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# Layer-dependent Schottky contact at TaX<sub>2</sub>–BY (X = S, Se, Te; Y = P, As, Sb) van der Waals interfaces

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The mechanical, thermal and dynamical stabilities, electronic structure, contact type, and height of the barrier at the interface of TaX<sub>2</sub> (X = S, Se, Te) and BY (Y = P, As, Sb) metal–semiconductor (MS) contact are investigated *via* first principles calculations. Binding energies, mechanical properties, phonon spectra and *ab initio* molecular dynamics (AIMD) simulations confirm the stabilities of these systems. TaX<sub>2</sub>–BY (X = S, Se, Te; Y = P, As, Sb) MS van der Waals heterostructures (vdWHs) are found to be metal with a Schottky contact at the interface. Formation of the n-type Schottky contact at the interface of TaX<sub>2</sub>–BY (X = S, Se, Te; Y = P, As, Sb) MS vdWHs favors electron conduction over hole conduction. Small (higher) effective mass (carrier mobility) make TaS<sub>2</sub>–BSb, TaSe<sub>2</sub>–BSb and TaTe<sub>2</sub>–BSb MS vdWHs, potential candidates for high speed nanoelectronic applications. Bader charge analysis shows that at the interface of TaX<sub>2</sub>–BY (X = S, Se, Te; Y = P, As, Sb) MS vdWHs, in TaX<sub>2</sub> (BP, BA) the electrons transfer from the TaX<sub>2</sub> layer to the BP and BA layer, while in TaX<sub>2</sub> (BSb) the electrons transfer from the BSb layer to TaX<sub>2</sub> layer.

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## 1. Introduction

After the successful development of graphene in 2004,<sup>1</sup> researchers isolated and studied more than a dozen 2D materials within less than a decade.<sup>2</sup> Therefore, the family of 2D materials extended from the carbon materials (graphene) to transition metal dichalcogenides (TMDCs),<sup>3</sup> MXene,<sup>4</sup> layered metal oxides<sup>5</sup> and many more<sup>6</sup> with insulating,<sup>7</sup> semiconducting,<sup>8</sup> semimetallic,<sup>9</sup> metallic<sup>10</sup> and superconducting nature.<sup>11</sup> The significant interest in 2D materials is attributed to their special physical characteristics that emerge *via* confinement of the transport of heat and charge to a plane.<sup>12</sup> The unique physical characteristics are expected to make a significant impact across various applications,<sup>13</sup> spanning from high-performance sensors,<sup>14</sup> storage,<sup>15</sup> catalysis,<sup>16</sup> inert coating,<sup>17</sup> electronic,<sup>18</sup> optoelectronic<sup>19</sup> and spintronic<sup>20</sup> devices. In the family of 2D materials, TMDCs with MX<sub>2</sub> (M = transition metal atom, X = chalcogen atom) general formula are of particular importance, where weak van der Waals (vdW) forces hold these layers together, allowing for their easy extraction from the bulk.<sup>21</sup> The simplicity of their preparation and diverse range of

characteristics, make them noteworthy in the realm of 2D materials.<sup>22</sup> Similarly, another class of 2D materials based on group III–V semiconductors has been explored both theoretically<sup>23,24</sup> and experimentally.<sup>25,26</sup> The direct band gap and hexagonal lattice structure, identical to graphene, render these materials promising for the next generation of nano<sup>27</sup> and optoelectronic device<sup>28</sup> applications.

The physical properties of the aforementioned 2D materials come with several key challenges<sup>29</sup> such as scalability, the production of high-quality materials with large surface area, and high cost. Current synthesis methods, like chemical vapor deposition (CVD), can be expensive and complex. Stability and durability of some 2D materials can be chemically reactive or sensitive to environmental factors such as air and moisture, which can degrade their properties over time.<sup>30,31</sup> Therefore, controlling the electronic properties and band gap of 2D materials is crucial, while some 2D materials are natural semiconductors, others, like graphene, require engineering to open a band gap for specific applications. Consequently, researchers have focused on the tuning of these materials *via* several techniques,<sup>32,33</sup> for their useful device applications.<sup>19</sup> In these techniques, stacking of 2D materials in the form of van der Waals heterostructures (vdWHs)<sup>34</sup> provides a flexible platform for exploring novel phenomena in the design of nanoelectronic devices.<sup>35</sup> Numerous vdWHs, particularly those in the form of semiconductor–semiconductor (SS) contact, have been extensively studied both theoretically<sup>36,37</sup> and experimentally<sup>38,39</sup> for their promising and remarkable applications in the field of optoelectronic devices.<sup>40</sup> The Schottky barrier (SB) in the metal

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and semiconductor (MS) vdWHs minimizes resistance at contact, hence tuning (enhancing) the polarity (selectivity) of carriers in the transistor channel (photovoltaic cells), therefore, playing a crucial role in devices.<sup>41,42</sup> These contacts (SS and MS) are fabricated *via* ultra-thin and flat surfaces without defects and with outstanding chemical (mechanical) stability (flexibility).<sup>43</sup>

Although, TMDCs have already been used in almost every MS contact,<sup>44–50</sup> a significant gap exists regarding the exploration of 2D TaX<sub>2</sub> (X = S, Se, Te) and BY (Y = P, As, Sb) MS contact. Therefore, in the present work, we have focused on the modelling of TaX<sub>2</sub>–BY MS vdWHs. Structural stability, electronic structure, contact type and height of the barrier of the modelled heterostructures are investigated, with the goal of exploring the potential applications of these materials in device fabrications.

## 2. Computational details

We used density functional theory (DFT) with the PWSCF code<sup>51</sup> with generalized gradient approximation (GGA) in the Perdew–Burke–Ernzerhof (PBE) style.<sup>52</sup> We fixed the convergence criteria for force to 10<sup>−3</sup> Å<sup>−1</sup> and energy to 10<sup>−5</sup> eV for the optimization/relaxation of the lattice constant/atomic positions. We also fixed the cut-off energy to 800 eV and used a 16 × 16 × 1 *k*-grid for the Brillouin zone integration. To mitigate interactions between neighbouring layers of atoms, we set a vacuum layer with a thickness of 25 Å.

Mechanical stability of these systems are examined using the energy-strain method in the VASPKIT code<sup>53</sup> and visualized with the ELATE software.<sup>54</sup> Thermal (dynamical) stabilities were investigated *via* AIMD (phonon) simulation (calculations).<sup>55,56</sup> In the case of thermal stability, *ab initio* molecular dynamics (AIMD) simulations,<sup>55</sup> through the Nose thermostat algorithm at a temperature of 300 K for a total of 6 ps with a time interval

of 1 fs are performed. For dynamical stability, we used a 3 × 3 × 1 supercell consisting of 45 atoms. We have also used density functional perturbation theory (DFPT) with the VASP code<sup>57</sup> to determine the harmonic second-order interatomic force constants (IFCs). In addition, we employed the PHONOPY code<sup>58</sup> to calculate the phonon dispersion using the frozen phonon approximation.

