Stability and Raman analysis of 1D carbon-boron nitride van der Waals heterostructure

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Abstract. In this work, we investigate the one dimensional van der Waals heterostructures formed by single-walled carbon nanotubes (SWCNTs) trapped inside single-walled boron nitride nanotubes (SWBNNTs) by a combination of molecular dynamics, the bond polarisability model, and the spectral moments method. Utilizing the Lennard-Jones potential, we examined the structural stability of the SWCNT(14,0)@SWBNNTs heterostructures. We calculated the optimal diameter of the host SWBNNTs at which the resulting SWCNT(14,0)@SWBNNTs heterostructures are stable. We then reported the Raman spectra of the SWCNT(14,0), SWBNNT(23,0), and SWCNT(14,0)@SWBNNT(23,0) calculated in the wavenumbers range of 0-1800 cm^{-1}. The structural stability of the SWCNT(14,0)@SWBNNT(23,0) coaxial heteronanotubes, as well as a possible charge transfer phenomenon occurring between the inner and the outer nanotubes, are investigated by analysing how encapsulation affects the Raman active modes of the guest SWCNT(14,0) and the host SWBNNT(23,0).

Keywords: SWCNTs, SWBNNTs, heteronanotubes, Raman.

1 Introduction

In the midst of the most prominent nanomaterials known for their fascinating physical properties that have stimulated researchers for the past 30 years, are Single-walled carbon nanotubes (CNTs) [1, 2]. Their specific honeycomb structure composed of sp^2 Carbon-Carbon bonds, forms rolled-up cylindrical graphene sheets. This covalent structure offers Single-walled CNTs high thermal conductivity and significant mechanical strength [3–7]. They have equally exceptional electronic properties. According to their chiral indices (n, m), they can be semiconducting or metallic [8, 9]. These outstanding properties make thase 1D nanomaterials potentially useful in several applications, including thermoelectric devices, transparent and flexible films, photovoltaic cells and transistors [9].

It should also be noted that, not just graphene, tubular structures can be formed using other 2D nanomaterials. In fact, Hexagonal boron nitride (h-BN) is 2D material which can

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form Single-walled boron nitride nanotubes (BNNTs) [10]. BNNTs are insulators with a large band-gap of around 5.5 to 6 eV independently of diameter or chirality, which inherit their 2D counterparts properties [11]. Equally, BNNTs show high thermal conductivity and mechanical strength [12–14], making them hopeful nanomaterials for various applications, including insulating components in nanodevices, as protective coatings or shells, and even in biocompatible materials for potential medical or biological applications [15–17].

The expansion of the potential applications of single-walled CNTs and BNNTs could be moreover performed by formation of the host/guest compounds with other nanomaterials, including nanowires, polymers, oligomers, or even more other types of nanotubes, resulting in 1D van der Waals (1D vdW) heterostructures [18–23]. Thanks to the recent advances in chemical vapor deposition techniques for nanomaterials, the experimental synthesis of these 1D vdW heterostructures have been enabled. Among them, single-walled CNTs encapsulated inside single-walled BNNTs (CNTs@BNNTs) are one of the simplest coaxial heteronanotubes with analogous layers of boron-nitrogen and carbon [19–21, 24, 25]. This is known as the 1D version of 2D vdW heterostructures formed by graphene and h-BN, which display unique physical properties and various applications. The weak vdW interactions subsisting between the guest single-walled CNTs and the host single-walled BNNTs, along with the inert surface of the host single-walled BNNTs can preserve the main physical properties of the guest single-walled CNTs, thereby maintaining their optoelectronic and thermoelectric properties. The 1D vdW heterostructures of CNTs@BNNTs is fascinating because the single-walled CNTs are protected and functionalized by dielectric single-walled BNNTs. The encapsulation inside allow to maintain the electronic behaviour of single-walled CNTs near the Fermi level, and it is expected to serve as the ultimate single-walled CNTs channel with a non-bonded surrounding dielectric layer, which allow to enhance its thermal conductance and make it more resistant to oxidation [26–28].

