Ab initio study on the electromechanical response of Janus transition metal dihalide nanotubes

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Abstract. We study the electronic response of Janus transition metal dihalide (TMH) nanotubes to mechanical deformations using Kohn–Sham density functional theory. Specifically, considering twelve armchair and zigzag Janus TMH nanotubes that are expected to be stable from the phonon analysis of flat monolayer counterparts, we first compute their equilibrium diameters and then determine the variation in bandgap and effective mass of charge carriers with the application of tensile and torsional deformations. We find that the nanotubes undergo a linear and quadratic decrease in bandgap with tensile and shear strain, respectively. In addition, there is a continual increase and decrease in the effective mass of electrons and holes, respectively. We show that for a given strain, the change in bandgap for the armchair nanotubes can be correlated with the transition metal’s in-plane $d$ orbital’s contribution to the projected density of states at the bottom of the conduction band.

1 Introduction

Nanotubes are hollow cylindrical structures whose diameters are the nanometer scale, with lengths that are orders of magnitude larger. These quasi one-dimensional materials, more than thirty of which have been synthesized since the pioneering work for carbon nanotubes [1], are known to display enhanced and exotic mechanical, electronic, optical, and thermal properties/behavior relative to their bulk counterparts [2–4]. Moreover, these properties differ based on the diameter/chirality of the nanotubes [5–10] and can be further controlled/tuned through external stimuli, such as addition of defects [11–13], electric field [14,15], magnetic field [16], temperature [17–19], and mechanical deformations [9,10,20–25], making them particularly suited for technological applications.

Among the nanotubes that have been synthesized, a large fraction are from the transition metal dichalcogenide (TMD) group [2–4], which consists of materials of the form MX$_2$, where M and X denote the transition metal and chalcogen, respectively. Given the large number of transition metal (34 in number) and chalcogen (4 in number) combinations (136 in number) that are possible, it is likely that even more TMD nanotubes will be synthesized in the future. However, such nanotubes are generally multiwalled and have large diameters that are typically in the range of 10–40 nm [2–4], a consequence of the relatively large bending moduli of TMD monolayers [26]. This limits the possibility of fascinating and novel properties that are associated with quantum confinement effects. Also, the large variations in the diameters makes systematic theoretical/computational studies extremely challenging.

The Janus TMD nanotube group [28], which consists of materials of the form MXY, where X and Y are different chalcogens, overcome many of the limitations of the TMD group. In particular, given the asymmetry in the system, single-walled Janus nanotubes become energetically more favorable than their flat counterparts [29,30], which significantly increases the likelihood of them being synthesized. Indeed, the WSSe nanotube has been recently synthesized [31]. Moreover, they have an energy minimizing diameter, typically in the range of 3–16 nm [30], which is much smaller than the corresponding values for TMD nanotubes, significantly increasing the likelihood of novel and exotic properties. In particular, recent work on the electromechanical response of Janus TMD nanotubes has shown that they have potential applications in mechanical sensors and semiconductor switches [32], similar to the case of TMD nanotubes [33]. It is therefore to be expected that at the very least, Janus TMD nanotubes also inherit the other applications of their non-Janus counterparts, including nano-electromechanical (NEMS) devices [34–36], biosensors [37], superconductive materials [18,19], and photodetectors [38–40].

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The Janus transition metal dihalide (TMH) nanotube group [41], which consists of materials of the form MXY, where X and Y are now different halogens, are likely to possess fascinating and exciting properties similar to those displayed in flat TMH monolayers [42,43] and their Janus variants [44,45], e.g., FeCl₂ is piezoelectric ferromagnetic with the Curie temperature around room temperature [42], and FeClBr and FeClF are ferrovalley materials based on their magnetic anisotropy [44,45]. Simultaneously, the nanotubes inherit the aforementioned advantageous features of being a Janus structure. However, the properties and behavior of these nanotubes have not been studied till now, providing the motivation for the current work. In particular, we study the electronic response of Janus TMH nanotubes to mechanical deformations using ab initio Kohn–Sham density functional theory (DFT) calculations. Specifically, considering twelve armchair and zigzag Janus TMH nanotubes that are expected to be stable, we first compute their equilibrium diameters and then determine the variation in bandgap and effective mass of charge carriers with the application of tensile and torsional deformations. Overall, we find that mechanical deformations represent a powerful tool for controlling the electronic properties of Janus TMH nanotubes.

