

Effective band structure control for single-atom-thick arsenic chain via strain manipulation by single-walled carbon nanotubes

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Abstract

Strain manipulation in low-dimensional material provides the chance to effectively and accurately modify their electronic and optoelectronic properties. Here, we synthesized small-diameter single-walled carbon nanotubes (SWCNTs) filled with the group V element arsenic (As) and discovered different crystal phases in SWCNTs with a narrow diameter distribution ($0.80 < d_t < 0.91$ nm). Gel permeation chromatography (GPC) was then applied for purification of as-filled SWCNTs by chirality, enabling an efficient enrichment of one-dimensional (1D) asymmetric zigzag As-based chains within the inner cavity of (7,5) and (8,4) SWCNTs. Photoluminescence and pressure-dependent Raman spectroscopic measurements were used as complementary tools to probe radial strain in these 1D heterostructures. In essence, pressure-dependent Raman measurements up to a medium-high pressure (~ 10 GPa) reveal that both metallic and semiconducting SWCNTs exhibit unconventional Raman mode frequency shifts and Raman intensity changes after filling, which was associated with abnormal lattice dynamics under pressure. Density functional theory (DFT) calculations reveal that asymmetric zigzag chains can transition from metallic to direct-bandgap semiconducting chains under certain compressive strain, likely due to the structure evolution of π -like valence bands. The large tunability of electronic bands together with clear knowledge of the local environment offer a useful platform for investigating strongly correlated electron states within 1D systems.

Introduction

Semimetals display with small indirect bandgaps show promising physical properties such as the presence of unusual topological quantum states¹, strong spin Hall effect^{2,3} and giant nonlinear optical response^{4,5}. Meanwhile, the unique electronic structure of nanoscale semimetals can also give rise to various interesting phenomena driven by strong electron correlation, such as ultrahigh electron mobility⁶ and the stability of superconductivity⁷. As is a group V element which exhibits a stable hexagonal buckled structure (known as gray As). Theoretical calculations indicate that both monolayer and layer-stacked gray As exhibit a small indirect bandgap, whose value depends on strain and crystal size⁸, making them an essential platform for discovering rich physics. Compared with 2D As crystals, experimental synthesis and investigations of their 1D analogues are still scarcely reported. It is essential to understand how the electronic band structure of atomic 1D As evolves as a function of lattice parameters, atomic structure and strain. The insight gained while analyzing such nanostructures could then be used to comprehend the behavior of a broad spectrum of materials.

Carbon nanotubes (CNTs) are imagined as rolled-up graphene, whose structure is described by the chirality indices (n,m). Among their unique properties is their ability to act as the smallest possible test tubes for studying structure-to-property relationships at the nanoscale. Such a vessel can potentially encapsulate various types of materials, including monoelements⁹, dye molecules^{10–13}, metal chalcogenides^{14–16}, metal particles^{17–19}, graphene nanoribbons^{20–22}, polar semiconductors²³, and

perovskites^{24–27}. Because the confined space of a SWCNT cavity restricts structures evolution, it can generate unconventional lattice structures such as 1D atomic chains or nanoclusters.

Here, we report the successful synthesis of SWCNTs encapsulated with As using a chemical vapor transfer (CVT) method with SWCNT diameters ranging from 0.5 nm to 1.4 nm. Based on subsequent gel permeation chromatography (GPC) experiments, As-filled semiconducting (7,5) and (8,4) were separated from the raw polychiral SWCNT mixture (Scheme 1). For raw SWCNTs with a diameter of about 0.8 nm, the encapsulated 1D As displayed three main structures: stretched symmetric zigzag chain, packed asymmetric zigzag chains, and discontinuous nanoclusters. Efficient refinement of the chain structure was confirmed by (7,5) and (8,4) SWCNT enrichment, with the majority found to be asymmetric zigzag chains. All discovered As chains were predicted to be metals. Core-level photoelectron emission spectra also revealed that the chemical environment of these atomic As chains was fundamentally different from that of gray As bulk crystals. Photoluminescence measurements revealed a mod family-dependent shift of the S_{11} emission peak, providing strong evidence of radial strain on (7,5) and (8,4) SWCNTs after zigzag As chains filled them. Based on subsequent pressure-dependent Raman measurements, an abnormal Raman mode frequency shift and Raman intensity change in these SWCNTs under pressure after the encapsulation of As were discovered. This may be ascribed to the radial strain induced by As filling and the resultant unusual lattice dynamics of the SWCNTs under elevated pressure.

Evolution of the electronic structure of the asymmetric zigzag As chains encapsulated in (7,5) and (8,4) SWCNTs as a function of radial compressive and tensile strain was then analyzed by the *ab initio* density functional theory (DFT) method, which indicates that an increased radial compressive strain can potentially turn the atomic chain into a direct-bandgap quasi-one-atom-thick semiconductor. The results shed light on the possibility of manipulating the nonlinear and magneto-optical response of extremely thin 1D heterostructures by strain engineering.

Results

Microstructure and steady-state spectroscopy

The UV-vis-NIR absorption spectrum of a solution of unseparated (mixed-chirality) SWCNTs (centrifuged but not purified via GPC) investigated in this study was shown in Figure S1. Absorption bands spanning the 950–1350 nm spectral region can be observed, which are assigned to the S_{11} transitions of SDS micelle-wrapped semiconducting SWCNTs with diameters of 0.55–1.2 nm according to the well-established empirical Kataura's model²⁸. In addition, the present absorption bands at 400–530 nm were assigned to the M_{11} transitions of metallic SWCNTs with diameters of ~ 0.8–0.95 nm, including (6,6), (7,7) and (8,5), as per results of our previous Raman characterizations²⁹.

The nanostructure of unseparated and chirality-separated As-filled SWCNTs was characterized based on high-angle annular dark field scanning transmission electron microscopic (HAADF-STEM) imaging (Fig. 1c-e). The As crystals found in polychiral SWCNTs showed various structural types (Fig. 1e). For

SWCNTs with diameters of 0.80–0.91 nm, zigzag chains and nanocluster chains are the dominant types of crystal phase. Noticeably, the zigzag chains display two structural types: symmetric chains showing a relatively wider bond angle and asymmetric chains comprising of closely packed As atoms and thus exhibiting much narrower bond angles. For SWCNTs with diameters on the order of 1 nm, a clear structural evolution can be observed, since wider chains such as ladder-shaped chains become the dominant type. This is similar to previous results, which revealed a dependence of As chain structure on SWCNT diameter³⁰. Additionally, chains with increased widths can also be observed, which are believed to be crystals filled inside SWCNTs wider than 1.1 nm (Figure S3). For separated (7,5) and (8,4) SWCNTs, the structural type of As crystals was clearly refined, with the majority displaying a zigzag shape. In comparison with zigzag chains discovered in unseparated, polychiral SWCNTs, the zigzag chains observed in (7,5)- and (8,4)-enriched sample are mainly asymmetric. The evolution of encapsulating chains with SWCNT diameter has been extensively studied and is interpreted as differences in formation energies³⁰. However, the structural evolution of atomic chains encapsulated inside SWCNTs with similar diameters is rarely reported. While formation energy plays a key role in altering chain structure, other factors, including charge-transfer effects and long-range dipole-dipole interactions can also affect the atomic arrangement of chains. For SWCNTs in their ground state, the dipole moment is zero. Additionally, since the material synthesis and imaging are performed under dry conditions, solvation effects are excluded. Therefore, the SWCNT and its external local environment would not favor long-range dipole-dipole interactions. If the encapsulated As chain has a large ground-state dipole moment, or if there is a strain effect or electronic coupling (e.g., charge transfer) between the encapsulated chain and the host SWCNT, the atomic structure of the chains could evolve.