Type (height) of the Schottky contact (barrier) is obtained using first principles calculations<sup>59</sup> using  $\Phi_{\text{Bn}} = E_{\text{CBM}} - E_{\text{F}}$  and  $\Phi_{\text{Bp}} = E_{\text{F}} - E_{\text{VBM}}$ , where  $E_{\text{CBM}}$  and  $E_{\text{VBM}}$  are the energies of the band edges of the semiconducting material and  $E_{\text{F}}$  is the Fermi level of the metallic material. Type (n and p) of the Schottky barrier without  $\Delta V$  were also calculated<sup>60</sup> using the Schottky–Mott rule;  $\phi_{\text{Bn}} = \phi_{(\text{metallic-monolayer})} - \chi_{(\text{MS-vdWH})}$  and  $\phi_{\text{Bp}} = I_{(\text{MS-vdWH})} - \phi_{(\text{metallic-monolayer})}$ , here  $\phi$ ,  $\chi$ , and  $I$  are the work function, electron affinity, and ionization energy, respectively, of the MS vdWHs and corresponding monolayers. Band bending was calculated<sup>61</sup> using  $\Delta\phi = \phi_{(\text{metallic-monolayer})} - \phi_{(\text{semiconducting-monolayer})}$ , where  $\phi_{(\text{metallic-monolayer})}$  and  $\phi_{(\text{semiconducting-monolayer})}$  denote the work function of the corresponding metallic and semiconducting monolayers, respectively, in the MS vdWHs.

## 3. Results and discussion

Although, monolayers of TaX<sub>2</sub> (X = S, Se, Te) and BY (Y = P, As, Sb) have already been investigated in detail in ref. 62 and 63. To verify our present approach, we have further calculated the electronic band structure of TaX<sub>2</sub> (X = S, Se, Te) and BY (Y = P, As, Sb). In agreement with ref. 62 and 63, TaX<sub>2</sub>(BY) monolayers exhibit a metallic (direct bandgap semiconducting) nature (see Fig. 1).

Therefore, using the optimized lattice constant of TaX<sub>2</sub> (X = S, Se, Te)<sup>64,65</sup> and BY (Y = P, As, Sb),<sup>66,67</sup> TaX<sub>2</sub>–BY MS contact in six different vdWH stacking configuration patterns are

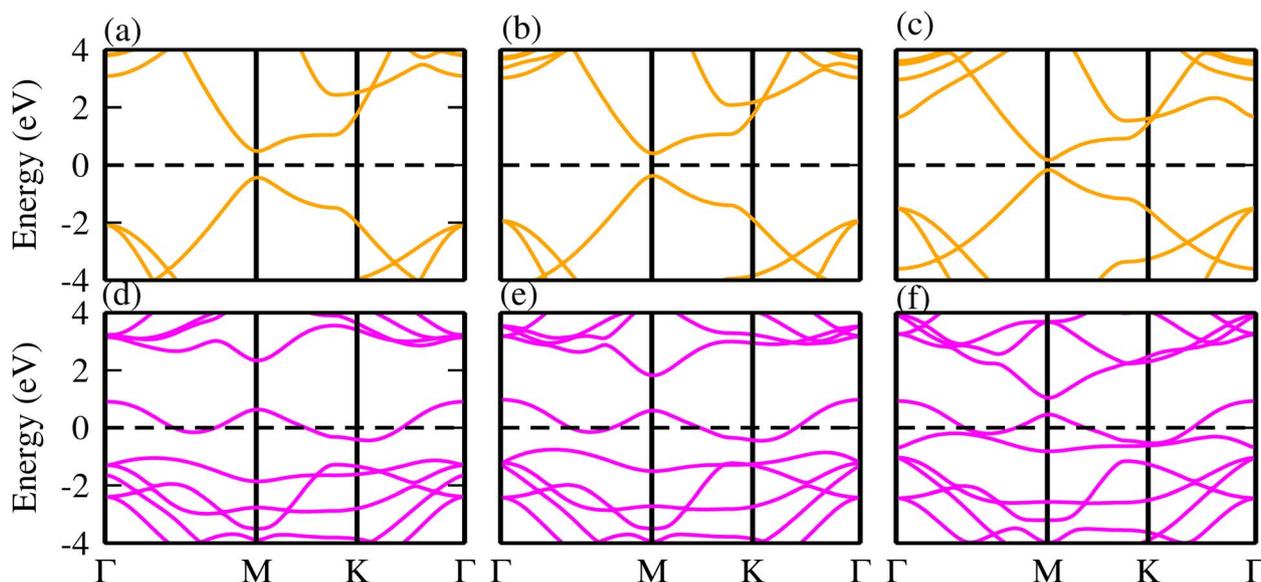


Fig. 1 Electronic band structures of (a) BP, (b) BAs, (c) BSb, (d) TaS<sub>2</sub>, (e) TaSe<sub>2</sub> and (f) TaTe<sub>2</sub> monolayers.



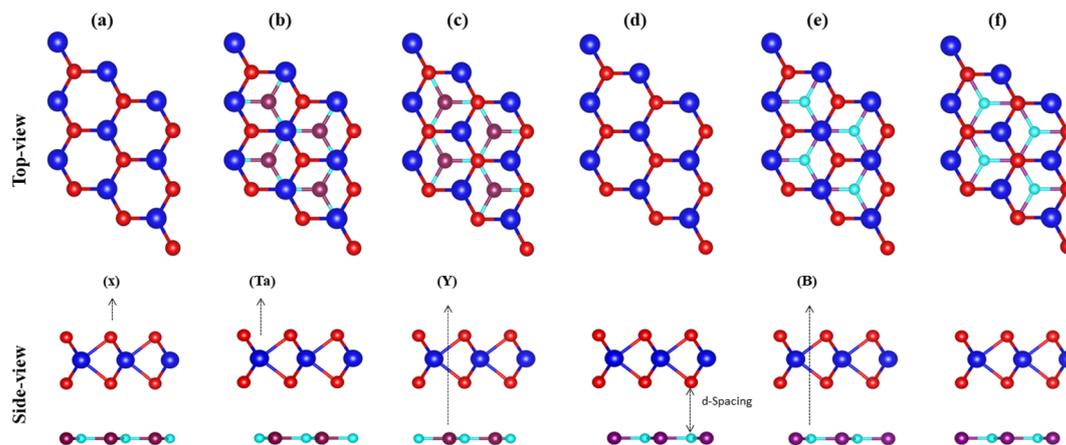


Fig. 2 Possible stacking configurations of  $\text{TaX}_2\text{-BY}$  ( $X = \text{S, Se, Te}$ ;  $Y = \text{P, As, Sb}$ ) MS vdWHs.

fabricated, see Fig. 2. In (a), the Ta(X) atom of the  $\text{TaX}_2$  layer is placed on top of the B(Y) atom of the BY layer. In (b), the Ta atom of the  $\text{TaX}_2$  layer is placed on top of the B atom of the BY layer, while the X(Y) atom of the  $\text{TaX}_2(\text{BN})$  layer is placed on the hexagonal centre. In (c), the X atom of the  $\text{TaX}_2$  layer is placed on top of the B atom of the BY layer, while the Ta(Y) atoms of  $\text{TaX}_2(\text{BY})$  are placed on the hexagonal centre. In (d), the Ta atom of the  $\text{TaX}_2$  layer is settled on top of the Y atom of the BY layer. In (e), the Ta atom of the  $\text{TaX}_2$  layer is stacked on top of the Y atom of the BY layer, while the X(B) atom of  $\text{TaX}_2(\text{BY})$  is placed on the hexagonal centre. In (f), the X atom of the  $\text{TaX}_2$  is settled on top of the Y atom of BY, while Ta(B) atoms are placed on the hexagonal centre.

