, studies of the Density of State (DOS) plots were conducted for

selected systems in order to detect the influence of adsorption of small  $H_2$  molecules on Ir/B co-doped SWCNT. As reported, all armchair CNTs demonstrate metallic properties showing zero bands around Fermi level (Itas *et al.*, 2022). In this work, a representative model of (8, 8) SWCNT was chosen to represent armchair CNTs in a pristine (pure/undoped) form. As can be seen in Figure 2 (a), (8, 8) SWCNT show metallic properties due to the presence of bands around HOMO-LUMO boundary which is in good agreement with the obtained experimental results. Moreover bands contours were seen crossing Fermi level forming intersections at two different Dirac points. This result is consistent with the DOS diagram obtained for the same system as shown in Figure 2 (b). More and also dense states are seen in the valence band than in the conduction bands. Higher peak was also observed at energy level corresponding to -7 eV. However due to the reported weak interactions between  $H_2$  molecules and C atoms in SWCNTs, we have decided to improve this through co-doping of transition metal and a hetero nonmetallic atom.

Through this, it is expected that the binding energies of the new developed nanotube will increase to pave way for  $H_2$  atoms to center around the region of the  $H_2$ -SWCNT interface.

As presented in Figure 3 (a), the bands projection around the center of the Fermi level was due to co-doping of Ir and B atoms. This does not physically change the electronic state of the SWCNT system. Therefore, co-doping does not change the electronic state of the pristine SWCNT although there were observed changes in the shape of the bands. More states are seen around Fermi level as shown in Figure 3 (b). Furthermore numerous peaks are seen in both valence and conduction bands due to perceived excitations by Ir and B atoms. When  $H_2$  molecule is adsorbed, they are centered around the Fermi energy level due to strong binding effects by Ir and B atoms (Zhiyuan *et al.*, 2017), they stay at the interface between  $H_2$ -SWCNT surfaces. Their adsorption does not change the metallic properties of the pristine SWCNT as shown in Figure 4 (a).

