

Electronic properties and phonon-limited carrier mobility in Janus CrBZTe₂ (Z = N, P, and As) monolayers: A first-principles study

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Abstract. In this work, we systematically investigate the structural, electronic, and carrier transport properties of Janus CrBZTe₂ (Z = N, P, and As) monolayers by using density functional theory. The calculations indicate that these Janus materials are dynamically and energetically stable, suggesting that they could be synthesised via conventional experimental techniques. While a CrBNTe₂ monolayer exhibits metallic behaviour, CrBPTe₂ and CrBAS₂Te₂ monolayers are direct band-gap semiconductors with relatively small band gaps of 0.83 and 0.72 eV, respectively, as obtained from HSE06 hybrid functional calculations. The out-of-plane structural asymmetry gives rise to a difference in the vacuum levels between the two surfaces of the proposed Janus CrBZTe₂ materials. Carrier mobility is further analysed by considering multiple scattering mechanisms to ensure reliable transport predictions. The results show that the semiconducting monolayers exhibit relatively low carrier mobility, with transport primarily limited by acoustic deformation-potential scattering. These findings provide fundamental insights into the physical properties of Janus monolayers and highlight their potential for future electronic applications.

Keywords: 2D Janus materials, electronic properties, phonon scattering, carrier mobility, density functional theory

1 Introduction

Since its discovery in 2004, graphene has revolutionised materials science [1], offering unparalleled carrier mobility, mechanical strength, and thermal conductivity for next-generation electronics [2]. These outstanding characteristics have stimulated extensive research efforts aiming at integrating graphene into nanoelectronic technologies and flexible electronic systems. However, despite its exceptional properties, graphene possesses an intrinsic limitation in electronic applications because of its zero band gap [3]. The absence of a finite band gap significantly

restricts its ability to achieve efficient switching behaviour in field-effect transistors, thereby limiting its direct use in digital nanoelectronics. To overcome this challenge, researchers have actively explored graphene-like materials with tunable electronic structures, including transition metal dichalcogenides [4], monochalcogenides [5], and the MA₂Z₄ family [6]. Importantly, a new class of asymmetric two-dimensional (2D) materials, known as Janus monolayers, has attracted considerable attention. The successful experimental fabrication of Janus MoSSe has opened new avenues for research in the field of 2D materials [7]. This structural asymmetry generates

an intrinsic dipole moment and leads to unique physical properties, including enhanced piezoelectricity, tunable band structures, strong Rashba spin splitting, and improved catalytic activity [8]. As a result, Janus materials offer significant advantages for applications in nanoelectronics, spintronics, photovoltaics, and photocatalysis [9].

The carrier mobility of a material plays a crucial role in determining device performance. Therefore, evaluating and optimising the carrier mobility of emerging materials are key steps in assessing their potential for next-generation nanoelectronic applications. Phonon scattering plays a dominant role in determining carrier mobility, as it acts as the primary intrinsic mechanism limiting the velocity of electrons and holes. In Janus structures, the broken inversion symmetry introduces additional scattering channels, such as polar optical phonon scattering, which further influences the effective mobility [10]. Therefore, incorporating multiple scattering mechanisms in carrier mobility calculations is necessary and helps improve the accuracy of the results [11].

In this work, we introduce a family of Janus CrBZTe_2 ($Z = \text{N, P, and As}$) monolayers and systematically investigate their structural, electronic, and carrier transport properties by using density functional theory (DFT). We carefully examine the stability of these crystals through the evaluation of both the phonon spectra and the cohesive energies. The electronic properties are analysed by examining the electronic band structures, which are calculated by using different exchange-correlation functionals. In particular, the carrier mobility is evaluated in detail by considering multiple scattering mechanisms. Furthermore, the variation trends in carrier mobility are analysed, and the dominant phonon-scattering mechanisms in each material are identified.