Binding energy<sup>68</sup> and the interlayer distance<sup>68</sup> (d) of all six patterns of  $\text{TaX}_2\text{-BY}$  MS vdWHs are calculated and presented in Table 1. Stacking (b) of  $\text{TaS}_2\text{-BP}$ , (b) of  $\text{TaS}_2\text{-BAS}$ , (b) of  $\text{TaS}_2\text{-BSb}$ , (e) of  $\text{TaSe}_2\text{-BP}$ , (b) of  $\text{TaSe}_2\text{-BAS}$ , (b) of  $\text{TaSe}_2\text{-BSb}$ , (e) of  $\text{TaTe}_2\text{-BP}$ , (e) of  $\text{TaTe}_2\text{-BAS}$  and (d) of  $\text{TaTe}_2\text{-BSb}$ , are found to be the most stable stacking configurations, based on the most smaller (higher) interlayer distance (binding energies),<sup>68</sup> see Table 1. The variation in stable stacking is due to the induced strain from the distinct chalcogen atoms and the dissimilar interface atoms. The optimized lattice constant and bond

length of the most stable stacking configurations are presented in Table 2. Before considering the stable stacking configurations for further investigation, we further confirmed the stability *via* calculating the mechanical properties of these systems.

Mechanical stability of the most stable stacking configurations of  $\text{TaX}_2\text{-BY}$  ( $X = \text{S, Se, Te}$ ;  $Y = \text{P, As, Sb}$ ) MS vdWH are assisted *via* the energy-strain method.<sup>69-71</sup> Using the hexagonal symmetry of  $\text{TaX}_2\text{-BY}$  MS vdWH, two independent elastic constants ( $C_{11}$  and  $C_{12}$ ), Young's modulus, shear modulus, and Poisson's ratios are calculated and presented in Table 2, that meet the Born criteria:  $C_{11} > 0$ ,  $C_{12} > 0$ , and  $C_{11} > |C_{12}|$ .<sup>69-71</sup> Therefore, these findings indicate the high mechanical stability of  $\text{TaX}_2\text{-BY}$  ( $X = \text{S, Se, Te}$ ;  $Y = \text{P, As, Sb}$ ) MS vdWH, in agreement with previous reports.<sup>69-71</sup>

Thermal stability in terms of the fluctuation energy as a function of time, of the energetically most favorable stacking configurations in  $\text{TaX}_2\text{-BY}$  ( $\text{TaS}_2\text{-BP}$ ,  $\text{TaS}_2\text{-BAS}$  and  $\text{TaS}_2\text{-BSb}$ ), are given in Fig. 3. One can observe that in the case of  $\text{TaS}_2\text{-BP}$ ,  $\text{TaS}_2\text{-BAS}$  and  $\text{TaS}_2\text{-BSb}$ , heterostructures after 4 ps, there is no structure distortion. Moreover, through the AIMD simulation, our results demonstrate that the geometrical structure of  $\text{TaS}_2\text{-BP}$ ,  $\text{TaS}_2\text{-BAS}$  and  $\text{TaS}_2\text{-BSb}$  is retained after 4000 step

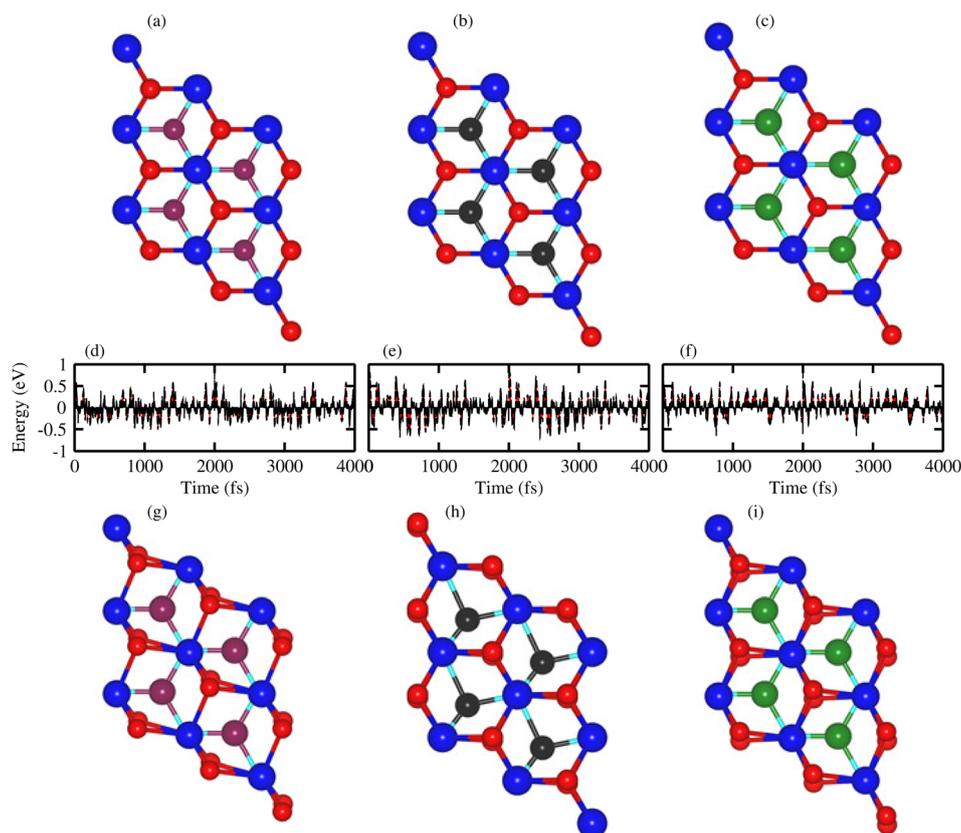
Table 1 Binding energy ( $E_b$  in eV) and interlayer distance ( $d$  in Å) of  $\text{TaX}_2\text{-BY}$  ( $X = \text{S, Se, Te}$ ;  $Y = \text{P, As, Sb}$ ) MS vdWHs in (a-f) stacking configurations

$\text{TaX}_2\text{-BY}$	$\text{TaS}_2\text{-BP}$	$\text{TaS}_2\text{-BAS}$	$\text{TaS}_2\text{-BSb}$	$\text{TaSe}_2\text{-BP}$	$\text{TaSe}_2\text{-BAS}$	$\text{TaSe}_2\text{-BSb}$	$\text{TaTe}_2\text{-BP}$	$\text{TaTe}_2\text{-BAS}$	$\text{TaTe}_2\text{-BSb}$
(a)	$E_b$	-0.010	-0.013	-0.025	-0.011	-0.013	-0.019	-0.011	-0.014
	$d$	3.549	3.542	3.062	3.620	3.638	3.574	3.889	3.834
(b)	$E_b$	-0.016	-0.019	-0.031	-0.017	-0.021	-0.028	-0.018	-0.023
	$d$	3.329	3.327	3.084	3.711	3.406	3.558	3.874	3.880
(c)	$E_b$	-0.011	-0.014	-0.024	-0.012	-0.015	-0.020	-0.012	-0.015
	$d$	3.378	3.385	3.657	3.444	3.454	3.642	3.626	3.601
(d)	$E_b$	-0.012	-0.016	-0.025	-0.014	-0.016	-0.021	-0.015	-0.018
	$d$	3.339	3.650	3.639	3.392	3.740	3.606	3.536	3.493
(e)	$E_b$	-0.015	-0.019	-0.030	-0.018	-0.021	-0.027	-0.019	-0.023
	$d$	3.638	3.661	3.628	3.317	3.765	3.781	3.476	3.486
(f)	$E_b$	-0.010	-0.013	-0.024	-0.010	-0.013	-0.018	-0.010	-0.012
	$d$	3.576	3.585	3.612	3.738	3.694	3.599	3.934	3.938