The remainder of this article is organized as follows. In Sect. 2, we list the Janus TMH nanotubes selected and detail the calculation of their electronic response to mechanical deformations. The results so obtained are presented and discussed in Sect. 3. Finally, we provide concluding remarks in Sect. 4.

2 Systems and methods

We consider zigzag and armchair variants of the following Janus TMH nanotubes: (i) M={Ti, Zr, Hf} and X,Y={Cl, Br, I}, with 2H-t symmetry [46,47]; and (ii) M={Fe} and X,Y={Cl, Br, I}, with 1T-o symmetry [46,47], all having the lighter halogen on the inner side. These represent the set of all Janus TMH nanotubes that have been predicted to be thermodynamically stable, i.e., energetically favorable relative to the corresponding TMH monolayers and 3D bulk structures, from first principles investigations [41]. Indeed, we have verified this result while determining the equilibrium diameters for the nanotubes below.

We perform all nanotube simulations using the Cyclix-DFT [48] feature—well tested in various physical applications [26,30,32,33,48–52]—in the state-of-the-art real-space DFT code SPARC [53–55]. In this formalism, as illustrated in Fig. 1, the cyclic and/or helical symmetry of the system is exploited to reduce all computations to a unit cell that contains only a small fraction of the atoms in the traditional periodic unit cell [5,48,56], e.g., the periodic unit cell for a (45,45) HfClBr nanotube with diameter ∼9 nm and an external twist of 6 × 10⁻⁴ rad/Bohr has 169,155 atoms, whereas the cyclic+helical symmetry-adapted unit cell has only 3 atoms (one of each chemical element), a number that remains unchanged by axial and/or torsional deformations. This symmetry-adaption provides tremendous computational savings, given that Kohn–Sham DFT computations scale cubically with system size.

In all simulations, we employ the Perdew–Burke–Ernzerhof (PBE) [57] exchange-correlation functional, and scalar relativistic optimized norm-conserving Vanderbilt (ONCV) [58] pseudopotentials with nonlinear core correction from the SPMS collection [59]. The equilibrium configurations for the flat monolayer counterparts so obtained (Supplementary Material) are in very good agreement with PBE results in literature [60], verifying the accuracy of the chosen pseudopotentials. Though PBE is known to generally underpredict the bandgap [60], it does provide good qualitative trends, making it a common choice for DFT calculations and Janus transition metal nanotubes in particular [61–67], motivating its selection here. Even quantitatively, sophisticated exchange-correlation functionals like hybrid are not necessarily more accurate for Janus...
The uncertainty in values accounts for the energy differences being smaller than the numerical accuracy in the calculations, i.e., $10^{-6}$ Ha/atom.
Fig. 2  a, b Variation of bandgap with axial strains; and c, d variation of bandgap with shear strains for the twelve armchair and zigzag Janus TMH nanotubes. e computed bandgap for the undeformed nanotubes vs. that predicted by the linear regression model. f coefficient of determination of the linear regression ($R^2$) for the linear and quadratic fits of the bandgap vs. axial and shear strains, respectively.

either Hf or Zr, which when subjected to axial strains, undergo an increase in bandgap at small strains, and then a monotonic decrease at larger strains. Similar trends have recently been predicted for the response of transition metal dichalcogenide (TMD) nanotubes [33] and their Janus counterparts [32]. However, the aforementioned exceptions are reversed, i.e., the bandgap of TMD nanotubes with Hf and Zr decreases linearly with axial strain, whereas the corresponding Janus variants demonstrate an increase and then decrease of the bandgap. In the case of TMD nanotubes, the linear decrease of bandgap with axial strains has also been predicted in Refs. [72–75]. The aforedescribed ability to strain engineer the bandgap in Janus TMH nanotubes has potential applications in devices, e.g., mechanical sensors [76–78].