In this work, structural stability and vibrational properties from Raman spectroscopy of 1D vdW heterostructures consisting of zigzag single-walled CNTs (14,0) trapped inside single-walled BNNTs, denoted as SWCNT(14,0)@SWBNNTS (see Fig. 1), is theoretically investigated using a hybrid approach integrating molecular dynamics, bond polarizability model, and spectral moments method. The optimization of the geometry of SWCNT(14,0)@SWBNNTS is carried out utilizing Lennard-Jones potential. After calculating the optimal diameter of the host SWBNNTs and demonstrating the most stable SWCNT(14,0)@SWBNNTs heterostructure, the Raman spectra of the pristine SWCNT(14,0) and SWBNNT(23,0) calculated in the wavenumber range of 0-1800 cm^{-1} before and after encapsulation are reported. Our purpose consists of probing the inter-walls interactions that subsist in such 1D vdW systems by analysing of the effects of the encapsulation on the Raman actives modes of the guest SWCNT(14,0) and those of the host SWBNNT(23,0).

2 Computational method

The simulation of Raman responses involves the acquaintance of the dynamical matrix as well as the polarizability tensor of the nanomaterials. The former primarily enables the determination of the positions of the wavenumbers of the Raman features, while the latter allows to define the intensities of the Raman lines. Taking advantage of molecular dynamics, a three-step methodology is adopted, involving the decomposition of coaxial heteronanotubes into two independent subsystems (SWCNTs and SWBNNTs), followed by the coupling of the guest and the host nanotubes using an appropriate empirical potential. Using this approach, Raman spectra of various 1D vdW heterostructures formed by SWCNTs and SWBNNTs en-

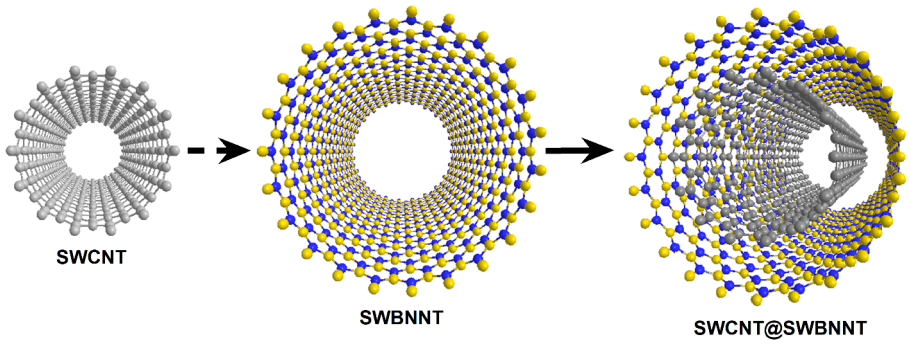

Figure 1. Schematic view of 1D carbon-boron nitride vdW heterostructure

capsulating oligothiophene derivatives, or SWCNTs filled with caffeine, and linear carbon chains can be effectively simulated as has been shown in our previous papers [29, 30].

Thus, Saito's force constant model is employed for the calculation of the dynamical matrix of the SWCNTs [31]. Then, Xiao's force constant model is employed for the calculation of the dynamical matrix of the SWBNNTs [32]. Lastly, as the pricipal binding mechanism in the coaxial heteronanotubes are the weak vdW interaction, the interactions between the inner SWCNTs and the outer SWBNNTs are characterized using lennard-Jones potential:

$$U_{ij}\left(r_{ij}\right) = \epsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - 2\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right]$$

with $\epsilon_{ij} = \sqrt{\epsilon_i \epsilon_j}$ and $\sigma_{ij} = \frac{\sigma_i + \sigma_j}{2}$. The parameters ($\epsilon_{ij}$; σ_{ij}) of Lennard-Jones that we used in our calculation for carbon, boron, and nitrogen atoms are (ϵ_{CC}=0.105 kcal.mol^{-1} ; σ_{CC}=3.851 Å), (ϵ_{BB}=0.180 kcal.mol^{-1} ; σ_{BB}=4.083 Å), and (ϵ_{NN}=0.069 kcal.mol^{-1} ; σ_{NN}=3.660 Å), respectively.