**Table 2** Lattice constant ( $a$  in Å), bond length (in Å), interlayer distance ( $d$  in Å), elastic constants ( $C_{11}$  and  $C_{12}$  in  $\text{N m}^{-1}$ ), Young's modulus ( $E$  in  $\text{N m}^{-1}$ ), shear modulus ( $G$  in  $\text{N m}^{-1}$ ), Poisson's ratio ( $\nu$ ), work function ( $\phi$  in eV), potential ( $\Delta V$  in eV), effective mass of the carriers ( $m_e^*$ ,  $m_h^*$ ), ionization energy ( $I$  in eV), electron affinity ( $\chi$  in eV), and band bending ( $\Delta W$  in eV) of  $\text{TaX}_2\text{-BY}$  ( $X = \text{S, Se, Te}$ ;  $Y = \text{P, As, Sb}$ ) MS vdWHs

$\text{TaX}_2\text{-BY}$	$\text{TaS}_2\text{-BP}$	$\text{TaS}_2\text{-BAs}$	$\text{TaS}_2\text{-BSb}$	$\text{TaSe}_2\text{-BP}$	$\text{TaSe}_2\text{-BAs}$	$\text{TaSe}_2\text{-BSb}$	$\text{TaTe}_2\text{-BP}$	$\text{TaTe}_2\text{-BAs}$	$\text{TaTe}_2\text{-BSb}$
$a$	3.26	3.35	3.51	3.34	3.43	3.61	3.46	3.54	3.72
M-X	2.46	2.48	2.52	2.58	2.60	2.64	2.79	2.79	2.78
B-N	1.88	1.94	2.08	1.93	1.98	2.10	1.99	2.05	2.32
$d$	3.33	3.33	3.08	3.32	3.41	3.56	3.48	3.49	2.29
$C_{11}$	299.38	282.34	252.80	254.77	252.49	226.39	142.89	156.02	159.40
$C_{12}$	84.46	82.65	73.65	79.53	69.60	64.49	62.46	72.88	42.81
$E$	275.55	258.15	231.34	299.95	233.31	208.02	115.58	121.98	147.90
$G$	107.46	99.85	89.57	87.62	91.45	80.95	40.21	41.57	58.29
$\nu$	0.282	0.239	0.291	0.312	0.276	0.285	0.437	0.467	0.269
$\Delta V$	4.93	2.22	4.88	7.23	4.41	2.67	4.74	1.64	2.53
$\phi$	4.01	3.92	3.65	3.81	3.82	3.63	3.28	3.58	4.01
$m_e^*$	0.71	0.61	0.43	0.79	0.68	0.48	0.94	0.79	0.57
$m_h^*$	0.66	0.57	0.41	0.75	0.65	0.47	0.91	0.77	0.55
$I$	4.65	4.59	4.58	4.82	4.79	4.73	5.11	5.05	5.38
$\chi$	4.65	4.58	4.57	4.81	4.79	4.70	5.10	5.04	5.36
$\Delta W$	0.23	0.23	0.23	0.24	0.24	0.24	0.32	0.29	0.24



**Fig. 3** *Ab initio* molecular dynamics simulation of (a, d, and g)  $\text{TaS}_2\text{-BP}$ , (b, e, and h)  $\text{TaS}_2\text{-BAs}$  and (c, f, and i)  $\text{TaS}_2\text{-BSb}$ , van der Waals heterostructures. Geometrical structure (a–c) before heating; (g–i) after heating with (d–f) fluctuating energy.

simulations and the average value of the total energy remains nearly constant. All these findings demonstrate that  $\text{TaS}_2\text{-BP}$ ,  $\text{TaS}_2\text{-BAs}$  and  $\text{TaS}_2\text{-BSb}$  are thermally stable at room temperature.

The phonon dispersion curves in Fig. 4 for the  $\text{TaS}_2\text{-BP}$ ,  $\text{TaS}_2\text{-BAs}$ , and  $\text{TaS}_2\text{-BSb}$  MS vdWHs show no imaginary frequencies throughout the Brillouin zone, confirming their dynamic stability. The lack of imaginary modes indicates that the atomic arrangements reside at a local minimum on the



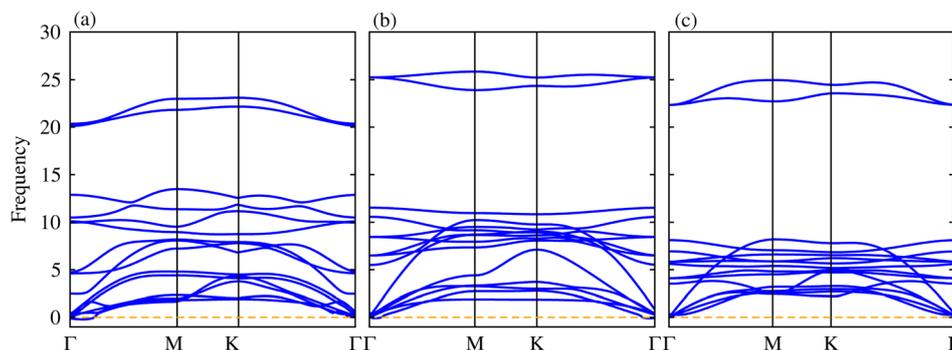


Fig. 4 Phonon dispersion curves of (a) TaS<sub>2</sub>-BP, (b) TaS<sub>2</sub>-BAs and (c) TaS<sub>2</sub>-BSb MS vdWHs.

potential energy surface, which is a key indicator of structural stability. Using the PBE functional, the electronic band structures are displayed in Fig. 5, where green (red) lines are attributed to the TaX<sub>2</sub>(BY) layers in TaX<sub>2</sub>-BY (X = S, Se, Te; Y = P, As, Sb) MS vdWHs. The electronic band structures in Fig. 5, show that all TaX<sub>2</sub>-BY (X = S, Se, Te; Y = P, As, Sb) MS vdWHs are metals with type-III band alignment<sup>72</sup> and look like the sum of band structure of TaX<sub>2</sub> and BY (Y = P, As, Sb) monolayers. The transition of BY (Y = P, As, Sb) to a metal is ascribed to the contribution of metallic states from TaX<sub>2</sub> (X = S, Se, Te) monolayer, enhancing its conductivity and making it suitable for various electronic applications involving Schottky contacts.