The purity of separated (7,5)- and (8,4)-enriched As chain-filled SWCNTs was examined by UV-vis-NIR absorption measurement. A profound enrichment of (7,5) and (8,4) can be achieved by choosing an equilibrating solution and eluent with a relatively high SDS concentration during the chromatography-based (GPC) purification (Fig. 2a). Repeated separation experiments also validated that the protocol reliably elevated the content of (7,5) and (8,4) SWCNTs (Figure S4). The enrichment of desired (n,m) species can further be demonstrated by results of photoluminescence excitation (PLE) measurements (Fig. 2c and 2d). By comparing the photoluminescence spectra of semiconducting unfilled SWCNTs ((7,5)- and (8,4)-enriched) and As chain-filled SWCNTs ((7,5)- and (8,4)-enriched), a mod family-dependent transition energy shift as a result of chain filling was revealed (Fig. 2e and 2f). This may indicate prominent radial strain in (7,5) and (8,4) SWCNT as a result of filling by As chains. Note that radial strain control in filled SWCNTs is an attractive topic and the strain-induced modulation of emission wavelength has also been reported for small-diameter semiconducting SWCNTs filled with n-hexane and cyclohexane³¹.

Raman G mode spectra of semiconducting unfilled ((7,5)- and (8,4)-enriched) and As-filled SWCNTs ((7,5)- and (8,4)-enriched) under 532 nm and 633 nm excitation were shown in Figure S5. Fitting the spectra with Lorentzian functions confirms that the G mode peaks consist of a series of longitudinal optical (LO) and transverse optical (TO) modes, expected for chiral SWCNTs. It was further found that As

filling resulted in almost no spectral shift, indicating a rather weak interaction between the encapsulated 1D As and the host SWCNTs.

Pressure-dependent Raman spectroscopy

To learn how chain type affects strain in SWCNTs, pressure-dependent Raman measurements on suspended As chain-filled SWCNTs were performed, as illustratively described by diagrams in Fig. 3a. The experiment was conducted using a standard diamond anvil cell (DAC). The SDS micelle-wrapped SWCNTs were extracted from the solvent by evaporating water and then redispersed in the pressure-transmitting medium, silicon oil. The force applied to the opposing diamond anvils is transmitted via pressure-transmitting medium onto individual As-filled SWCNTs. Raman spectra were recorded during compression and decompression. Pressure-dependent spectra of various tested samples, including unfilled and As-filled semiconducting/mixed-chirality SWCNTs, were presented in Fig. 3b-i. Only strong RBMs were observed in the spectra of unfilled and As-filled mixed-chirality SWCNTs, which is potentially attributed to a much higher fraction of non-armchair metallic SWCNTs in these samples. For As chain-filled semiconducting SWCNTs (i.e., (7,5)- and (8,4)-enriched species), the RBMs vanished completely under as a low pressure as 0.3 GPa (Fig. 3f). Moreover, the G mode of (7,5) and (8,4) was also strongly suppressed under such a pressure (Fig. 3g). In contrast, the RBMs of As-filled SWCNTs with similar diameters (0.80–0.91 nm) in the mixed-chirality sample remained observable under a pressure of up to 5.2 GPa (Fig. 3h).

A more pronounced reduction in Raman intensities for As chain-filled (7,5)- and (8,4)-enriched sample is tentatively attributed to a larger extent of radial stress as a result of size mismatch between the SWCNTs and asymmetric zigzag chain. Nonetheless, since the Raman intensity of SWCNTs can be affected by several factors, including changes of the density of states (DOS), Raman scattering cross section (or polarizability), lattice distortion, and the interaction between SWCNTs and the environment³³, one needs to conduct comprehensive analyses to investigate all the above effects. Hence, we further measured the pressure-dependent Raman characteristics of unfilled mixed-chirality and semiconducting SWCNTs, and then investigated the Raman mode frequency shift ($d\omega/dP$) and Raman intensity change (dI/dP) of different SWCNT samples before and after filling with As.

For these analyses, the experimental Raman spectra were background-subtracted and deconvoluted. The background-subtracted spectra under various pressures for these SWCNT samples were displayed in Figures S6-11. Lorentzian functions were chosen to fit the Raman modes of different (n,m) species, except for the G+ modes of non-armchair metallic SWCNTs, which display an asymmetric line profile as a result of strong electron-phonon coupling³⁴. For such modes, an asymmetric Lorentzian function, named the Breit-Wigner-Fano (BWF) function, was applied for the simulation, which is expressed as follows:

$$I(\omega) = I_0 \frac{[1 + (\omega - \omega_0)/q\Gamma]^2}{1 + [(\omega - \omega_0)/\Gamma]^2}$$

1

where Γ and q are the Raman linewidth and a parameter describing electron-phonon coupling, respectively.

Pressure-dependent frequency shift of the G mode ($d\omega(G)/dP$) of unfilled species were investigated first (see Fig. 4a and 4c, and Figure S12-13). It appears that the variation of $\omega(G)$ with pressure for these unfilled mixed and semiconducting SWCNTs can both be fitted with a linear function, with slopes associated with different tangential modes (LO and TO modes). Moreover, for unfilled mixed-chirality SWCNTs, the gradients corresponding to the pressure-increasing and pressure-decreasing runs were found to show a non-negligible difference. Frequency shift of RBM with pressure ($d\omega(RBM)/dP$) for these unfilled SWCNTs was then studied. RBM spectra of the unfilled unseparated SWCNTs and semiconducting SWCNTs were found to be best fitted by 5 and 3–5 Lorentzian functions, respectively, which is interpreted as a drastic pressure-induced change in the spectral profile of semiconducting species. The two most intense RBMs were chosen to analyze the variation of $\omega(RBM)$ with pressure for each sample. It was found that one (and two) of RBM(s) of the semiconducting (mixed-chirality) sample displayed a trend described well by a second-order polynomial function, in the low-to-medium pressure region. The only exception is the lower-frequency RBM of the unfilled semiconducting sample, which follows a linear trend. All $d\omega(G)/dP$ and $d\omega(RBM)/dP$ determined from the fits, alongside the corresponding mode Grüneisen parameters γ_i calculated based on $\gamma_i = B d \ln \omega / dP$, where B is linked to isothermal volume compressibility, were displayed in Table S1 (B is assumed to be 13 GPa for unfilled SWCNTs).

Previous reports studied pressure-dependent Raman spectra of bundled SWCNTs and surfactant-coated individualized SWCNTs, which showed different $d\omega/dP$ characteristics. Venkateswaran and colleagues first reported the pressure-dependent Raman features of bundled SWCNTs using a methanol-ethanol mixture as the pressure transmitting medium³⁵. They found that the consideration of van der Waals interaction between SWCNTs and the intercalation effect (molecules of the pressure transmitting medium penetrating through the intertube space) affected the pressure-induced phenomenon, which gives rise to different theoretical models. These are: (i) the entire bundle is subjected to an external compression, or, (ii) the individual SWCNTs are each compressed symmetrically, and intertubule coupling is ignored, or, (iii) the pressure-transmitting medium is allowed to penetrate the interstitial channels between SWCNTs and thereby exert a $\sin^2 3\theta$ force on the SWCNTs. Kappes and co-workers studied the Raman features of surfactant micelle-coated individualized small-diameter semiconducting SWCNTs³⁶. They showed that the pressure-dependent frequency shift of either RBM or the G mode for these SWCNTs followed a linear trend unless a non-hydrostatic condition was reached. In our current study, the pressure-dependent frequency shifts of the RBM and G mode for unfilled SWCNTs are best fitted by a second-order polynomial and a linear function, respectively, which strongly suggests the