To correlate the bandgap variation with changes in the electronic structure, we compute the atomic orbital projected density of states (PDOS) for the Janus TMH nanotubes at all the configurations studied in this work, i.e., equilibrium and axially/torsionally deformed (Supplementary Material). For armchair nanotubes, we find that the transition metal’s in-plane $d$ orbital, i.e., $d_{yz}$ orbital, is dominant near the edges of the bandgap—exception being when the transition metal is iron, for which the $d_{xz}$ orbital is dominant—making it the focus of study here. In addition, the changes that occur with deformation are more significant at the upper edge of the bandgap, i.e., bottom of the conduction band, therefore the analysis here is restricted to that region. In Fig. 3, for each of the five axial and shear strains considered, we plot the change in bandgap vs. the contribution of the transition metal’s $d_{yz}$ orbital to the PDOS at the bottom of the conduction band. We observe that for a given strain, the change in bandgap is well correlated with the transition metal’s $d_{yz}$’s contribution to the PDOS, with the average coefficient of determination of the linear regression for axial and shear strains being 0.77 and 0.72, respectively. The importance of $d_{yz}$ in determining the response is to be expected, given its in-plane nature, which means that it is the most likely to undergo significant changes for the deformations considered. Note that the total PDOS contribution of all the orbitals at a given angular momentum remains unchanged, from which it can be inferred that
there is no rehybridization of the orbitals upon the application of axial/torsional deformations.

In Fig. 4, we present the variation in the difference between the effective mass of holes and electrons (holes minus electrons) with axial and shear strains for the Janus TMH nanotubes. Based on whether this quantity is positive or negative, the material can be classified as a n-type or p-type semiconductor, respectively. In particular, if the effective mass of electron is greater than that of the hole, then the mobility of electrons is lower, translating to a lower conduction of electrons, making it a p-type semiconductor, and vice versa [79]. We observe from the figure that all the Janus TMH nanotubes are p-type semiconductors in their undeformed state, differing from TMD and Janus TMD nanotubes, which are generally n-type semiconductors [32,33]. On the application of axial and torsional deformations, there is a continuous increase and decrease in the effective mass of electrons and holes, respectively. We have observed similar trends for the TMH nanotubes (Supplementary Material), with the effective mass values for the Janus variants lying in between the parent TMH nanotubes. Exceptions to this are again the TMH nanotubes with Hf and Zr, which when subjected to axial strains, experience first a decrease (increase) and then increase (decrease) in the effective mass of electrons (holes). Similar trends have recently been predicted for TMD [33] and Janus TMD [32] nanotubes. However, as in the case of the bandgap, the aforementioned exceptions are reversed between the TMD nanotubes and their Janus variants. The predicted hole mobility enhancement [80,81] makes the Janus TMH nanotubes more dominant p-type semiconductors, which has applications in devices such as MOSFET transistors [82,83].

Fig. 3 The change in bandgap for the twelve armchair Janus TMH nanotubes vs. the percentage contribution of the transition metal’s $d_{yz}$ orbital to the PDOS at the bottom of the conduction band.

Fig. 4 Variation of the difference in charge carriers’ effective mass (holes minus electrons) with axial and shear strains for the twelve armchair and zigzag Janus TMH nanotubes.
4 Concluding remarks

In this work, we have performed ab initio Kohn–Sham DFT calculations to study the electronic response of Janus TMH nanotubes to mechanical deformations. Specifically, considering twelve armchair and zigzag Janus TMH nanotubes at their equilibrium diameters—predicted to be stable based on the phonon analysis of flat monolayer counterparts—we have determined the variation in bandgap and effective mass of charge carriers with the application of tensile and torsional deformations. We have found that the nanotubes undergo a linear and quadratic decrease in bandgap with tensile and shear strain, respectively. Simultaneously, there is a continual increase and decrease in the effective mass of electrons and holes, respectively. We have found that for a given strain, the change in bandgap for armchair nanotubes can be correlated with the transition metal’s in-plane $d$ orbital’s contribution to the projected density of states at the bottom of the conduction band.

Overall, the current work shows that mechanical deformations represent a powerful tool to control the electronic properties of Janus TMH nanotubes, with applications in devices such as sensors and MOSFET transistors. The study of the optical and thermal deformations presents itself as a worthy subject for further investigation. The extension of such studies to multiwalled nanotubes is also an interesting topic for research that is currently being pursued by the authors.

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Author contributions

All of the authors contributed equally to this work.

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