PDOS of the TaX<sub>2</sub>-BY MS vdWHs are presented in Fig. 6, and show that the main contributions at the Fermi level are due to

the Ta-d ( $d_{3z^2-r^2}$ ,  $d_{xy}$ ) and (S, Se, Te)-p orbital of the TaX<sub>2</sub> monolayers (crossing the Fermi level); while both the valence and conduction band without crossing the Fermi level, are due to the B- $p_x$  and (Y = P, As, Sb)- $p_z$  orbitals of the BY monolayer. After stacking, the TaX<sub>2</sub> monolayer shifts the conduction band minimum (CBM) of the BY layer toward the Fermi level due to the difference in electronegativity. The position of these orbitals near to the Fermi level in the valence and conduction bands show that the band structure of BY and TaX<sub>2</sub> monolayers are well preserved in the TaX<sub>2</sub>-BY MS vdWHs. The minimum (maximum) of the conduction (valence) band is due to the Ta- $d_{3z^2-r^2}$  (Ta- $d_{x^2-y^2}$ ,  $d_{xy}$ ) orbital with a very small contribution from the Ta- $d_{x^2-y^2}$  and  $d_{xy}$  orbitals, see Fig. 6. The B- $p_x$  and  $p_y$  orbital dominate the valence band minimum (VBM), with a small

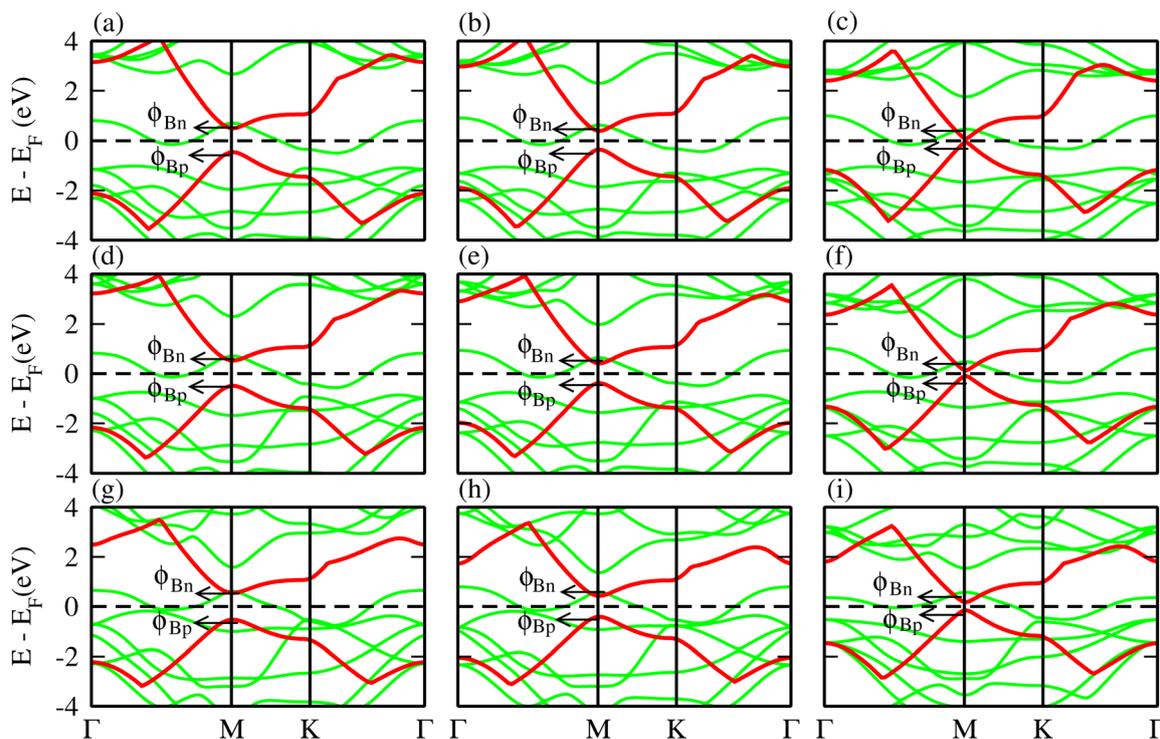


Fig. 5 Electronic band structure of (a) TaS<sub>2</sub>-BP, (b) TaS<sub>2</sub>-BAs, (c) TaS<sub>2</sub>-BSb, (d) TaSe<sub>2</sub>-BP, (e) TaSe<sub>2</sub>-BAs, (f) TaSe<sub>2</sub>-BSb, (g) TaTe<sub>2</sub>-BP, (h) TaTe<sub>2</sub>-BAs and (i) TaTe<sub>2</sub>-BSb MS vdWHs.



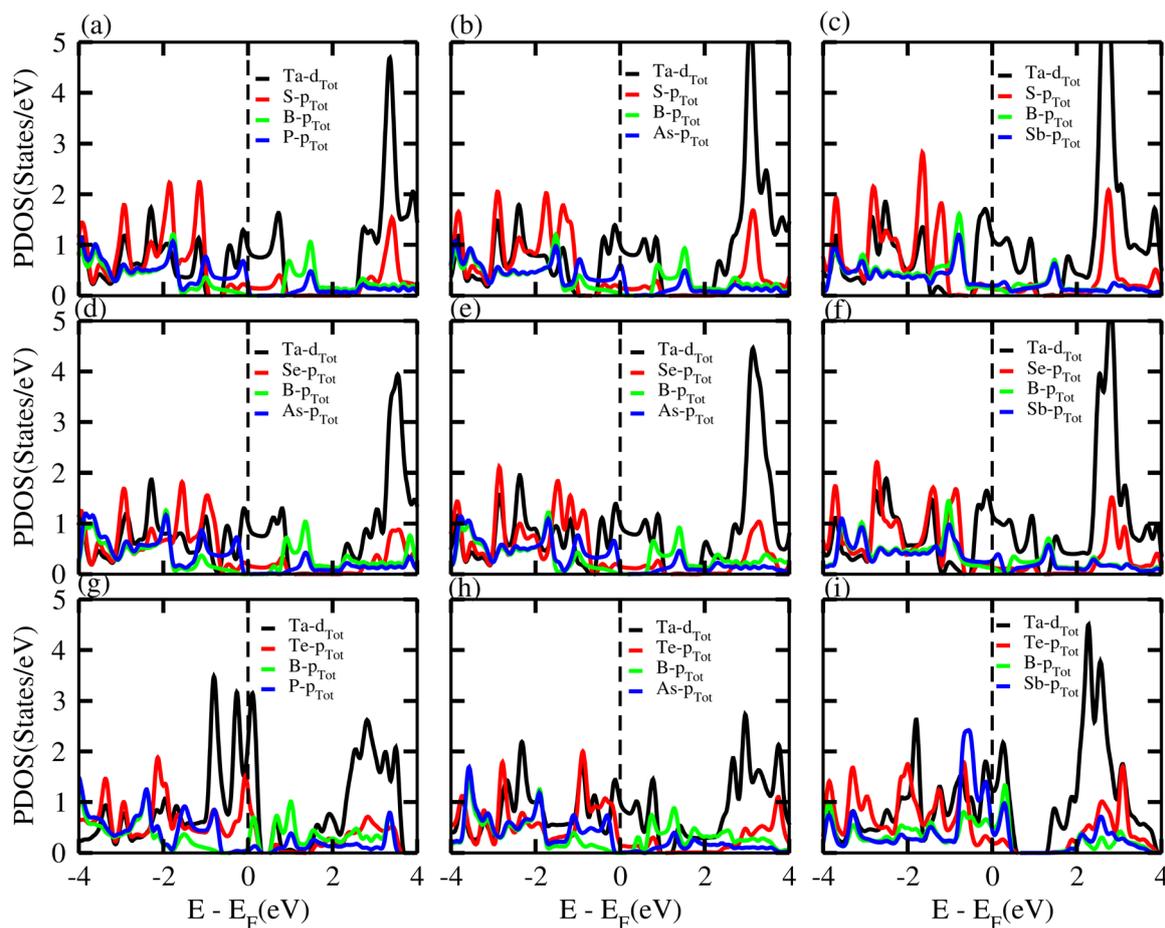


Fig. 6 PDOS of (a)  $\text{TaS}_2$ -BP, (b)  $\text{TaS}_2$ -BAs, (c)  $\text{TaS}_2$ -BSb, (d)  $\text{TaSe}_2$ -BP, (e)  $\text{TaSe}_2$ -BAs, (f)  $\text{TaSe}_2$ -BSb, (g)  $\text{TaTe}_2$ -BP, (h)  $\text{TaTe}_2$ -BAs and (i)  $\text{TaTe}_2$ -BSb, vdWHs.