rebundling of SWCNTs. It is thus suspected that the relatively poorer solubility of SDS micelle-coated SWCNTs in silicon oil caused partial bundling of individualized SWCNTs. This hypothesis is supported by the fact that SDS may assume the reverse micelle configuration in silicon oil, or the micellization of this surfactant is prohibited altogether, given the hydrophobic nature of this liquid medium. Under such circumstances, two unfavorable effects are in force, which decrease the propensity of SWCNTs for individualization. First, non-polar silicon oil molecules can replace SDS on the SWCNT surface. Second, since both the solvent and the solute are hydrophobic in nature, silicon oil molecules and SWCNTs compete for access to SDS. The pressure-dependent frequency shifts of G modes and RBMs of As-filled SWCNTs were studied in the next section (see Fig. 4e and 4g, and Figure S14). It was revealed that the BWF line and G+ mode of As-filled mixed-chirality SWCNTs displayed remarkably different variation trends: $d\omega(\text{G}+)/dP$ shows a clear linear characteristic, while $d\omega(\text{BWF})/dP$ features a significantly large value up to 1 GPa followed by quite a small change at higher pressure. The variation of $\omega(\text{RBM})$ with pressure for these SWCNTs could be fitted with a second-order polynomial up to 3 GPa. For As chain-filled (7,5) and (8,4)-enriched species, only the variation feature of the G+ mode was investigated, attributed to the relatively low intensity of RBMs. It was shown that their pressure-dependent $\omega(\text{G}+)$ exhibited a clear second-order polynomial behavior up to 5 GPa. Gradients for $d\omega(\text{G})/dP$ and $d\omega(\text{RBM})/dP$ determined from the fits were summarized in Table S2.

The pressure-dependent frequency shift of G modes indicates that encapsulating As atomic chains/nanoclusters within SWCNTs affects both semiconducting and metallic SWCNTs. Two scenarios were considered to interpret this result: changes in forces on SWCNT under pressure after As filling, and filling-induced changes in van der Waals interactions between the SWCNTs and/or that between the SWCNT and adsorbed silicon oil molecules.

The intensity change of G mode peaks ($dI(\text{G})/dP$) for different samples was subsequently investigated (see Fig. 4b, 4d, 4f and 4h). $I(\text{G}+)$ and $I(\text{BWF})$ of unfilled mixed-chirality SWCNTs feature a steady decrease with pressure, while those of As-filled unseparated SWCNTs show an abrupt decrease below 0.5 GPa but a moderate change beyond 0.5 GPa. Additionally, the reversibility of the intensity of unfilled SWCNTs was remarkably better than that of As-filled SWCNTs. $I(\text{G}+)$ of unfilled semiconducting SWCNTs fluctuated within a pressure range up to 9.3 GPa, while $I(\text{G}-)$ of these SWCNTs increased sharply beyond 5 GPa. $I(\text{G}+)$ of As chain-filled semiconducting SWCNTs dropped immediately at 0.3 GPa, but recovered to some extent at higher pressure. For unfilled semiconducting SWCNTs, the reversibility of Raman intensity is sufficiently high. For As chain-filled semiconducting SWCNTs, however, a comparatively poorer reversibility (about one third of the original value) was found, which is similar to that of As-filled unseparated SWCNTs.

Previous studies reported Raman intensity changes of bundled SWCNTs, surfactant micelle-coated individualized SWCNTs and fullerene-filled SWCNTs (peapods) under pressure^{35–37}. Presumably, four reasons account for the observed changes: (i) lattice distortion and deformation (such as faceting³⁸), which lead to a change in the optical transition linewidth and hence the Raman scattering cross section of SWCNTs. (ii) Structure change as a result of interaction between the host SWCNT and guest material.

(iii) Chemical damage on SWCNTs due to the irreversible reaction of the SWCNT sidewall with surrounding molecules (e.g., the pressure-transmitting medium), which is supposed to occur at a high pressure (over 10 GPa in oil). (iv) Transferring into a relatively more non-hydrostatic condition, which leads to the scattering of Raman intensity. A significant faceting effect is not expected since no anomalous mode frequency shift was observed in experiments here. We first examined the resonance condition referring to the SWCNT diameter-dependent optical transition energies ($E_{ii} \sim d_t$), which were calculated based on a theoretical model accounting for many-body interactions³⁹:

$$E_{ii} = a \left[\frac{p}{d_t} + b \frac{p}{d_t} \log \left(\frac{c}{p/d_t} \right) \right] + \frac{\beta_p}{d_t^2} \cos 3\theta + \frac{\gamma}{d_t}$$

2

where p is related to the transition order. In this model, the linear term ap/d_t represents the quantum confinement of the 2D electronic structure of graphene, the logarithmic term accounts for many-body electron interactions, the chiral angle-dependent term corrects for a variation with the SWCNT chirality, and γ/d_t takes into account the diameter-dependent exciton binding energy. It was shown from the $E_{ii} \sim d_t$ plot for SWCNTs belonging to mode families 12–29 that the metallic (7,7) and (8,5) are in resonance under 532 nm excitation (Figure S15). The two species are believed to be abundant in the mixed-chirality SWCNTs used in this study, which rationalizes the high intensities of RBMs. The semiconducting species in the investigated samples, including (6,4), (6,5), (7,5), (7,6), (8,4) and (9,4), cannot be resonantly excited under such conditions. Owing to the resonance effect as well as a predicted small electron-phonon (or exciton-phonon, if excitonic effect is taken into account)⁴⁰ coupling matrix element⁴¹, the weak RBM intensities of semiconducting species can be expected.

Bearing these assumptions in mind, the abrupt decrease in intensities of G modes for As-filled mixed-chirality and semiconducting SWCNTs at low pressures is likely associated with a filling-induced abnormal lattice distortion (or deformation) resulting from radial strain under pressure. We did not provide any more direct evidence for a filling-induced change in the van der Waals forces in the current study, which theoretically may be achieved from Lennard-Jones simulations. Lastly, we plotted the Grüneisen parameters γ_i for various SWCNT samples to show more directly the effect of filling, as displayed in Figure S16. Since the variation of γ_i as a result of As filling appears to be dependent on the electronic structure of SWCNT, pressure-dependent Raman spectroscopy is a complementary tool to photoluminescence characterization to systematically investigate the radial strain effect of the encapsulated inorganic atomic chain on the host SWCNT.

Core-level and valence band electronic structures of chains

Since As has fully occupied d orbitals whilst partially occupied p orbitals, these p orbitals would influence the nature of As-As bonds. The core-level photoelectron spectra of the material were studied by

X-ray photoelectron spectroscopy (XPS). Figure 5a shows the As 3d spectra of As chain-filled (7,5) and (8,4) (denoted as “GP”), As chain-filled mixed-chirality SWCNTs (“C”), as-synthesized As chain-filled SWCNTs that were not pre-purified via centrifugation (“UC”), and mechanically exfoliated 2D gray As sheets (“NS”). The main observed differences between these spectra can be summarized as follows: (i) GP and C display split 3d peaks, which present at almost the same binding energies despite a difference in the chain structure, and (ii) UC and NS display a more prominent As-O 3d peak compared to the other two samples. Since the encapsulated As chains should be stable against oxidation, the emergence of the As-O 3d peak is indicative of the presence of bulk As crystals. The UC sample was not pre-purified by centrifugation, and there can be a lot of remaining bulk crystal residuals, which can account for such an effect. For As, spin-orbit coupling leads to a doublet feature of the 3d peak ($3d_{5/2}$ and $3d_{3/2}$)⁴². The vanished split 3d peak in the UC and NS samples is probably due to the significant inhomogeneity of the bulk crystals.