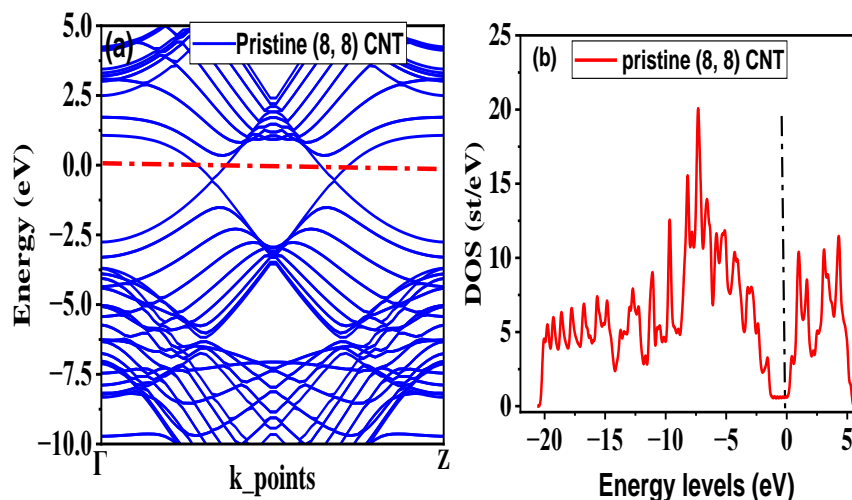


Figure 2. Electronic bands and DOS for pristine (8, 8) SWCNT

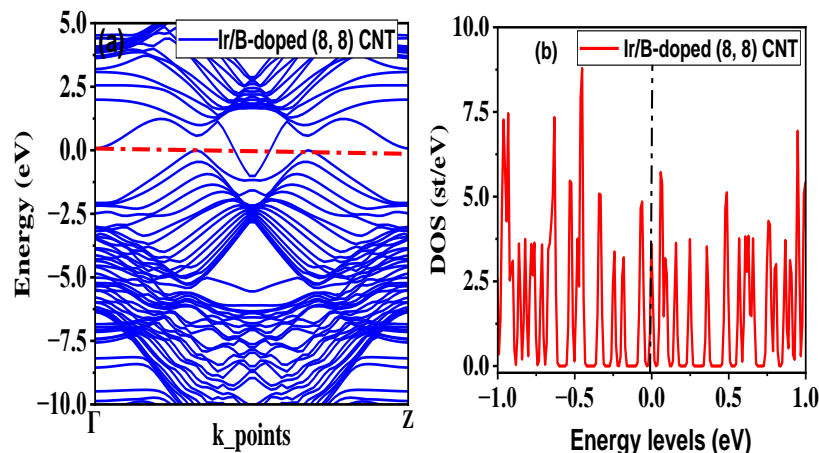


Figure 3. Electronic bands and DOS for Ir/B co-doped SWCNT

The two peaks at -4.5 eV and -5.1 eV shown in Figure 4 (b) are due to confinement of the adsorbed  $H_2$  molecule by the co-doped SWCNT. Some intermediate levels were introduced due to the observed changes in the bands and DOS of the co-doped system, these levels have some contribution in the band calculations. In terms of adsorption,

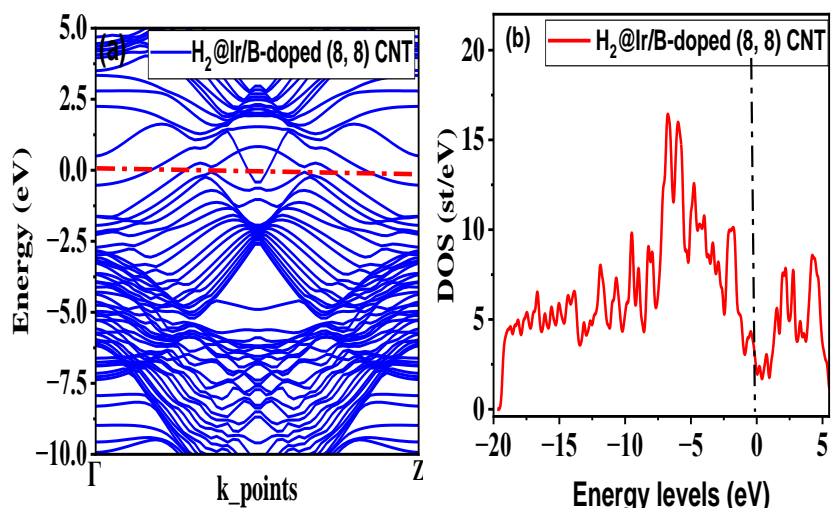


Figure 4. Electronic bands and DOS for  $H_2$  adsorbed Ir/B co-doped SWCNT system

### 3.4 Local density of states

The local density of state is a space resolved parameter which describes the total contribution of orbital subshells in an electronic interactions process (Sachs *et al.*, 2011). We now consider the discussion on the charge redistributions as a result of adsorbents. The contribution of these adsorbents to coulomb scattering is a direct function of changes in the electrostatic potential and also to the partial charges from the shift of core level (Ignatchenko and Tsikalov, 2017). This work discusses the level of charge transfer between C, B and Ir after adsorbing  $H_2$  molecule. To demonstrate the amount of  $H_2$  adsorption in this work, we have calculated the LDOS of the  $H_2$  adsorbed Ir/B co-doped SWCNT around the Brillouin zone. Different contributions by p' orbitals of C, B and Ir and also d' and f' orbitals were shown in Figure 5 (a), details of individual orbitals participations are shown in Figure 5 (b).

Highest occupation of states are reported by d' orbital of Ir atom which can be justified by d' orbital peaks in Figure 5 (b) which is highest at 1.8. Therefore  $H_2$  molecules were centered on Fermi level. The second highest participation was recorded by p' orbital of B atom. So increase in the efficiency is mainly due to p' and d' orbitals of B and Ir respectively as also agreed with obtained properties of other nanotubes (Balarabe *et al.*, 2023). Therefore as a result of co-doping, LDOS demonstrated a significant jump at edges of the

variations in inter frontier molecular orbital eigenvalue is mostly accompanied by changes in optical characteristics. Therefore the effects of addition of Ir and B impurities to the pristine SWCNT is not charge oriented, as such external field may not affect its adsorption behavior.

allowed bands through transition from one layer to another.