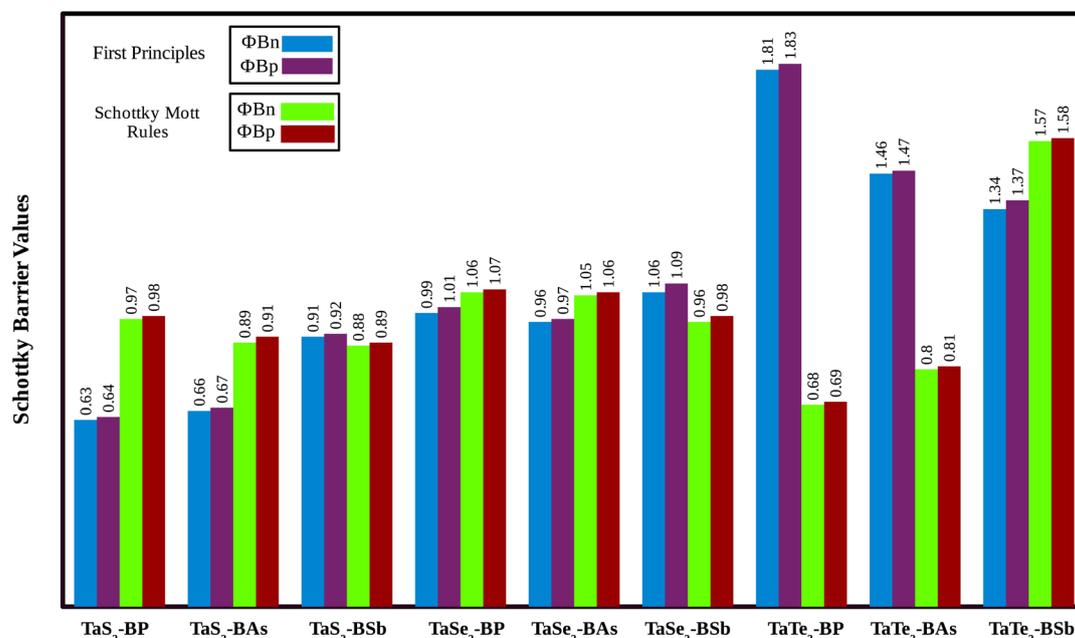


Fig. 7 Schottky barrier height calculated using the Schottky–Mott rule and first principles calculation of  $\text{TaX}_2$  ( $X = \text{S}, \text{Se}, \text{Te}$ )– $\text{BY}$  ( $Y = \text{P}, \text{As}, \text{Sb}$ ) MS vdWHs.



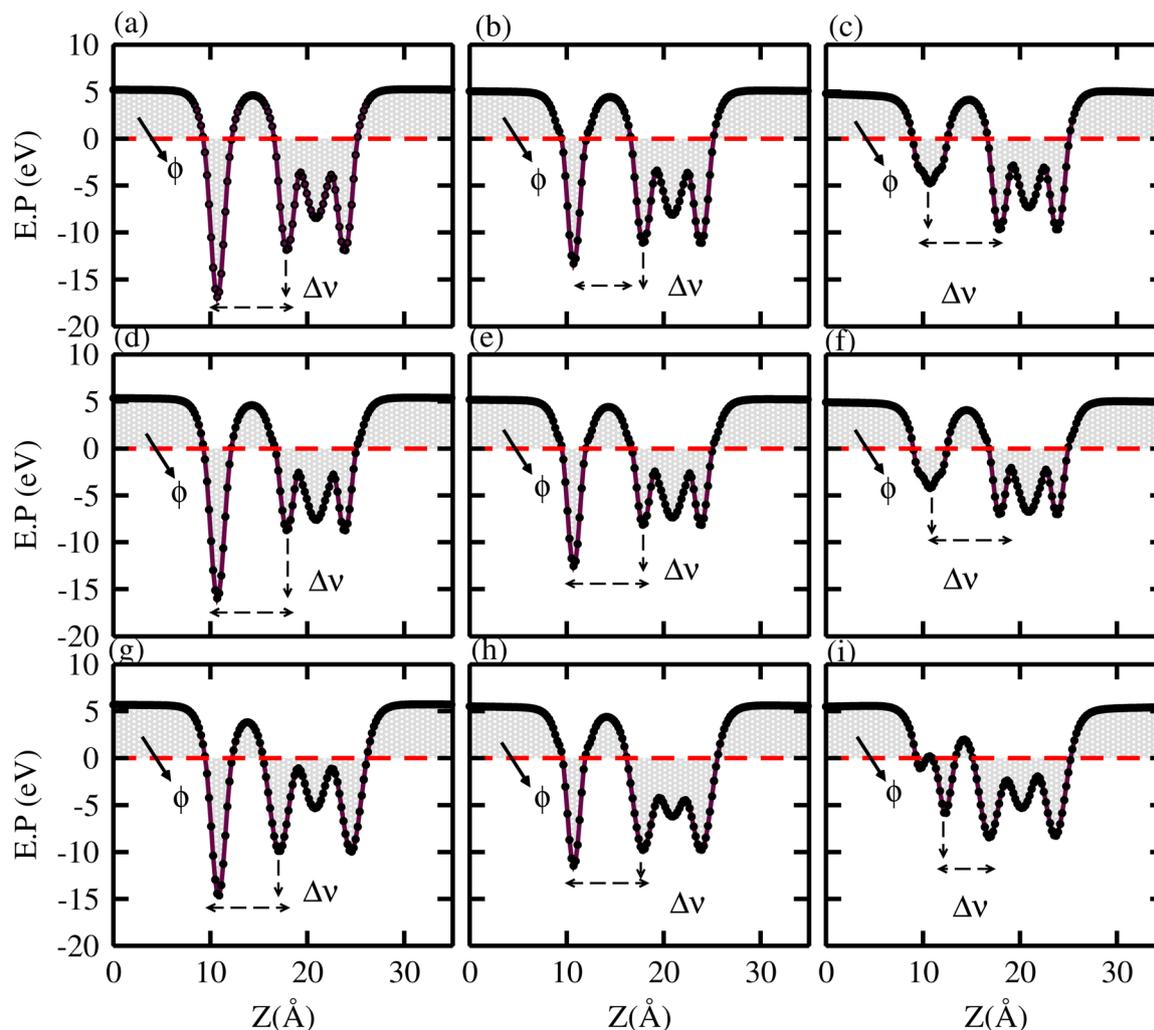


Fig. 8 Average electrostatic potential of (a) TaS<sub>2</sub>-BP, (b) TaS<sub>2</sub>-BAS, (c) TaS<sub>2</sub>-BSb, (d) TaSe<sub>2</sub>-BP, (e) TaSe<sub>2</sub>-BAS, (f) TaSe<sub>2</sub>-BSb, (g) TaTe<sub>2</sub>-BP, (h) TaTe<sub>2</sub>-BAS, and (i) TaTe<sub>2</sub>-BSb, MS vdWHs.

contribution from the B-p<sub>z</sub> orbitals. Through modelling TaX<sub>2</sub>-BY MS vdWHs, we found that strain is induced in the corresponding monolayers due to the lattice mismatch, tuning the coupling between the orbitals of the TMDCs (Ta-d) and chalcogen atoms ((S, Se, Te)-p). Therefore, splitting in the bonding and antibonding states of BY monolayers in TaX<sub>2</sub>-BY MS vdWHs fluctuates, and hence the position of the contributing orbital at the Fermi level varies.