One the other hand, the polarizability tensor is calculated using the bond polarizability model [33]. The values of the empirical bond polarizability parameters of the SWCNTs and SWBNNTs are taken from reference [31]. Finally, the Raman responses of the investigated 1D vdW heterostructures of SWCNTs@SWBNNTs are performed by employing spectral moments method [34].

3 Results

3.1 Structural stability of SWCNT(14,0)@SWBNNTs

This section focuses on the structural stability of the 1D vdW heterostructures of SWCNTs@SWBNNTs. In the following calculations, SWCNTs@SWBNNTs heterostructures consisting of zigzag SWCNT(14,0) trapped into SWBNNTs are chosen as the largest coaxial heteronanotubes, where the diameter of the inner SWCNT(14,0) is 1.0968 *nm*. The first matter to be addressed when exploring the structural stability of such systems is the optimal diameter of the outer SWBNNTs at which the resulting 1D vdW heterostructures of SWCNT(14,0)@SWBNNTs are stable. As the interactions between the guest SWCNT(14,0) and the host SWBNNTs are ruled via the weak vdW interactions, the relaxation of the heterostructures is achieved through the minimization of Lennard-Jones potential. The calculation of the Lennard-Jones potential as a function of the diameter of the host SWBNNTs is

illustrated in Fig. 2. Thus, the results show that the equilibrium spacing between the sidewalls of the SWCNT(14,0) and SWBNNTs corresponds to a minimum of energy calculated aroud at 1.80 *nm*. Consequently, the optimal diameter of SWBNNTs of about 1.80 *nm*, like SWBNNT(23,0), is the most convenient for trapping SWCNT(14,0), where the optimal spacing between the sidewalls of the guest SWCNT(14,0) and the host SWBNNT(23,0) is at 0.36 *nm*.