The structures of valence bands of various As chains were further investigated by *ab initio* DFT method. The analyzed chain structures were not relaxed for calculation. The energy dispersion relations of the symmetric zigzag chain, asymmetric zigzag chain, and ladder chain were computed and displayed in Fig. 5b-d. All these chains displayed a metallic nature, unlike their 2D analogues, confirmed to be semimetals.⁸ Compared to the band structures of the symmetric and asymmetric zigzag chains, that of the ladder chain is characterized by the presence of multiple valence bands, which show strong crossing. This produces multiple electron and hole pockets, indicating the complex electronic and optoelectronic behavior of ladder chains.

Discussion

It has been found that strain manipulation can induce a metal-insulator transition (MIT) or topological phase transition in various materials^{8, 43–47}, driven by purely a structural (crystal symmetry) changes⁴⁵, or by, mechanisms such as Peierls instability⁴⁸. These phenomena are essential to the research on superconductivity and the stability of the antiferromagnetic (AFM) phase. Therefore, it is of great interest to investigate how radial strain influences the evolution of the electronic structure of atomic As chains and to elucidate the underlying mechanism.

Figure 6 shows the electronic band structure of asymmetric As chains as a function of compressive or tensile strain. For the structure without stress, the two bands above the Fermi Level were found to nearly cross at the V_1 valley. With increased tensile strain toward + 5%, the two bands clearly crossed. By comparison, with compressive strain toward – 5%, the upper band rose notably, and a gap emerged between the two bands. Since the positions of the minimum of the upper band and the maximum of the lower band almost align in the reciprocal space, the result indicates the possibility of creating a direct bandgap semiconducting chain. The effective mass ratio for charge carriers at the band edges, m_e^*/m_h^* , was estimated to be about 0.4, indicating higher electron mobility than that of holes. The potentially high

conductivity of zigzag As chains means they might perform similarly to metallic SWCNTs and graphene⁴⁹.

The electronic bands of this As chain near the Fermi Level comprise both a non-dispersive and a highly dispersive band. It was shown that the contributing orbitals to the two bands were quite different. The non-dispersive band mainly displays the p_y character, while the highly dispersive band has mixed p_x , p_z , and s character. For the highly dispersive band, the energy at the Γ point moved downward by 0.481 eV under radial compressive strain of 5%, while it moved upward by 0.447 eV under tensile strain of 5%. For the non-dispersive band, in contrast, the energy at the Γ point moved upward or downward by only 0.066 eV or 0.077 eV under 5% radial compressive or tensile strain, respectively. With further increases in radial strain, a change in band ordering is expected.

Similar to 2D Group V crystals, 1D As chains should also contain both σ and π (anti-) bonds⁵⁰. By altering radial strain, the overlap between p orbitals can change in accord with interatomic distance. This causes valence bands to rise or shift downward, as expected and clearly demonstrated by our *ab initio* DFT calculations above. We deduce that one electronic band close to the Fermi Level is σ -like, while the other is π -like. To further validate the hypothesis, one can calculate and analyze the characteristics of frontier orbitals of the As atomic chain under strain, which was not carried out in the current study. Since a more or less obvious change in the valence band structure of an asymmetric zigzag As chain under radial strain can be demonstrated, it is anticipated that the metallicity and charge mobility of the material can also be effectively altered via strain manipulation.

Additionally, a notable change in the p orbital and π bond characteristics of As chains under radial strain is expected, which indicates that the van der Waals (vdW) interaction (π - π interaction) between the As chain and the sidewall of SWCNT is modified accordingly. According to the results of our Raman measurement (see Figure S5), a negligible shift of the G+ band as a result of As chain filling was found, indicating a rather weak van der Waals interaction between the As chain and (7,5) or (8,4) SWCNTs. By cautiously examining the Raman features of the same (n,m) SWCNT species encapsulating other types of As atomic chains (e.g., symmetric zigzag chains), a clear relationship between the strength of host SWCNT-guest chain interaction and strain effect can hopefully be obtained. Such approach could enable quantitative research on electron correlation in a 1D system in the presence of screened Coulomb forces. For example, by involving methods based on the 1D Hubbard model.

Conclusion

In conclusion, we identified three main crystal phases of 1D atomic As in SWCNTs with diameters between 0.80 and 0.91 nm: symmetric zigzag chain, asymmetric zigzag chain, and nanocluster chain. We reported efficient separation of asymmetric zigzag As chain-filled (7,5) and (8,4) SWCNTs from mixed-chirality As-filled SWCNTs via GPC experiments. The photoluminescence and pressure-dependent Raman measurements were revealed to be efficient and complementary tools for evaluating the effect of radial strain on 1D As encapsulated in SWCNTs with a specific (n,m). Electronic structures of different

types of ultrathin As chains were investigated by XPS measurements and the *ab initio* DFT method. A remarkable change in the electronic characteristics of asymmetric zigzag As chains as a function of radial strain experienced within the narrow cavity of small SWCNTs was demonstrated, which is tentatively attributed to the structure evolution of π -like valence bands. The reported methodology is supposed to serve as guidance how to quantitatively study strongly correlated electron states within 1D systems.

Experimental Section

Material

CoMoCAT SWCNTs (ref no.: 775533) were used as raw SWCNTs. Sodium dodecyl sulfate (SDS) was purchased from Sigma-Aldrich (ACS reagent, $\geq 99.0\%$). As was purchased from Sigma-Aldrich (99.999%). Hydrogels made from a cross-linked copolymer of allyldextran and N,N'-methylene bis(acrylamide) (Sephacryl S-200) were purchased from GE Healthcare.

Filling Experiment

To perform the filling experiment, raw SWCNT powder and As powder were mechanically mixed, transferred into a quartz ampule, and sealed under high vacuum. The ampule was heated to 900 °C for 12 h to initiate the filling process.

SWCNT Purification

Chirality-refined SWCNTs were obtained by gel permeation chromatography (GPC) as described in previous work^{51–53}. The raw unfilled and As-filled SWCNTs were thoroughly dispersed in 2 wt. % aqueous SDS solutions via tip sonication. Persistent SWCNT bundles and catalyst particles introduced during SWCNT synthesis, which detached from SWCNTs during agitation, were removed by centrifugation at a high force of 150,000 $\times$ g. The as-centrifuged SWCNT dispersion is called the stock solution. This stock solution was then loaded into a hydrogel column equilibrated with aqueous SDS solutions of various concentrations. SDS solutions with increasing concentrations (i.e., 0.25, 0.5, 1, 1.5, 2 and 5 wt. %) were applied to elute the SWCNT species adsorbed on the gel bead. Typically, semiconducting SWCNTs can be enriched at a highly concentrated eluent. The concentration of the equilibrating solution did not significantly affect semiconducting purity of SWCNTs. However, both a highly concentrated eluent and the equilibrating solution were required to separate As-filled (7,5) and (8,4) SWCNTs.

ADF-STEM Imaging and EDX Analysis

High-angle annular dark-field scanning transmission electron microscopic microscopy (ADF-STEM) imaging of SWCNT samples was performed using a Thermo Scientific Themis Z microscope at an acceleration voltage of 300 kV and a condenser lens aperture size of 50 μm . The tested samples were prepared by dropcasting the semiconducting SWCNT solution onto a lacey carbon grid followed by baking the grid in a vacuum oven for 12 hours. Afterward, the grid was treated with argon plasma to remove organic compounds further. To reduce the effect of carbon buildup, beam showering was performed before imaging.