Furthermore, for the use of TaX<sub>2</sub>-BY (X = S, Se, Te; Y = P, As, Sb) MS vdWHs in device applications, effective mass and carrier mobility are investigated and related by  $\mu = e\tau/m^*$ .<sup>73</sup> Thus, to evaluate the carrier mobility of TaX<sub>2</sub>-BY MS vdWHs, effective mass is calculated using<sup>74</sup>  $\frac{1}{m^*} = \frac{1}{\hbar} \frac{\partial^2 E(K)}{\partial K^2}$  where,  $\hbar$  is Planck's constant and  $K$  is the wave vector. Based on the above equation, using the parabolic fitting of the CB and VB of TaX<sub>2</sub>-BY MS vdWHs, the calculated effective mass for electrons (holes) are given in Table 2. Quite a small effective mass in the case of TaS<sub>2</sub>-BSb, TaSe<sub>2</sub>-BSb and TaTe<sub>2</sub>-BSb MS vdWHs, exhibit high

carrier mobility, and hence show potential for efficient nano-electronic devices.

Relative locations of the metal (TaX<sub>2</sub>) with semiconductor (BY) band edges in TaX<sub>2</sub>-BY (X = S, Se, Te; Y = P, As, Sb) MS vdWHs establish the Schottky or ohmic junctions across the interface. Tuning the Schottky barrier (SBH) can change the current flow across the interface of the TaX<sub>2</sub>-BY (X = S, Se, Te; Y = P, As, Sb) MS vdWHs, hence boosting the device performance.<sup>75,76</sup> The band structures in Fig. 5 indicate that the Fermi level of TaX<sub>2</sub> (metal layer) sits in the band edges of BY (semiconductor layer), and hence establish Schottky contacts<sup>77</sup> at the interface of TaX<sub>2</sub>-BY MS vdWHs. The type of Schottky contact (n-type or p-type) is obtained using the Schottky-Mott rule,<sup>78</sup> see computational details. The calculated values of the Schottky barrier  $\phi_{\text{Bn}}$  and  $\phi_{\text{Bp}}$  using first principles calculations and the Schottky-Mott rule, are given in Fig. 7, which shows that  $\phi_{\text{Bn}}$  of all stacking configurations is smaller than  $\phi_{\text{Bp}}$ , suggesting that they form an n-type Schottky contact. Therefore, the MS vdWHs under consideration favor electron conduction over hole



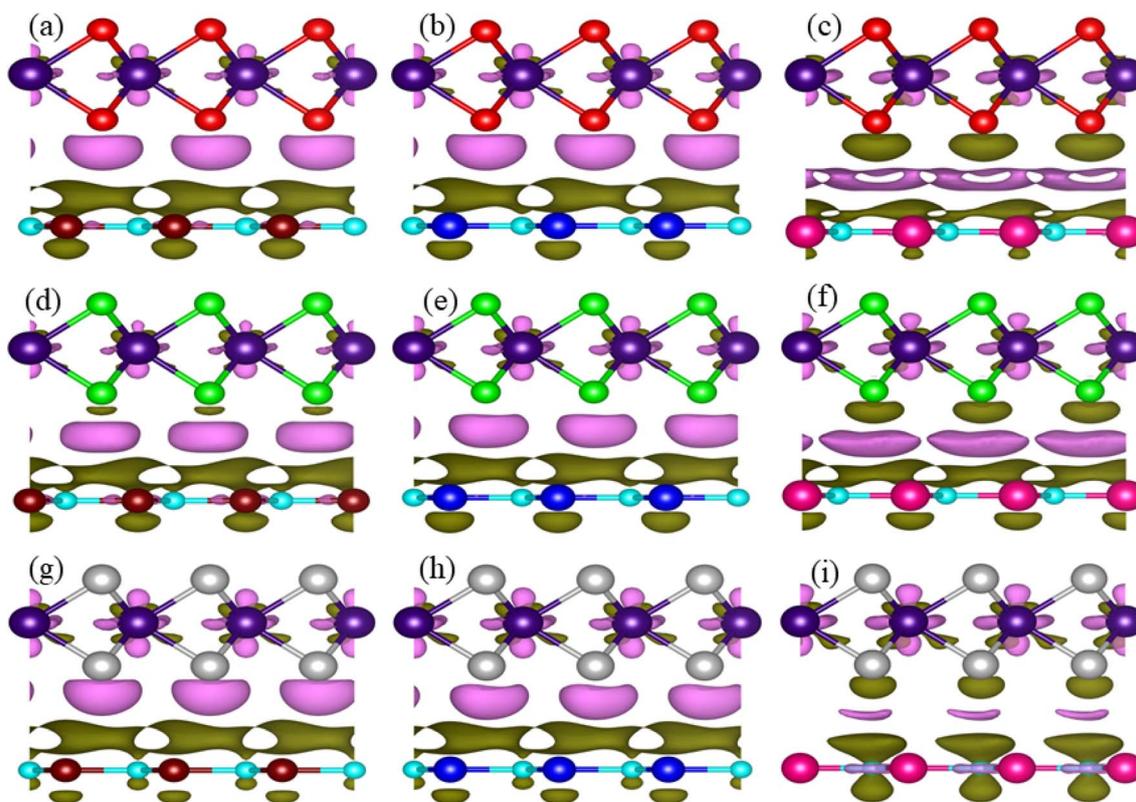


Fig. 9 Charge density difference of (a) TaS<sub>2</sub>-BP, (b) TaS<sub>2</sub>-BAS, (c) TaS<sub>2</sub>-BSb, (d) TaSe<sub>2</sub>-BP, (e) TaSe<sub>2</sub>-BAS, (f) TaSe<sub>2</sub>-BSb, (g) TaTe<sub>2</sub>-BP, (h) TaTe<sub>2</sub>-BAS, and (i) TaTe<sub>2</sub>-BSb, MS vdWHs.

conduction, and hence have significant implications in transistors, sensors, photodetectors, and other electronic components.<sup>79</sup> It is clearly observed that the SBH increases (decreases) from P to As to Sb in TaS<sub>2</sub>-BY (TaTe<sub>2</sub>-BY) MS vdWHs. Moreover, the metallic nature of these heterostructures suppress the metal induced gap states (MIGS) in BY (Y = P, As, Sb) monolayers, hence, leading to weak Fermi Level Pinning (FLP). Weak vdW interactions redistribute the charge density at the interface, see Fig. 9 (discussed later on), and hence establish interface dipoles (ID). Therefore, neglecting the metal semiconductor interaction (without considering  $\Delta V$ ) should ideally follow the predictions of the Schottky-Mott rule. Therefore, type (n and p) of the Schottky barrier without  $\Delta V$  were also calculated<sup>60</sup> using  $\phi_{\text{Bn}} = \phi_{\text{(metallic-monolayers)}} - \chi_{\text{(vdWH)}}$  and  $\phi_{\text{Bp}} = \chi_{\text{(vdWH)}} - \phi_{\text{(metallic-monolayers)}}$ . These IDs may lead to deviation from the Schottky-Mott limit, due to shifting of the electronic levels and FLP effect at the interface from their original positions.<sup>80</sup> The band bending of the TaX<sub>2</sub>-BY systems reveals the presence of both p-type and n-type Schottky barrier even without the transfer of charge between the corresponding monolayers. When  $\Delta\phi$  is greater than 0 or  $\Delta\phi$  is less than 0, it signifies the formation of n-type and p-type Schottky contacts.<sup>50</sup> In the TaX<sub>2</sub>-BY vdWHs under study,  $\Delta\phi$  is greater than 0, see Table 2. This observation suggests that charge will preferentially flow from metal to semiconductor, indicating n-type contact due to the high values of  $\Delta\phi$  (greater than 0), which demonstrate that holes will flow from TaX<sub>2</sub> to the BY layer. The controllable electronic properties

and formation of the Schottky contact in TaX<sub>2</sub>-BY MS vdWHs makes it a potential candidate for Schottky nanodevices.<sup>50</sup>