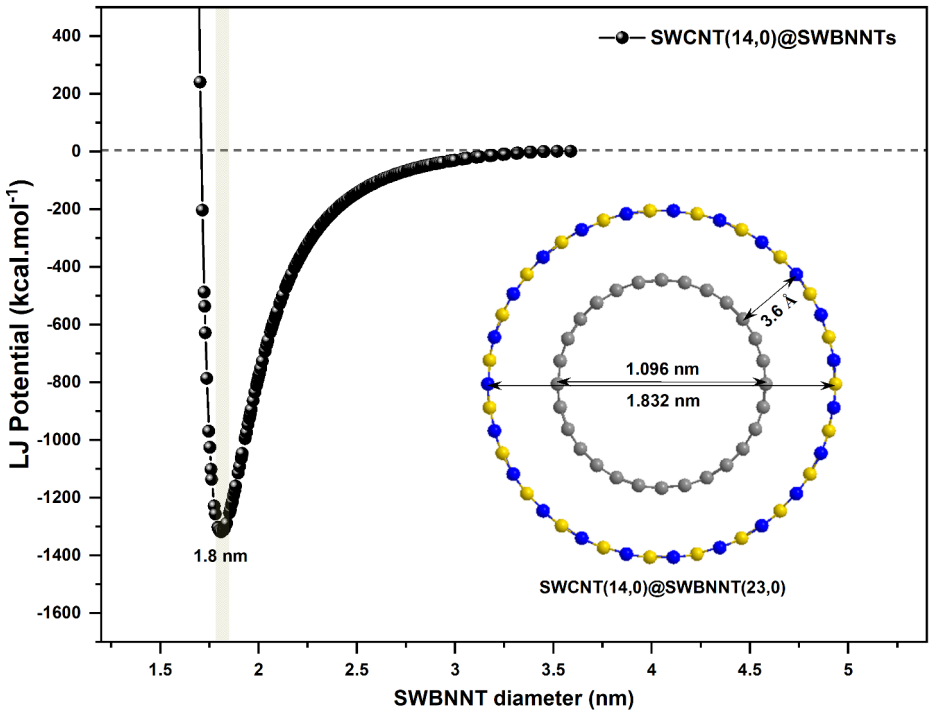

Figure 2. Lennard-Jones potential as a function of SWBNNT diameters

3.2 Raman spectra of SWCNT(14,0)@SWBNNT(23,0)

Raman spectroscopy plays a major role in nanomaterial science, especially in the study of the SWCNTs and SWBNNTs functionalized by encapsulation with divers chemical substances [35, 36] . The effects of the filling on the Raman active modes have been demonstrated to be pertinent to investigate the stability of the filled nanotubes, as well as the existence of an eventual charge transfer phenomenon [37, 38]. Likewise, Raman spectroscopy is expected to be a relevant tool of characterization for the 1D vdW heterostructures of SWCNTs@SWBNNTs. Thereby, we calculated the Raman spectra of the SWCNT(14,0)@SWBNNT(23,0) heterostructure. SWBNNT(23,0) was chosen as the host for the guest SWCNT(14,0), because its diameter of 1.83 *nm*, corresponds to the optimal value found in the precedent section, which allows the trapping of SWCNT(14,0). In the following section, the effects of encapsulation on the Raman-active modes of the guest SWCNT(14,0) and those of the host SWBNNT(23,0) are investigated.

The Raman spectra of the empty SWCNT(14,0), SWBNNT(23,0), and SWCNT(14,0)@SWBNNT(23,0) heterostructure calculated within the wavenumber

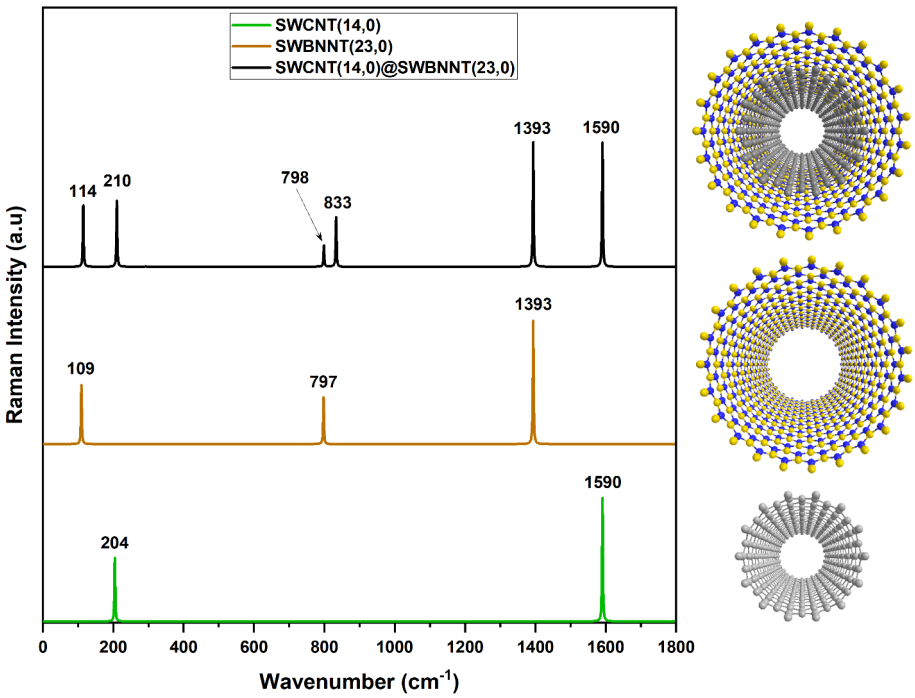

Figure 3. Raman spectra of empty SWCNT(14,0), SWBNNT(23,0), and the resulting SWCNT(14,0)@SWBNNT(23,0) heterostructure

range of 0–1800 cm^{-1} are shown in Fig. 3. The calculated Raman spectrum within the bond polarizability model of the empty SWCNT(14,0) comprises two features: (i) radial breathing modes (RBM), which are observed in the lower wavenumbers region of 100–400 cm^{-1}, that correspond to the coherent vibrations of all the carbon atoms in the nanotube's radial direction; and (ii) the tangential modes (TM) in the higher wavenumbers region of 1580–1600 cm^{-1}, so-called G-band, which belong to tangential motions of all carbon atoms [39].