### 3.5 $H_2$ adsorption properties

The  $H_2$  adsorption properties of the Ir/B co-doped SWCNT were investigated from the optical response of the system to incident electromagnetic photon in terms of imaginary dielectric functions. This is because optical parameters such as reflection, extinction coefficients, absorption and optical conductivity are calculated from the imaginary part of the dielectric function. Higher peaks in the imaginary dielectric spectrum report higher absorption. Moreover; absorptions are higher in the region of lower reflections. In this work we have investigated the imaginary dielectric functions of the pristine (8, 8) SWCNT, Ir/B-doped SWCNT and the  $H_2$  adsorbed Ir/B-doped SWCNT separately. The studies were also conducted in both parallel (z) and perpendicular (x) to the nanotubes. From the results shown in Figure 6, all the systems demonstrated optical potentials in both parallel and perpendicular directions. However, lower dielectric peaks were observed with (8, 8) SWCNT which is evident that it cannot give a perfect and strong binding energies for adsorption (Renáta and Andrej, 2011). As the pristine SWCNT is doped with Ir and B atoms, significant increase in the dielectric peaks were observed as demonstrated in Figure 6 (b). But the dielectric behaviors of the Ir/B doped SWCNT is more symmetric in the parallel direction than in the perpendicular direction. This can be justified by the



presence of peaks at 2.51 and 17.55 for perpendicular and parallel respectively. Figure 6 (c) presents the aftermath of H<sub>2</sub> adsorption by Ir/B co-doped SWCNT system. Significant increase in the dielectric adsorption peaks were seen to rise above 20. This is evident the binding energy needed by (8, 8) SWCNT

to adsorb H<sub>2</sub> molecule is significantly enhanced by co-doping Ir and B atoms. Furthermore adsorptions are more in parallel than perpendicular because of the higher aspect ratio (length to diameter) of the SWCNT (Manoj *et al.*, 2015).