Steady-state Spectroscopic Characterizations

Steady-state UV-vis-NIR absorption measurements were performed on an Agilent Cary 5000 instrument. Solutions stored in a 1 cm-beam path quartz cuvette were measured. PLE measurements were performed on an Edinburgh FLS 1000 instrument. The near-infrared fluorescence from semiconducting SWCNTs was collected in a right-angle geometry and detected by a liquid nitrogen-cooled near-infrared single-photon photomultiplier detector. Variations in excitation power and detector sensitivity were corrected. Raman measurements were performed using a Renishaw InVia Reflex spectrometer under an excitation wavelength of either 532 nm or 633 nm, operated with a 1800 l/mm diffraction grating. A 50 $\times$ infinity-corrected objective was used for the measurement.

Pressure-dependent Raman Measurement

High-pressure conditions were generated using a diamond anvil cell (DAC) equipped with T301 steel gaskets for sample sealing. Silicone oil was employed as the pressure-transmitting medium and maintained quasi-hydrostatic conditions up to approximately 4 GPa⁵⁴. The pressure inside the DAC was determined from ruby fluorescence shifts measured with a BETSA system and calibrated using the IPPS-Ruby Eq. 5⁵.

In situ Raman measurements were performed on a Horiba LabRAM HR Evolution spectrometer using a 50 $\times$ super long-working distance Olympus objective, a 532 nm laser (5 mW), and a 600 grooves mm^{-1} grating. Spectra were recorded in the range of 100–4800 cm^{-1} with an acquisition time of 60 s and a confocal hole of 1000 μm . The calibration uncertainty of the Raman shift was controlled within $\pm 0.5 \text{ cm}^{-1}$.

X-ray Photoelectron Spectroscopy

XPS measurement was performed on a ThermoFisher Scientific ESCALAB Xi + XPS Microprobe system. The tested samples are filtered SWCNT thin films and as-purchased As powders deposited on silicon wafers. To remove organic compounds from SWCNT films manufactured using materials previously

separated via GPC, the samples were cleaned by gas cluster ion sputtering. The binding energy scale was calibrated with Au 4f₇, Ag 3d₅, and Cu 2p₃ core levels.

Computational Method

First-principles calculations were performed within the framework of density functional theory (DFT) using the Vienna Ab initio Simulation Package (VASP). Ion-electron interactions were described via the projector-augmented wave (PAW) method, whereas electronic exchange-correlation effects were addressed within the generalized gradient approximation (GGA) using the Perdew-Burke-Ernzerhof (PBE) functional. A plane-wave energy cutoff of 400 eV was adopted, and an energy convergence threshold of 10^{-6} eV per unit cell was imposed. Long-range van der Waals (vdW) interactions were accounted for through the DFT-D3 correction scheme. A 25 Å vacuum layer was added along the xy-plane to eliminate spurious adjacent supercell interactions, with Brillouin zone (BZ) sampling confined to the Γ -point, while the periodic z-direction was sampled with a denser k-point mesh. Radial strain was simulated by adjusting the lattice constant along the x- or y-direction while optimizing the perpendicular lattice and all atomic positions, with strains ranging from – 5% to + 5%.

Declarations

Data availability

The data that support the findings and result analysis of this study are included in the article and its Supplementary Information. Additional data are available from the corresponding author upon reasonable request.

ASSOCIATED CONTENT

Supporting Information

The following files are available free of charge.

More UV-vis-NIR absorption spectra of unseparated (centrifuged but not purified via GPC) and GPC-purified SWCNT solutions. HAADF-STEM image of wide As chains in large-diameter SWCNTs. G mode Raman spectra of (7,5) and (8,4) SWCNTs under the excitation wavelengths of 532 nm and 633 nm. Pressure-dependent Raman characteristics of different SWCNT samples. Simulated diameter-dependent optical transition energies of SWCNTs belonging to mod families 12-29. Parameters of fits to the pressure-induced Raman frequency change of various samples and the calculated Grüneisen parameters γ_i .

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Author Contributions

X. Z. synthesized the material and performed various steady-state spectroscopic measurements. L. G. performed HAADF-STEM measurement. X. G. performed pressure-dependent Raman measurements. Z. H. analyzed the HAADF-STEM images and various steady-state spectroscopic data. Y. W. and Z. H. completed ab initio DFT calculations and analyzed the data. Z. H., S. Q., D. J. and L. K. wrote the manuscript. H. Y., H. O., R. A., M. B., G. S., Y. Z. contributed to manuscript revision.

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Notes

Any additional relevant notes should be placed here.

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Scheme 1

Scheme 1 is available in the Supplementary Files section.