On the other hand, the calculated Raman spectrum of the empty SWBNNT(23,0) within the bond polarizability model is characterized by three features : (i) the RBM located in the lower wavenumbers range of 100–400 cm^{-1}), which belong to the coherent vibrations of all boron and nitrogen atoms of the nanotube in the radial direction; (ii) the out-of-plane radial buckling modes (R) observed in the intermediate wavenumbers region of 790-830 cm^{-1}), where the boron and nitrogen atoms move inwards or outwards in the nanotube's radial direction; and (iii) the TM located in the higher wavenumbers region of 1380-1400 cm^{-1}), corresponding to the well-known E^{2g} in-plane vibrational mode of the h-BN networks [39]. Analysing the effects of encapsulation on these Raman ative modes is notably relevant to answer the questions about of the structural stability of such 1D vdW heterostructure, and the charge transfer phenomenon between the guest SWCNT(14,0) and the host SWBNNT(23,0), which are the main focus of this investigation.

For the Raman spectrum of the SWCNT(14,0)@SWBNNT(23,0) heterostructure, it seems to be as a superposition of both Raman spectrum of the guest SWCNT(14,0) and that of the host SWBNNT(23,0). However, attentive analysis reveals several modifications typical

of the interwall interactions between the guest SWCNT(14,0) and the host SWBNNT(23,0) in the resulting SWCNT(14,0)@SWBNNT(23,0) heterostructure.

We start with the effect of the encapsulation on the RBM of the nanotubes observed in the lower wavenumbers range of 100-400 cm^{-1}. The symmetric contraction and expansion motions of the inner SWCNT(14,0) and that of the outer SWBNNT(23,0) in the radial direction are influenced under encapsulation effects. In fact, the RBM of the SWCNT(14,0) located at 204 cm^{-1}, and that of SWBNNT(23,0) situated at 109 cm^{-1}, show a wavenumber up-shift by about 6 cm^{-1}, and 5 cm^{-1}, respectively, after encapsulation in the spectrum of SWCNT(14,0)@SWBNNT(23,0) heterostructure.

In fact, the RBM is a common feature of the nanotube-like systems that play a significant role in characterising and identifying of the the geometric structure of the nanotubes. The importance of the RBM derives from the fact that its wavenumber is inversely proportional to the nanotube's diameter [30, 31, 40]. However, although the existence of numerous theoretical investigations on the RBM wavenumber of the SWBNNTs, few experimental data are available [41, 42]. By contrast, numerous studies on the RBM of SWCNTs have been published in the literature, particularly those concerning the encapsulation of organic molecules inside SWCNTs [21, 37], where the RBM show systematic wavenumber up-shifts of around 2-5 cm^{-1} after filling. In General, the shifts of the RBM could be originated from vdW interaction or charge transfer, or from competition between these two effects. However, as demonstrated in our previous works [29, 30], charge transfer can be ruled out as the cause of the RBM shifts, and it was found that only the vdW interaction affects the shift of the RBM. Therefore, the up-shifts in the RBM of a few cm^{-1} can provide evidence for the structural stability of the selected SWCNT(14,0)@SWBNNT(23,0) heterostructure.

Next, regarding the R mode of the SWBNNT(23,0), which is located within the intermediate wavenumber range of 790-820 cm^{-1}, the encapsulation impacts the inward or outward radial vibration of the boron and nitrogen atoms of the SWBNNT(23,0). This is demonstrated by an upshift in the R mode wavenumber of approximately 1 cm^{-1}), accompanied by an additionnal mode peaking at 833 cm^{-1}. Following the conclusion about the effect of the encapsulation on the RBM, and the fact that the RBM and the R mode are relatively similar, leads us to assume that the influence on the R mode induced by the guest SWCNT(14,0) could arise from the same effect that produces the up-shift of the RBM.

On the other hand, for the TM of the nanotubes located in the higher wavenumbers region of 1385-1405 cm^{-1}, and 1580-1600 cm^{-1}, for SWBNNT(23,0) and SWCNT(14,0), respectively, no shifts are observed in the spectrum of SWCNT(14,0)@SWBNNT(23,0) heterostructure as illustrated in Fig. 3. The encapsulation does not affect the positions of the peaks of either nanotube's TM. The no change after encapsulation in the TM peak positions evince the absence of an eventual charge transfer between the guest SWCNT(14,0) and the host SWBNNT(23,0), which is consistent with the expected large band-gap of the SWBNNTs [11].