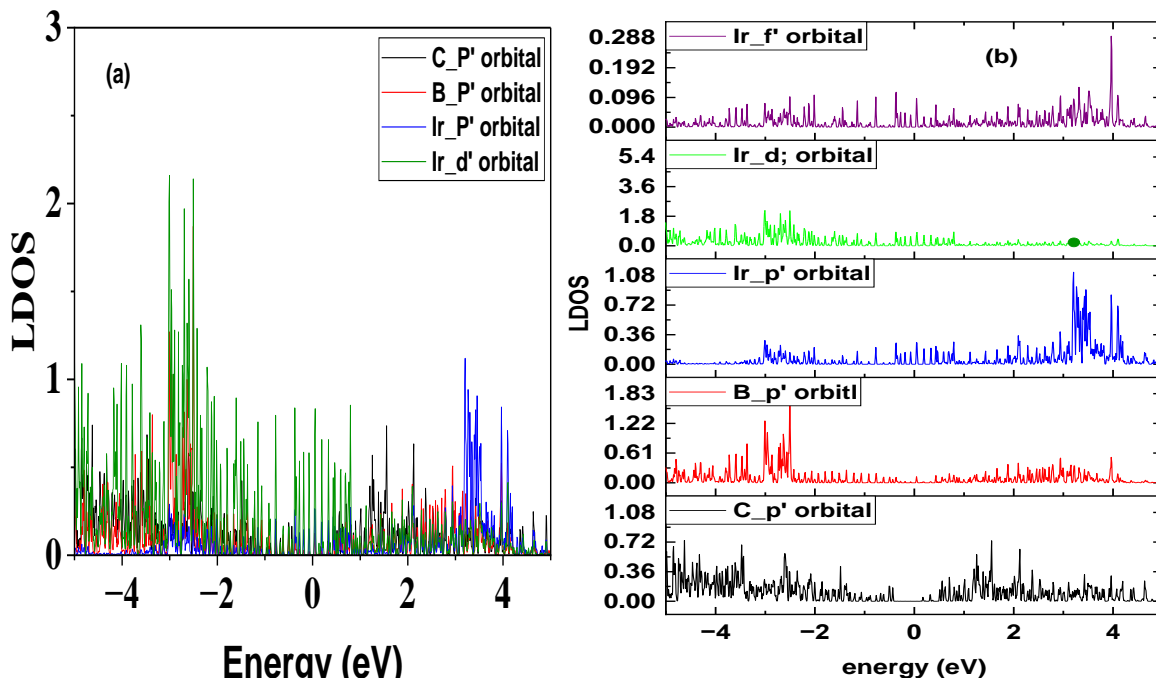


Figure 5. LDOS for the H<sub>2</sub> adsorbed Ir/B co-doped SWCNT

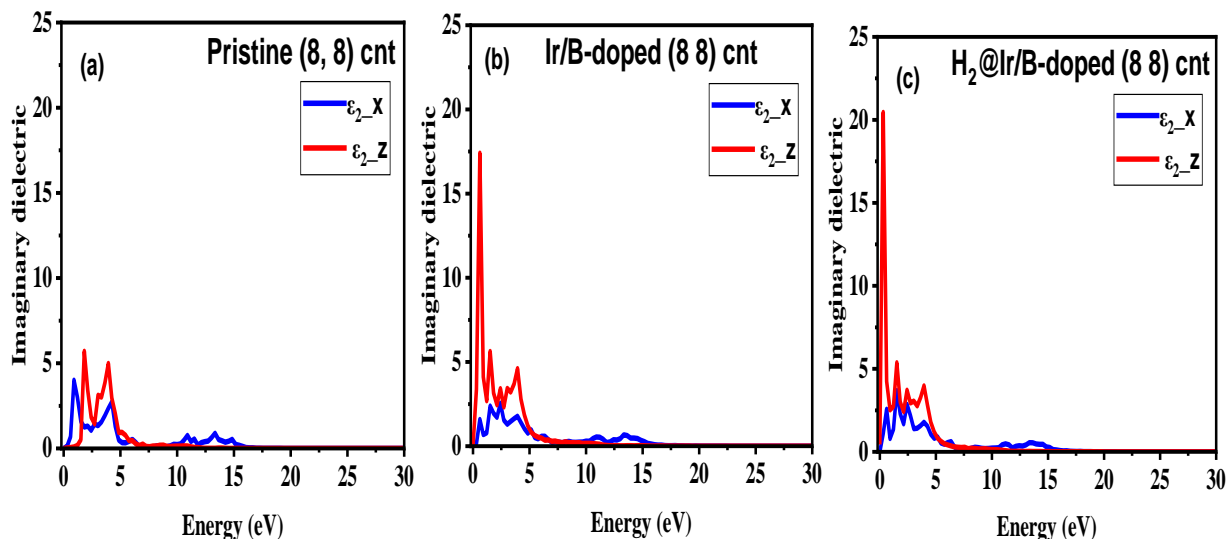


Figure 6. Optical absorption spectrum of (a) SWCNT, (b) Ir/B co-doped SWCNT and (c) H<sub>2</sub> adsorbed Ir/B co-doped SWCNT

### 3.6 Effects of H<sub>2</sub>-Ir/B co-doped SWCNT distance (*d*) on the adsorption efficiency

To further get the best, precise and efficient results on the potentials of Ir/B co-doped SWCNT structure, we have conducted our calculations across different

distance of H<sub>2</sub> molecule to the co-doped SWCNT which is denoted by *d* and measured in angstrom (Å). The studies were conducted by altering *d* to 6.12 Å, 6.45 Å and 7.77 Å respectively. All the calculations were ensured under ambient temperature and pressure.

Data were obtained in terms of the optical absorption coefficient ( $\alpha$ ) which is a function of the imaginary dielectric function. As presented in Figure 7, higher H<sub>2</sub> adsorption was observed for  $d = 6.45 \text{ \AA}$  (Figure 7 (b)), while lower adsorption was recorded for  $6.77 \text{ \AA}$  (Figure 7 (c)). Optimum H<sub>2</sub> adsorption was obtained for  $d = 6.12 \text{ \AA}$ . In the case of  $6.12 \text{ \AA}$  and  $6.45 \text{ \AA}$  spectrum shown in Figures 7 (a) and (b). The H<sub>2</sub> adsorption was symmetric in the direction along (parallel) to the nanotubes axes. Therefore, higher peaks were obtained. As such the Ir/B co-doped SWCNT can excellently store H<sub>2</sub> energy when the nanotube and H<sub>2</sub> molecules align in the same parallel directions and this agrees well with the reported hydrogen adsorption properties of carbon nanotubes (Itas *et al.*, 2022). More adsorption peaks appear as the H<sub>2</sub>-SWCNT distance ( $d$ ) is further increased from  $6.12 \text{ \AA}$  to  $6.45 \text{ \AA}$ . Outside this range, adsorption drastically diminished as reported in Figure 7 (c), therefore for better performance the H<sub>2</sub>- SWCNT distance must be the range  $6 \text{ \AA}$ - $6.5 \text{ \AA}$ .