Figures

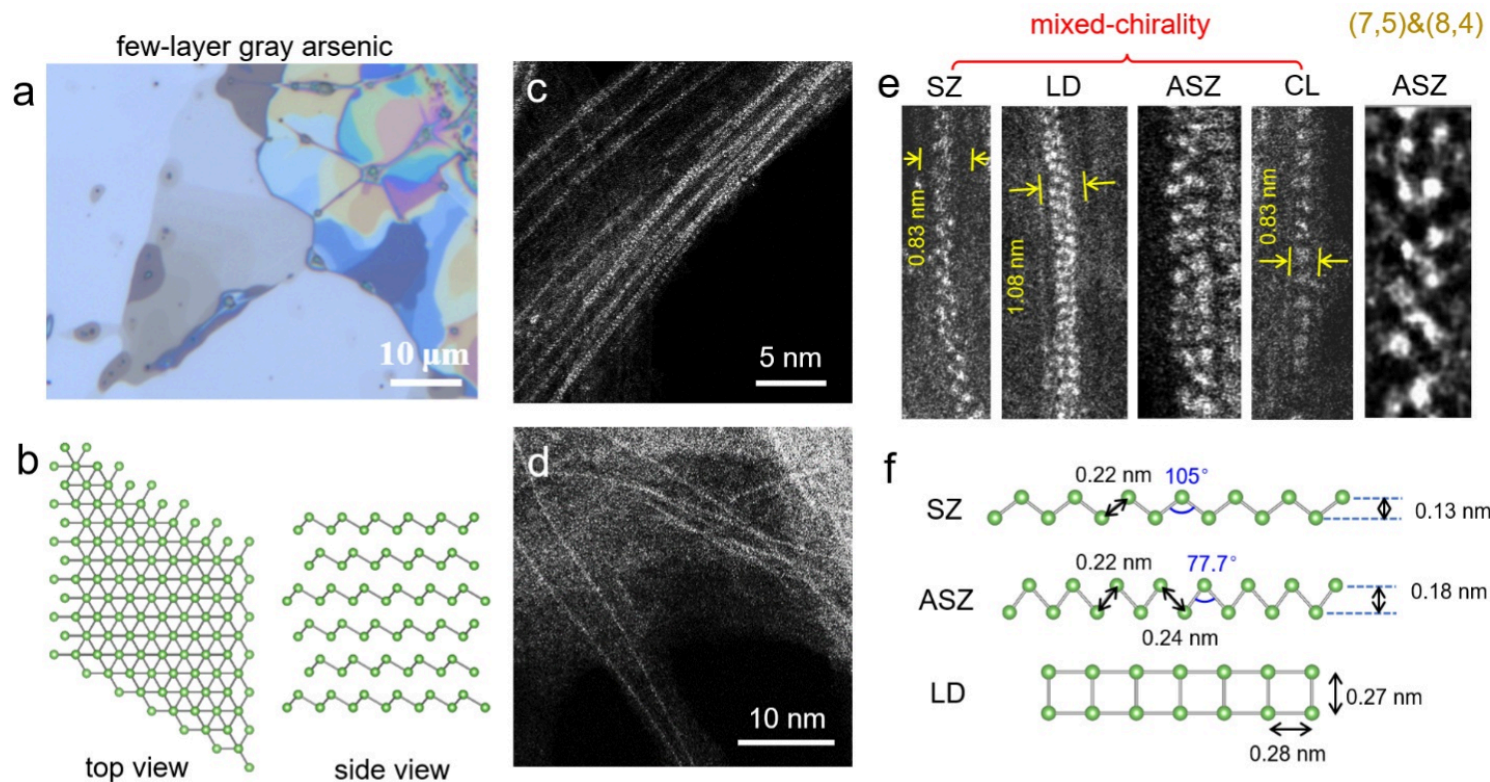


Figure 1

(a) An optical microscopic image of few-layer gray As. (b) Top and side views of the hexagonal buckled (ABC-stacking) structure of gray As. (c,d) HAADF-STEM images of (c) mixed-chirality SWCNTs and (d) (7,5)- and (8,4)-enriched SWCNTs filled by 1D As. (e) Zoomed-in images of selected chains from mixed-chirality and (7,5)- and (8,4)-enriched SWCNTs. The annotations above the images indicate the chain structures: SZ-symmetric zigzag, LD-ladder, ASZ-asymmetric zigzag, CL-nanocluster. (f) The structure models and corresponding lattice parameters of the symmetric zigzag, asymmetric zigzag, and ladder chains.

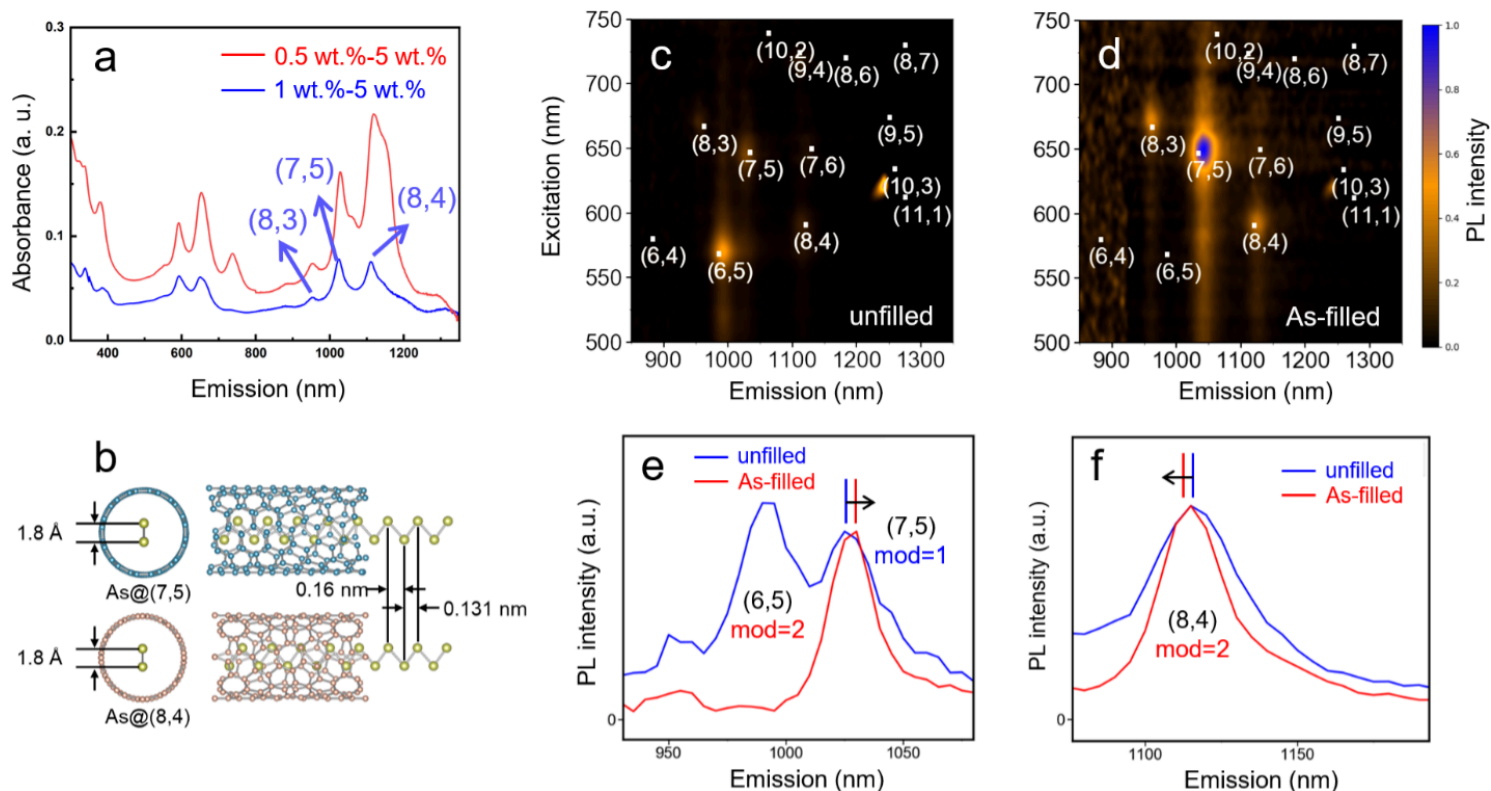


Figure 2

(a) UV-vis-NIR absorption spectra of semiconducting As-filled SWCNTs separated via GPC. Using an equilibrating solution and eluent with a high SDS concentration led to more efficient separation of (7,5) and (8,4) SWCNTs. (b) Structure models of asymmetric zigzag As chain-filled (7,5) and (8,4) SWCNTs. (c,d) Photoluminescence excitation maps of semiconducting unfilled ((7,5)- and (8,4)-enriched) and As-filled SWCNTs ((7,5)- and (8,4)-enriched). The presence of (6,5) SWCNTs in the first photoluminescence excitation map is related to their intrinsically high brightness. Interestingly, upon As filling, the signals from (6,5) SWCNTs diminishes³². (e,f) Photoluminescence spectra of unfilled and As-filled SWCNTs mentioned above at the excitation wavelengths of 645 nm and 590 nm, respectively.