4 Conclusion

In conclusion, the structural stability and vibrational properties from Raman spectroscopy of 1D vdW heterostructures formed by zigzag SWCNT(14,0) trapped inside SWBNNTs were theoretically investigated using a hybrid approach integrating molecular dynamics, the bond polarizability model, and the spectral moments method. The structural stability of the SWCNT(14,0)@SWBNNTs heterostructures was examined through calculating the optimal diameter of the SWBNNTs at which the resulting SWCNT(14,0)@SWBNNTs heterostructures are stable utilizing the Lennard-Jones potential. It turned out that the best practical host SWBNNTs allowing the accommodation of the guest SWCNT(14,0) are those possessing

diameters of around 1.80 *nm*, like SWBNNT(23,0), where the optimal spacing between the sidewalls of the inner SWCNT(14,0) and the outer SWBNNT(23,0) is at 0.36 *nm*. Next, we reported the calculated Raman spectra of the pristine SWCNT(14,0) and SWBNNT(23,0) before and after encapsulation. The structural stability and the appearance of a prospective charge transfer phenomenon in the SWCNT(14,0)@SWBNNT(23,0) coaxial heteronanotubes have been explored by analysing the effects of the encapsulation on the Raman active modes of the guest SWCNT(14,0) (RBM and TM), and those of the host SWBNNT(23,0) (RBM, R mode and TM). The up-shifts of a few cm^{-1} in the RBM of the nanotubes under the effects of the encapsulation provided the first evidence for the structural stability of the trapped SWCNT(14,0) inside the SWBNNT(23,0) cavity distinguished by its optimal diameter. Additionally, the behaviour of the R mode of the host SWBNNT(23,0) under encapsulation effects provided supplementary evidence to support the predicted structural stability of the selected SWCNT(14,0)@SWBNNT(23,0) heterostructure. On the other hand, no shifts were observed in the spectrum of the SWCNT(14,0)@SWBNNT(23,0) heterostructure for the TM of the nanotubes located in the higher wavenumber region. The absence of change after encapsulation in the TM peak positions excludes the possibility of a charge transfer phenomenon occurring between the guest SWCNT(14,0) and the host SWBNNT(23,0), which is consistent with the expected large band-gap of the SWBNNTs.

References

[1] H.M. Dewey, A. Lamb, J. Budhathoki-Uprety, Recent advances on applications of single-walled carbon nanotubes as cutting-edge optical nanosensors for biosensing technologies. Nanoscale (2024).

[2] V.N. Popov, Carbon nanotubes: properties and application. Mater. Sci. Eng. R Rep. **43**, 61–102 (2004).

[3] J. Hone, M. Whitney, C. Piskoti, A. Zettl, Thermal conductivity of single-walled carbon nanotubes. Phys. Rev. B **59**, R2514 (1999).

[4] A.V. Savin, B. Hu, Y.S. Kivshar, Thermal conductivity of single-walled carbon nanotubes. Phys. Rev. B **80**, 195423 (2009).

[5] A. Cao, J. Qu, Size dependent thermal conductivity of single-walled carbon nanotubes. J. Appl. Phys. **112**, 1 (2012).

[6] X. Lu, Z. Hu, Mechanical property evaluation of single-walled carbon nanotubes by finite element modeling. Compos. Part B Eng. **43**, 1902–1913 (2012).

[7] N.A. Sakharova, A.F.G. Pereira, J.M. Antunes, C.M.A. Brett, J.V. Fernandes, Mechanical characterization of single-walled carbon nanotubes: Numerical simulation study. Compos. Part B Eng. **75**, 73–85 (2015).

[8] M.V. Kharlamova, Advances in tailoring the electronic properties of single-walled carbon nanotubes. Prog. Mater. Sci. **77**, 125–211 (2016).

[9] M. Ouyang, J.-L. Huang, C.M. Lieber, Fundamental electronic properties and applications of single-walled carbon nanotubes. Acc. Chem. Res. **35**, 1018–1025 (2002).