### 3.7 Effects of temperature

This work also investigated the effects of temperature on the hydrogen adsorption efficiency of the co-doped SWCNT. Calculations were performed by keeping optimum value of  $d$  to  $6.45 \text{ \AA}$  constant while the temperature is further increased to  $650, 700,$  and  $750 \text{ }^\circ\text{C}$ . From the results, it is evident that temperature changes significantly affects the adsorption behaviors of the co-doped SWCNT. H<sub>2</sub> is weakly adsorbed when temperature is high, therefore increase as the temperature increased the amount of the H<sub>2</sub> adsorbed decreases. Based on this results, it can be reported that the Ir/B co-doped SWCNT demonstrated superficial H<sub>2</sub> gas adsorption capacity. This is because density of the H<sub>2</sub> gas increased near the surface of the co-doped SWCNT.

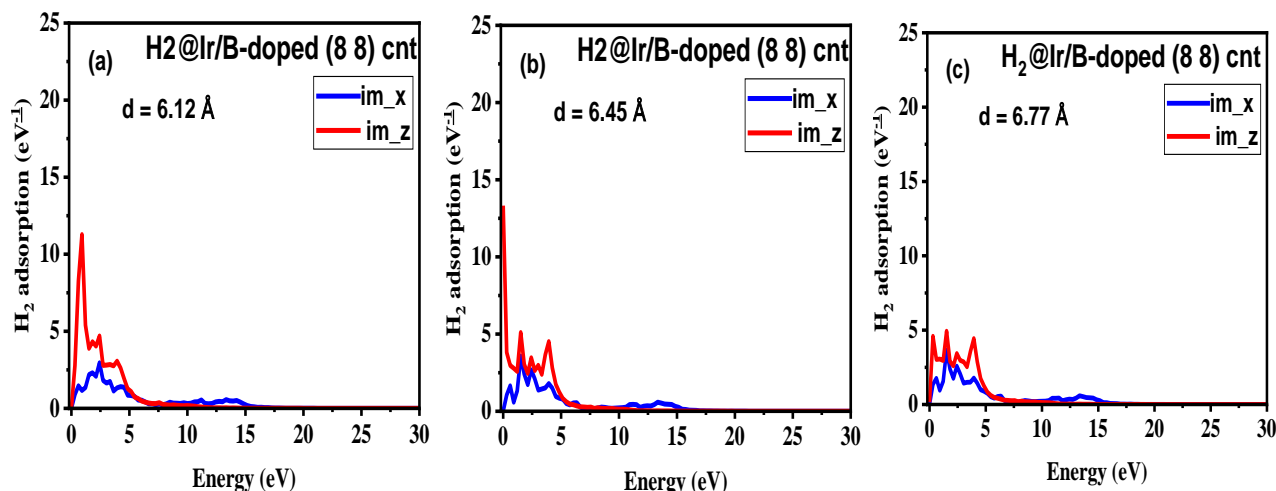


Figure 7. H<sub>2</sub> adsorption spectrum of Ir/B co-doped SWCNT under various  $d$ .