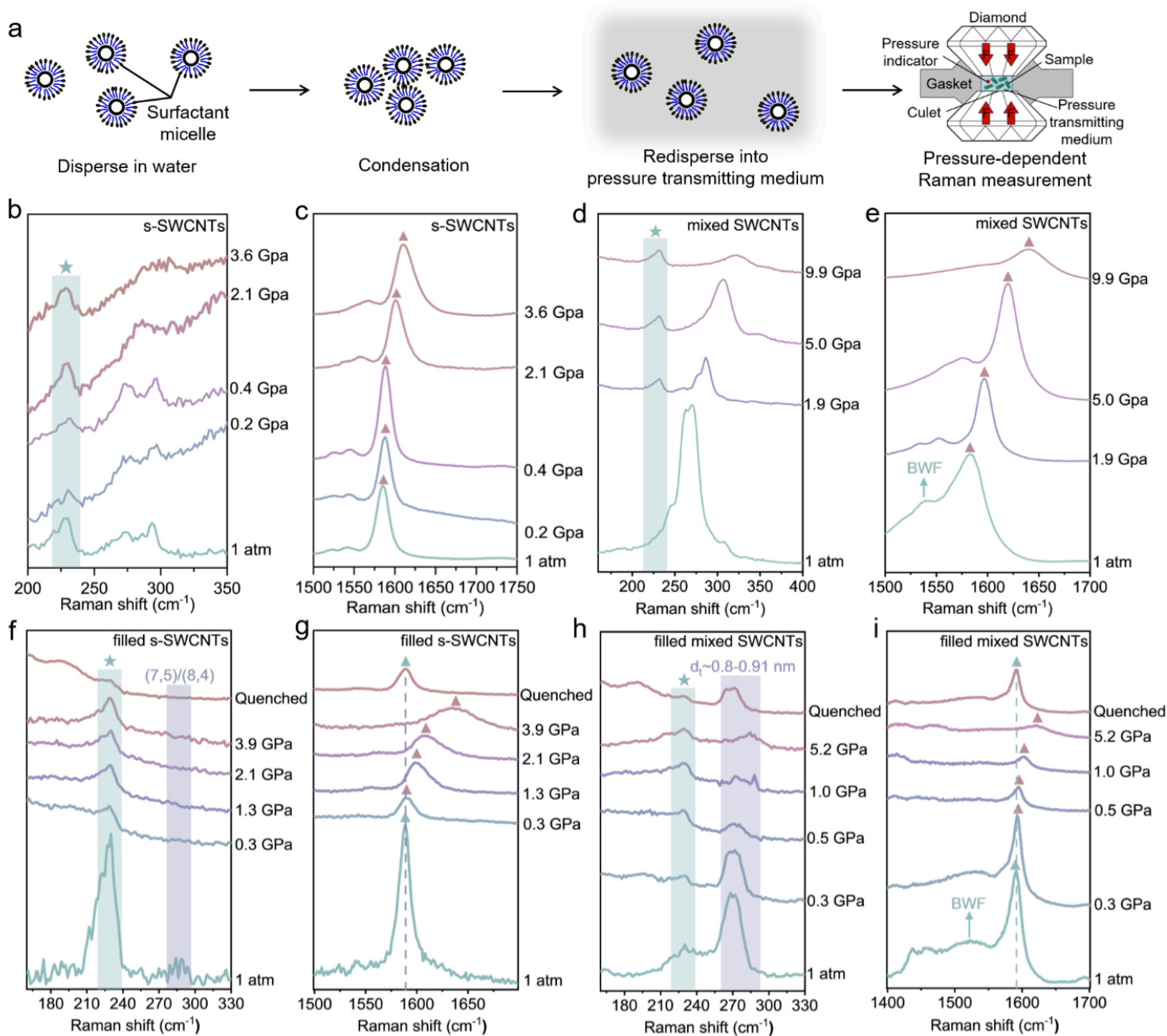


Figure 3

(a) Diagrams illustratively show the method to prepare dispersed SWCNT samples for pressure-dependent Raman spectroscopic measurement. (b-i) RBM and G mode spectra of (b,c) unfilled (7,5)- and (8,4)-enriched SWCNTs, (d,e) unfilled mixed-chirality SWCNTs, (f,g) As chain-filled (7,5)- and (8,4)-enriched SWCNTs, and (h,i) As-filled mixed-chirality SWCNTs under various pressures (background signals were not removed). The bands indicated by stars in panels b, d, f and h are peaks do not originate from SWCNTs. The spectra are not normalized in order to demonstrate the actual intensity changes with pressure. Dashed lines in panels g and i illustrate the frequencies of G+ peaks before pressure increase, indicating a high recovery of peak position following the pressure increasing and decreasing run.

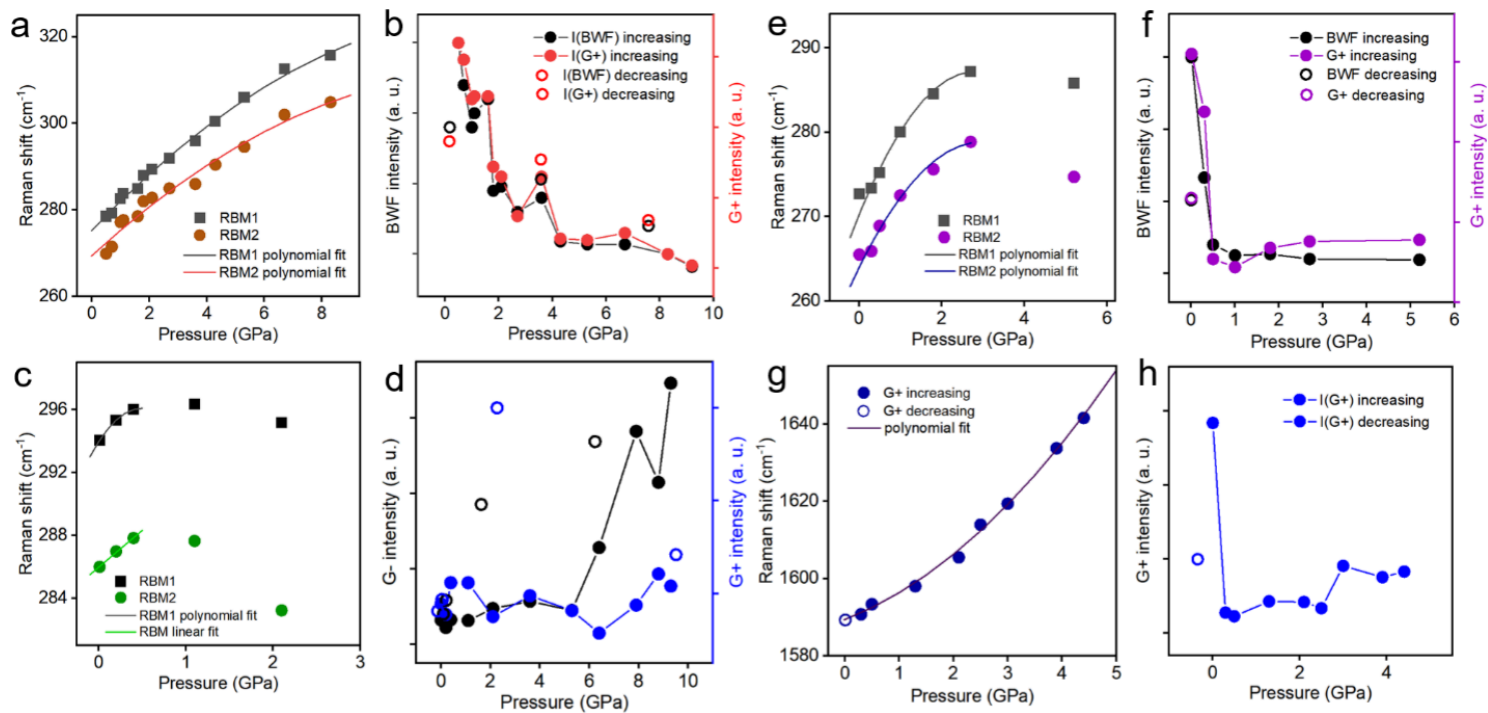


Figure 4

Pressure-dependent frequencies and intensities of Raman modes of (a,b) unfilled mixed-chirality (unseparated) SWCNTs, (c,d) unfilled semiconducting ((7,5)- and (8,4)-enriched) SWCNTs, (e,f) As-filled mixed-chirality SWCNTs and (g,h) As chain-filled semiconducting ((7,5)- and (8,4)-enriched) SWCNTs. Data points in panels b, d, f, g, and h contain values measured during pressure-increasing and pressure-decreasing runs.