2 Computational methods

All calculations based on first principles were performed within the framework of DFT by using the Vienna *Ab initio* Simulation Package (VASP) [12, 13]. The interaction between electrons and ions was described by using the projector augmented-wave formalism [14]. A plane-wave basis set with a kinetic energy cutoff of 600 eV was adopted to ensure computational accuracy. The Brillouin zone was sampled by using a $12 \times 12 \times 1$ Monkhorst-Pack k -point grid. To eliminate artificial interactions between periodic replicas, we introduced a vacuum spacing of 25 Å along the out-of-plane direction. Structural optimisations were carried out until the residual forces on each atom were smaller than 10^{-3} eV/Å, while the electronic self-consistent field iterations were converged to 10^{-6} eV. Dipole corrections were applied to properly account for the built-in electric field arising from the structural asymmetry. The dynamical stability of the systems was further assessed by calculating phonon dispersion relations with the finite-displacement approach implemented in the PHONOPY code [15]. To evaluate electronic properties, we utilised two exchange-correlation approximations. The generalised gradient approximation with the Perdew-Burke-Ernzerhof (PBE) functional [16] was adopted to capture general electronic trends. To ensure a more accurate description of the band structures, we employed the Heyd-Scuseria-Ernzerhof (HSE06) hybrid functional [17]. This included a standard mixing parameter of $\alpha \otimes 0.25$ and a screening parameter of $\mu \otimes 0.2 \text{ Å}^{-1}$ to ensure high-fidelity bandgap predictions. Carrier mobility behaviours were computed by using the AMSET code [18], which evaluates transport coefficients based on the ground-state electronic structures obtained from VASP. To accurately model mobility, we incorporated several intrinsic and extrinsic scattering mechanisms, including acoustic deformation potential (ADP), ionised

impurity (IMP), piezoelectric (PIE), and polar optical phonon (POP) scattering. The total carrier mobility was calculated by using Matthiessen's rule [11].

3 Results and discussion

Fig. 1 illustrates the crystal structure of the Janus CrBZTe₂ (Z = N, P, and As) monolayers. These structures consist of five atomic sublayers stacked in a Te-Cr-Z-B-Te sequence. In the ground state, the Janus CrBZTe₂ belongs to the *P3m1* space group. The optimised lattice constants for CrBNTe₂, CrBPTe₂, and CrBAsTe₂ monolayers are 3.31, 3.41, and 3.48 Å, respectively. The lattice constants of the CrBZTe₂ monolayers increase progressively as the atomic constituent Z evolves from N through P to As. The lattice constants of CrBZTe₂ are comparable with those of the similar structures, such as CrSi₂Z₄ (from 2.84 to 3.68 Å) and CrGe₂Z₄ (from 3.06 to 3.78 Å) [19]. The thickness of the monolayers Δh , defined as the vertical distance between the two Te atomic layers, is 5.39, 5.96, and 6.16 Å for CrBNTe₂, CrBPTe₂, and CrBAsTe₂ structures, respectively. The calculated structural parameters for the proposed Janus CrBZTe₂ materials are summarised in Table 1.

Furthermore, the charge density difference, shown in Fig. 1b, is presented to provide a better understanding of the chemical bonding characteristics. The distribution of the iso-surfaces reveals a significant charge redistribution upon the formation of the crystal lattice from isolated atoms. A pronounced accumulation of electron density (yellow regions) is observed around the Cr sites, reflecting the localised nature of the *d*-orbitals and their interaction with the neighbouring B and Z atoms. Conversely, the cyan regions situated between the B and Z atoms indicate a depletion of charge, characteristic of strong polar covalent bonding.