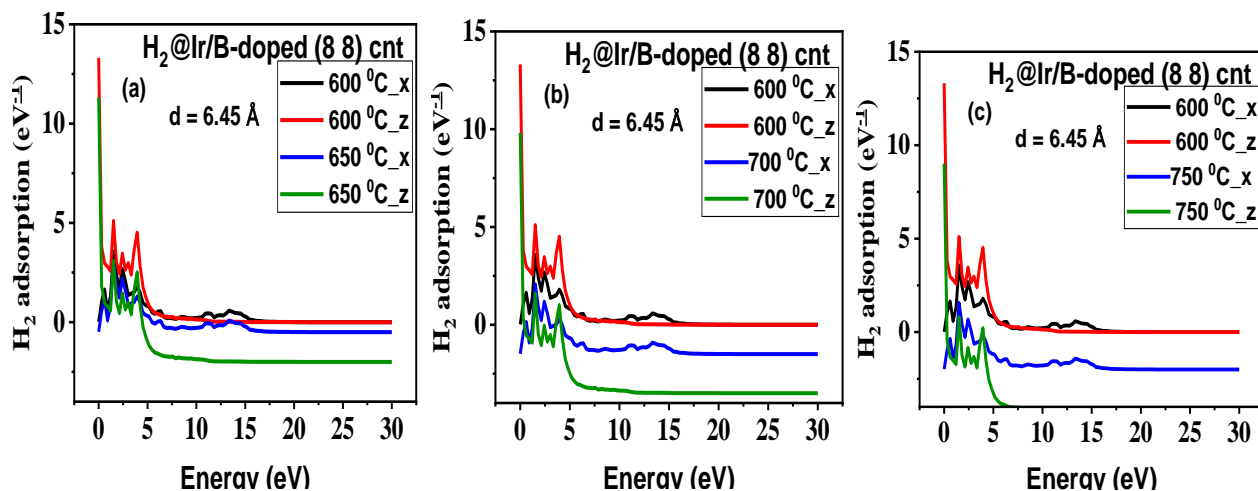


Figure 8. H<sub>2</sub> adsorption spectrum of Ir/B co-doped SWCNT under various temperatures

Gibbs free energy changes are negative, and also entropy changes are negative which in turn reduce the level of decrease of the release of the H<sub>2</sub> molecule. Figure 8 (a) Presents the adsorption values of the co-doped system under 600 °C and 650 °C respectively, results were calculated in both parallel and perpendicular directions.

Adsorption dropped from 13.4 and 3.7 in perpendicular and parallel to 11.3 and 2.9 respectively after increasing the temperature. This reduced the efficiency of the Ir/B doped-SWCNT adsorption by 27.6 % in parallel and 25.7 % in perpendicular. Further increase in temperature to 700 and 750 °C produced results obtained in Figures 8 (b) and (c) respectively. It can be seen also from all the Figures, H<sub>2</sub> adsorption are higher in lower energy ranges from 0 eV to 5 eV. The rate of H<sub>2</sub> adsorption by Ir/B co-doped SWCNT decreases with increase in temperature. Therefore, the Ir/B doped-CNT system works excellently as hydrogen storage candidate at room temperature. Furthermore, negative adsorption intensities were recorded by temperature increase by 650, 700 and 750 °C, this can be termed as exothermic adsorption. Based on this, it can be demonstrated that H<sub>2</sub> adsorption by co-doped SWCNT undergoes endothermic adsorption under ambient temperature and shows exothermic adsorption under higher temperatures.

#### 3.8 Effects of electric field

To further understand the efficiency of the fabricated armchair Ir/B-doped SWCNT structure, we studied the effects of applying external electric field of 0.1V/Å with different distances of the H<sub>2</sub> molecule, and the electric field are applied transverse to the nanotubes axes. The results were compared on the geometric and band structure of the nanotubes in the presence and absence of external electric field. Applying electric field transverse to all the three configurations of the nanotubes does not change the structure of nanotubes. Similarly, no effects were observed for band structure. By increasing the electric field from 0.1V/Å to 0.3V/Å, a slight shift in energy was observed for nanotubes under 6.45 Å and 6.77 Å IWD, although this does not change the size of the band gap. Further increase in the electric field makes no significant changes in the CBNNT band structure. However, there was slight change in the nanotube diameter under 6.12 Å IWD.

#### 4.0 Conclusions

To conclude this work, hydrogen energy is a remarkable tool to replace the existing fossil fuel due to its cleanliness, sustainability, and renewability with a significantly reduced impact on the global environment. This research employed a new technique of improving the performance efficiency of SWCNT in terms of hydrogen energy storage by co-doping of transition metal and non-metallic atoms. Studies were

conducted via DFT approach implemented in Quantum ESPRESSO and thermo-pw codes. Co-doped SWCNT were found to be more efficient within a specific range of distance of H<sub>2</sub> molecules from the co-doped system, it also performs best under ambient temperature. Numerous peaks are seen in both valence and conduction bands due to perceived excitations by Ir and B atoms. When H<sub>2</sub> molecule is adsorbed, they are centered around the Fermi energy level due to strong binding effects by Ir and B atoms. Introducing transition metals and hydrogen bonding clusters inside SWCNTs can enhance the uptake and release of hydrogen by and from the carbon nanotubes at practical temperatures and pressures. These impeded clusters should be capable of bonding large amounts of hydrogen with favorable thermodynamics and enhanced kinetics while the transition metals catalyze the hydrogen to react with the clusters/nanotubes system.

#### Declarations

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##### Ethics approval and consent to participate

Not Applicable

##### Consent for publication

All authors have read and consented to the submission of the manuscript.

##### Availability of data and material

Not Applicable.

##### Competing interests

All authors declare no competing interests.

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