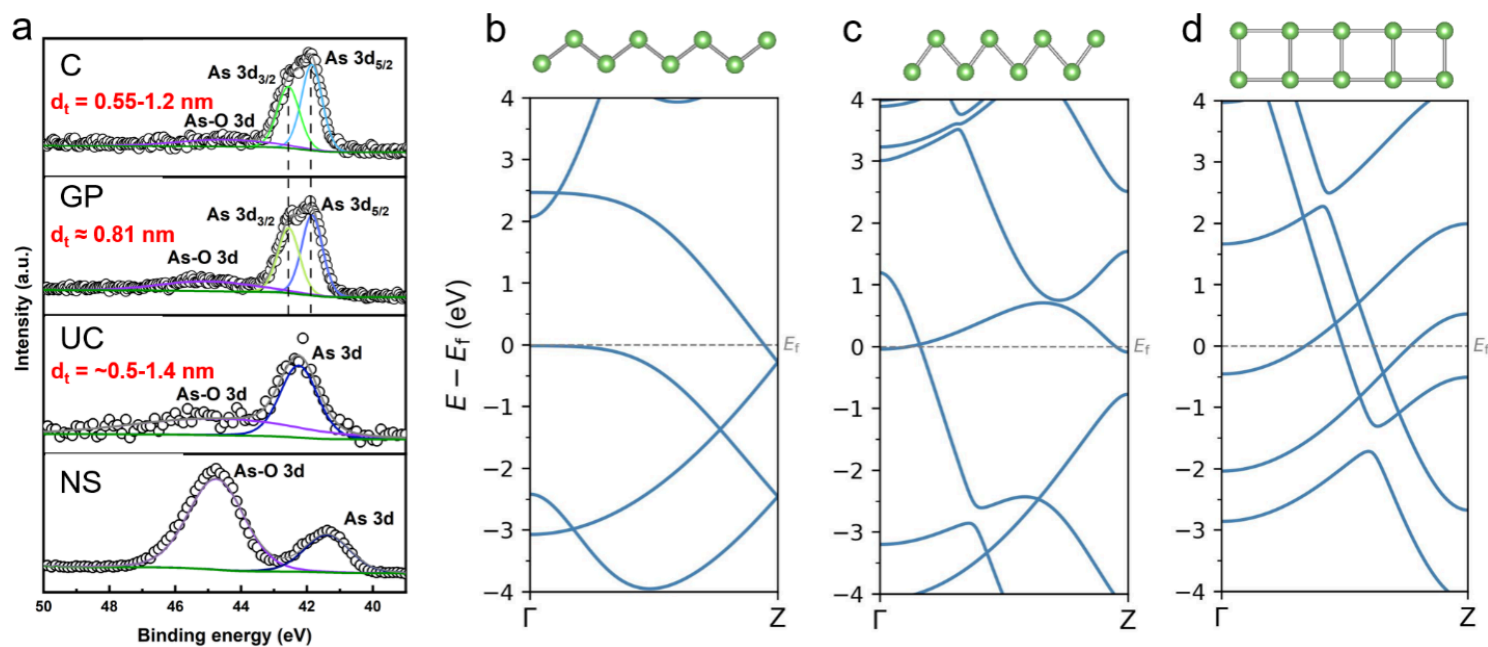


Figure 5

(a) XPS As 3d spectra of As chain-filled mixed-chirality SWCNTs (C, centrifuged but not purified via GPC), As chain-filled (7,5) and (8,4) (GP), as-synthesized As chain-filled SWCNTs that were not pre-purified via centrifugation (UC), and mechanically exfoliated 2D gray As sheets (NS). (b-d) Calculated single-particle picture electronic band structures of a symmetric zigzag As chain, an asymmetric zigzag As chain and a ladder As chain.

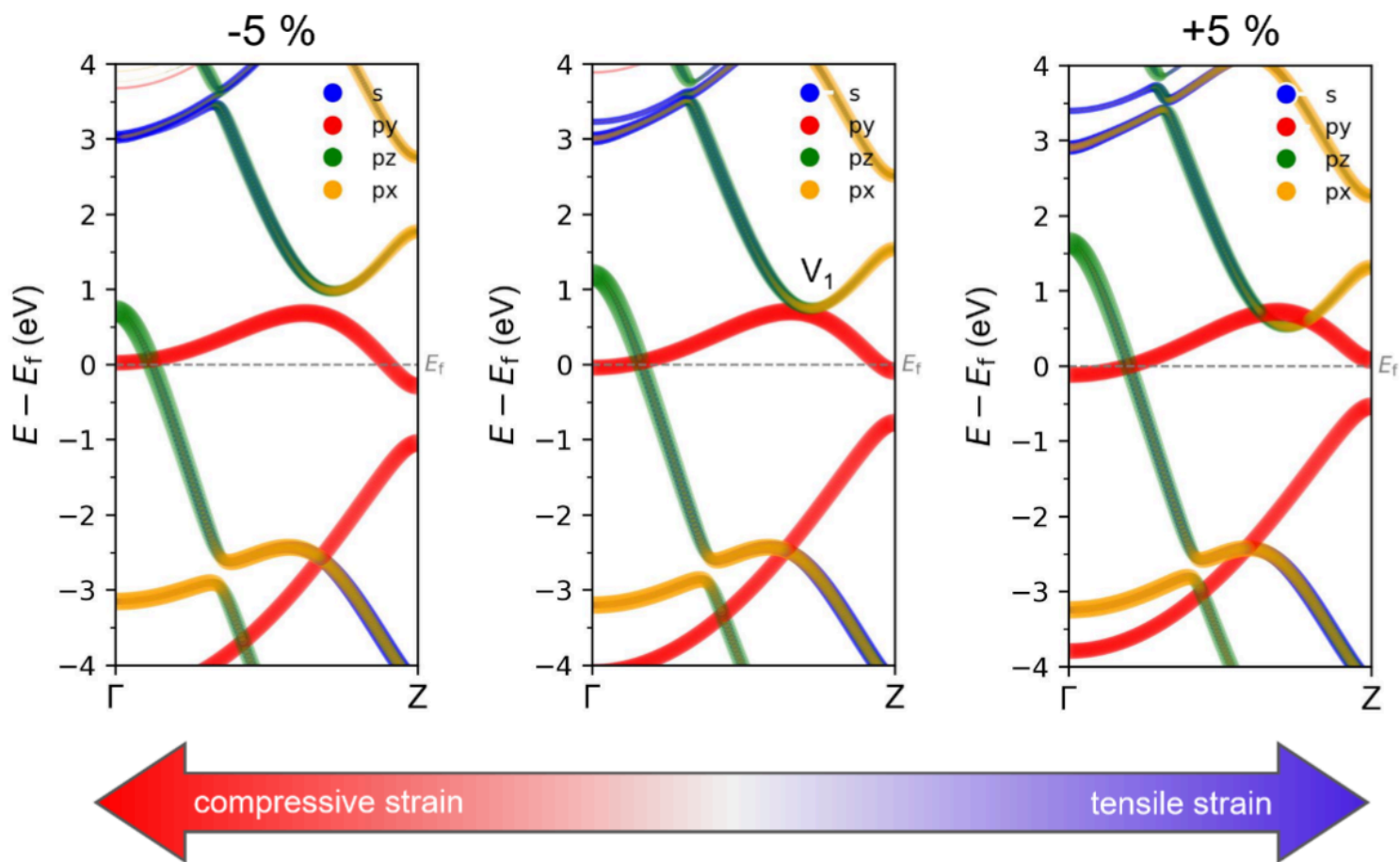


Figure 6

Calculated electronic band structures and the orbital contributions of an asymmetric zigzag As chain under radial compressive or tensile strain.

Supplementary Files

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