[10] N.G. Chopra, R.J. Luyken, K. Cherrey, V.H. Crespi, M.L. Cohen, S.G. Louie, A. Zettl, Boron nitride nanotubes. Science **269**, 966–967 (1995).

[11] X. Blase, A. Rubio, S.G. Louie, M.L. Cohen, Stability and band gap constancy of boron nitride nanotubes. Europhys. Lett. **28**, 335 (1994).

[12] T. Li, Z. Tang, Z. Huang, J. Yu, A comparison between the mechanical and thermal properties of single-walled carbon nanotubes and boron nitride nanotubes. Physica E **85**, 137–142 (2017).

[13] C.W. Chang, A.M. Fennimore, A. Afanasiev, D. Okawa, T. Ikuno, H. Garcia, D. Li, A. Majumdar, A. Zettl, Isotope effect on the thermal conductivity of boron nitride nanotubes. Phys. Rev. Lett. **97**, 085901 (2006).

[14] L. Vaccarini, C. Goze, L. Henrard, E. Hernandez, P. Bernier, A. Rubio, Mechanical and electronic properties of carbon and boron–nitride nanotubes. Carbon **38**, 1681–1690 (2000).

[15] H.M. Ghassemi, R.S. Yassar, On the mechanical behavior of boron nitride nanotubes. (2010).

[16] J.H. Kim, T.V. Pham, J.H. Hwang, C.S. Kim, M.J. Kim, Boron nitride nanotubes: synthesis and applications. Nano Convergence **5**, 1–13 (2018).

[17] C. Zhi, Y. Bando, C. Tang, D. Golberg, Boron nitride nanotubes. Mater. Sci. Eng. R Rep. **70**, 92–111 (2010).

[18] J.W. Kang, H.J. Hwang, Comparison of C_{60} encapsulations into carbon and boron nitride nanotubes. J. Phys.: Condens. Matter **16**, 3901 (2004).

[19] J. Guo, R. Xiang, T. Cheng, S. Maruyama, Y. Li, One-dimensional van der Waals heterostructures: A perspective. ACS Nanosci. Au **2**, 3–11 (2021).

[20] S. Cambré, M. Liu, D. Levshov, K. Otsuka, S. Maruyama, R. Xiang, Nanotube-based 1D heterostructures coupled by van der Waals forces. Small **17**, 2102585 (2021).

[21] C. Allard, L. Alvarez, J.-L. Bantignies, N. Bendiab, S. Cambré, S. Campidelli, J.A. Fagan, E. Flahaut, B. Flavel, F. Fossard *et al.*, Advanced 1D heterostructures based on nanotube templates and molecules. Chem. Soc. Rev. (2024).

[22] C.M. Homenick, D. Bennett, H. Li, Y. Martinez-Rubi, M.B. Jakubinek, L. Gaburici, O. Kodra, Z. Jakubek, K.S. Kim, B. Simard *et al.*, Low-Temperature Triazine Functionalization of Boron Nitride Nanotubes for Applications from Drug Delivery to Advanced Composites. ACS Appl. Nano Mater. **6**, 21079–21091 (2023).

[23] M.V. Kharlamova, Filled carbon nanotubes: promising material for applications. Nanomaterials **13**, 2472 (2023).

[24] R.S. Jones, B. Maciejewska, N. Grobert, Synthesis, characterisation and applications of core–shell carbon–hexagonal boron nitride nanotubes. Nanoscale Adv. **2**, 4996–5014 (2020).

[25] R. Arenal, A. Lopez-Bezanilla, In situ formation of carbon nanotubes encapsulated within boron nitride nanotubes via electron irradiation. ACS Nano **8**, 8419–8425 (2014).

[26] R. Xiang, T. Inoue, Y. Zheng, A. Kumamoto, Y. Qian, Y. Sato, M. Liu, D. Tang, D. Gokhale, J. Guo *et al.*, One-dimensional van der Waals heterostructures. Science **367**, 537–542 (2020).