In the case of TaX<sub>2</sub>-BY MS vdWHs, the TaX<sub>2</sub> (BP, BAS) layer exhibits shallower (deeper) potential confirming charge transfer from TaX<sub>2</sub> to the BP and BAS layer. On the contrary, in the case of TaX<sub>2</sub> (X = S, Se, Te)-BSb, the TaX<sub>2</sub> (BSb) layer is deeper (shallower), which confirms the transfer of charge from the BSb layer to TaX<sub>2</sub>, due to the fact that BSb has a higher work function than TaX<sub>2</sub>. The calculated  $\Delta V$  varies within (1.64 to 7.23 eV) due to the difference in electronegativity among the atoms<sup>81</sup> at the interface. For both TaX<sub>2</sub> and BY monolayers in the form of TaX<sub>2</sub>-BY MS vdWHs, the electrostatic potential effectively controls charge movement at the interface, contributing to increased energy conversion efficiency. The work function ( $\phi$ ) of TaX<sub>2</sub>-BY MS vdWHs – defined as the difference between the vacuum level and Fermi level – was calculated using average electrostatic potential as displayed in Fig. 8.  $\phi$  predominantly depends on the condition of the material surface due to changes in surface electric field settings and electron distribution at the interface. The calculated  $\phi$  for of TaX<sub>2</sub>-BY MS vdWHs lies in the range 3.285–4.009 eV, see Table 2, which shows the potential for field effect transistors.<sup>82</sup>

To see the contact charge redistribution, we have calculated the charge density difference of the TaX<sub>2</sub>-BY (X = S, Se, Te; Y = P, As, Sb) MS vdWHs using<sup>83,84</sup>  $\nabla\rho = \rho_{\text{MSvdWHs}} - \rho_{\text{monolayer-I}} - \rho_{\text{monolayer-II}}$ . In the case of TaX<sub>2</sub>-BY (X = S, Se, Te; Y = P, As) MS vdWHs, charge depletion (accumulation) around the TaX<sub>2</sub> (BP)



**Table 3** Charge redistribution at the interface of TaX<sub>2</sub>-BY (X = S, Se, Te; Y = P, As, Sb) MS vdWHs: e<sup>-</sup> (h<sup>+</sup>) shows transfer of electrons (holes) from one layer to another

TaX <sub>2</sub> -BY	TaS <sub>2</sub> -BP	TaS <sub>2</sub> -BAS	TaS <sub>2</sub> -BSb	TaSe <sub>2</sub> -BP	TaSe <sub>2</sub> -BAS	TaSe <sub>2</sub> -BSb	TaTe <sub>2</sub> -BP	TaTe <sub>2</sub> -BAS	TaTe <sub>2</sub> -BSb
TaX <sub>2</sub>	0.026 (h <sup>+</sup> )	0.038 (h <sup>+</sup> )	0.065 (e <sup>-</sup> )	0.013 (h <sup>+</sup> )	0.024 (h <sup>+</sup> )	0.050 (e <sup>-</sup> )	0.001 (h <sup>+</sup> )	0.008 (h <sup>+</sup> )	0.033 (e <sup>-</sup> )
BY	0.027 (e <sup>-</sup> )	0.039 (e <sup>-</sup> )	0.065 (h <sup>+</sup> )	0.012 (e <sup>-</sup> )	0.025 (e <sup>-</sup> )	0.051 (h <sup>+</sup> )	0.001 (e <sup>-</sup> )	0.009 (e <sup>-</sup> )	0.032 (h <sup>+</sup> )

layer indicates loss (gain) of electrons in TaX<sub>2</sub> (BP, BAS). For TaX<sub>2</sub>-BSb MS vdWHs, TaX<sub>2</sub> (BSb) gain (loss) of electrons in this region makes an electron (hole)-rich region.<sup>85</sup> The BSb layer becomes a depletion region with fewer electrons, resulting in a hole-rich environment, while the TaX<sub>2</sub> layer accumulates electrons and becomes electron-rich as shown in Fig. 9. Quantitative behaviour of charge transfer, analysed *via* Bader charges, show a maximum of 0.065409e and minimum of 0.000399e transferred from TaX<sub>2</sub> to the BY monolayer, see Table 3. The phenomena of the transfer of charge shows a strong interlayer coupling and vdWh interaction established at the interface of TaX<sub>2</sub> and BY monolayers in TaX<sub>2</sub>-BN MS vdWHs. A charge transportation built-in-electric field in the interface, creates a region where charges are separated, generating an electric field at the interface<sup>86</sup> which enhances the carrier mobility along with the number of carriers (holes and electrons). A similar result is also confirmed *via* experiments in graphene/GaSe<sup>87</sup> and graphene/MoS<sub>2</sub>.<sup>88</sup> Ionization potential (*I*);  $I = E_{\text{vac}} - E_{\text{VBM}}$ , for the TaX<sub>2</sub>-BY MS contact in Table 2, helps in determining the Schottky barrier height, crucial for understanding the behavior of MS contacts.

## 4. Conclusion

Using DFT calculations and electronic band structure, the contact (barrier) type (height) at the interface of TaX<sub>2</sub>-BY (X = S, Se, Te; Y = P, As, Sb) MS vdWHs are investigated. The stability of these systems are confirmed *via* binding energies, mechanical (Born criteria), properties, AIMD simulation and phonon spectra calculations. Electronic band structures confirm the metallic behaviour of TaX<sub>2</sub>-BY MS vdWHs with weak vdW interactions in the corresponding monolayers. The quite small effective mass in the case of TaS<sub>2</sub>-BSb, TaSe<sub>2</sub>-BSb and TaTe<sub>2</sub>-BSb MS vdWHs, exhibit high carrier mobility and hence show potential for high speed nanoelectronic applications. n-type Schottky contact at the interface of TaX<sub>2</sub>-BY MS vdWHs favor electron conduction over hole conduction, hence has significant applications in transistors, sensors, photodetectors, and other electronic components. Large potential drop in the case of TaS<sub>2</sub>-BP, TaS<sub>2</sub>-BSb, TaSe<sub>2</sub>-BP, TaSe<sub>2</sub>-BAS and TaTe<sub>2</sub>-BP of the TaX<sub>2</sub>-BY MS vdWHs, suggests a considerable electrostatic field at the interface, which controls the charge transportation and strengthens the power conversion efficiency. Analysis of the Bader charges, show that a maximum (minimum) of 0.065409 (0.000399)e are transferred from the TaX<sub>2</sub>(BY) monolayer. The work function for the TaX<sub>2</sub>-BY MS contact lies in the 3.285–4.009 eV range, which shows potentiality for FET.

## Data availability

The data that support the findings of this study are available on request from the corresponding author.

## Conflicts of interest

There are no conflicts to declare.

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