[27] K. Otsuka, T. Sugihara, T. Inoue, W. Jia, S. Matsushita, T. Saito, M. Lee, T. Taniguchi, K. Watanabe, G. Pitner *et al.*, Coaxial boron nitride nanotubes as interfacial dielectric layers to lower interface trap density in carbon nanotube transistors. Nano Res. **16**, 12840–12848 (2023).

[28] H. Suzuki, M. Kishibuchi, K. Shimogami, M. Maetani, K. Nasu, T. Nakagawa, Y. Tanaka, H. Inoue, Y. Hayashi, Memristive behavior in one-dimensional hexagonal boron nitride/carbon nanotube heterostructure assemblies. ACS Appl. Electron. Mater. **3**, 3555–3566 (2021).

[29] Y. Kensi, J. Chenouf, B. Fakrach, S.A.A. Abdelkader, A.H. Rahmani, H. Chadli, A. Rahmani, 1D van der Waals heterostructures based on single-walled carbon nanotubes encapsulating linear carbon chains: Stability and charge transfer evidence from Raman spectroscopy. Appl. Surf. Sci. **611**, 155692 (2023).

[30] O. Elouardi, J. Chenouf, S. Elhadfi, Y. Kensi, S.A.A. Abdelkader, B. Fakrach, A.H. Rahmani, H. Chadli, A. Rahmani, Energetics and Raman spectroscopy of organic molecules encapsulated in single-walled boron nitride nanotubes: The example of π-conjugated oligothiophenes. Synth. Met. **311**, 117811 (2025).

[31] R. Saito, T. Takeya, T. Kimura, G. Dresselhaus, M.S. Dresselhaus, Raman intensity of single-wall carbon nanotubes. Phys. Rev. B **57**, 4145 (1998).

[32] Y. Xiao, X.H. Yan, J.X. Cao, J.W. Ding, Y.L. Mao, J. Xiang, Specific heat and quantized thermal conductance of single-walled boron nitride nanotubes. Phys. Rev. B **69**, 205415 (2004).

[33] S. Guha, J. Menendez, J.B. Page, G.B. Adams, Empirical bond polarizability model for fullerenes. Phys. Rev. B **53**, 13106 (1996).

[34] C. Benoit, E. Royer, G. Poussigue, The spectral moments method. J. Phys.: Condens. Matter **4**, 3125 (1992).

[35] M.S. Dresselhaus, G. Dresselhaus, R. Saito, A. Jorio, Raman spectroscopy of carbon nanotubes. Phys. Rep. **409**, 47–99 (2005).

[36] R. Arenal, A.C. Ferrari, S. Reich, L. Wirtz, J.-Y. Mevellec, S. Lefrant, A. Rubio, A. Loiseau, Raman spectroscopy of single-wall boron nitride nanotubes. Nano Lett. **6**, 1812–1816 (2006).

[37] M.V. Kharlamova, C. Kramberger, Spectroscopy of filled single-walled carbon nanotubes. Nanomaterials **12**, 42 (2021).

[38] M.V. Kharlamova, Kinetics, Electronic Properties of Filled Carbon Nanotubes Investigated with Spectroscopy for Applications. Nanomaterials **13**, 176 (2022).

[39] J. Chenouf, S. Elhadfi, S.A.A. Abdelkader, B. Fakrach, A. Rahmouni, A.H. Rahmani, Raman spectroscopy of carbon nanotubes embedded in boron nitride nanotubes: Insights into the origin of the observed shifts. Diam. Relat. Mater, 112989 (2025).

[40] B. Akdim, R. Pachter, X. Duan, W.W. Adams, Comparative theoretical study of single-wall carbon and boron-nitride nanotubes. Phys. Rev. B **67**, 245404 (2003).

[41] D. Ciuparu, R.F. Klie, Y. Zhu, L. Pfefferle, Synthesis of pure boron single-wall nanotubes. J. Phys. Chem. B **108**, 3967–3969 (2004).

[42] T. Shiratori, I. Yamane, S. Nodo, R. Ota, T. Yanase, T. Nagahama, Y. Yamamoto, T. Shimada, Synthesis of Boron Nitride Nanotubes Using Plasma-Assisted CVD Catalyzed by Cu Nanoparticles and Oxygen. Nanomaterials **11**, 651 (2021).