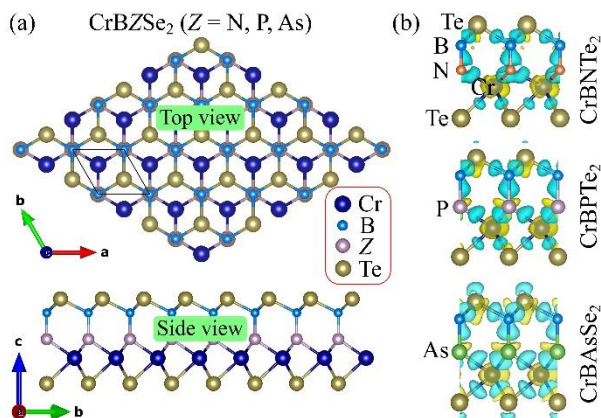


Fig. 1. Crystal structures (a) and differential charge density with an iso-value of $0.005 \text{ e}/\text{\AA}^3$ (b) of Janus CrBZTe₂ (Z = N, P, and As) monolayers. The yellow and cyan iso-surfaces in (b) represent electron accumulation and depletion, respectively

To evaluate the structural stability, we next calculated the cohesive energy to assess the strength and stability of the internal chemical bonding. The cohesive energy of the Janus CrBZTe₂ monolayers is defined by the following expression [20]:

$$E_{\text{coh}} = \frac{E_{\text{tot}} - (n_{\text{Cr}}E_{\text{Cr}} + n_{\text{B}}E_{\text{B}} + n_{\text{Z}}E_{\text{Z}} + n_{\text{Te}}E_{\text{Te}})}{n_{\text{Cr}} + n_{\text{B}} + n_{\text{Z}} + n_{\text{Te}}} \quad (1)$$

where E_{tot} is the total energy of the Janus CrBZTe₂ monolayer; E_i and n_i ($i = \text{Cr, B, Z, and Te}$) represent the energies of the isolated atoms and their respective counts within the unit cell.

The calculated results for the cohesive energy of CrBNTe₂, CrBPTe₂, and CrBAsTe₂ are -6.04 , -5.60 , and -5.36 eV , respectively. These values are comparable with those of similar structures, including MBNS₂ ($M = \text{Ti, Zr, and Hf}$) [21] and WBAsX₂ ($X = \text{S, Se, and Te}$) [22]. The negative values of the cohesive energies indicate that all three structures are energetically favourable and thermodynamically stable. This suggests that the constituent atoms prefer to remain bound within the lattice rather than exist as isolated atoms, highlighting the strong bonding interactions that stabilise the structures. A more negative cohesive energy corresponds to stronger intralayer bonding. Our calculations show that the

monolayers exhibit large cohesive energies, and the chemical bonds in the CrBNTe₂ monolayer are the most stable.

To further assess the stability of the proposed monolayers, we calculated their phonon dispersion spectra to evaluate the dynamical stability. The phonon dispersion spectrum of the

CrBZTe₂ monolayer consists of 15 vibrational branches, which arise from the five atoms present in the primitive unit cell (Fig. 2). The absence of imaginary frequencies throughout the Brillouin zone further confirms the dynamical stability of the CrBZTe₂ monolayer, suggesting that its experimental synthesis could be feasible.

Table 1. Lattice constant a (Å), bond length d (Å), monolayer thickness h , cohesive energy E_c (eV/atom), PBE/HSE06 bandgap E_g (eV), vacuum level different $\Delta\Phi$ (eV), and work function on the bottom/top side $\Phi_{1/2}$ (eV) of Janus CrBZTe₂ (Z = N, P, and As) monolayers. M refers to metal.

	a	$d_{\text{Te-Cr}}$	$d_{\text{Cr-Z}}$	$d_{\text{Z-B}}$	$d_{\text{B-Te}}$	Δh	E_{coh}	E_g^{PBE}	E_g^{HSE06}	$\Delta\Phi$	Φ_1	Φ_2
CrBNTe ₂	3.31	2.64	2.14	1.42	2.25	5.39	-6.04	M	M	0.01	4.07	4.08
CrBPTe ₂	3.41	2.63	2.34	1.88	2.24	5.96	-5.60	0.54	0.83	0.82	5.60	4.78
CrBAsTe ₂	3.48	2.63	2.45	2.01	2.27	6.16	-5.36	0.46	0.72	0.66	4.61	3.95

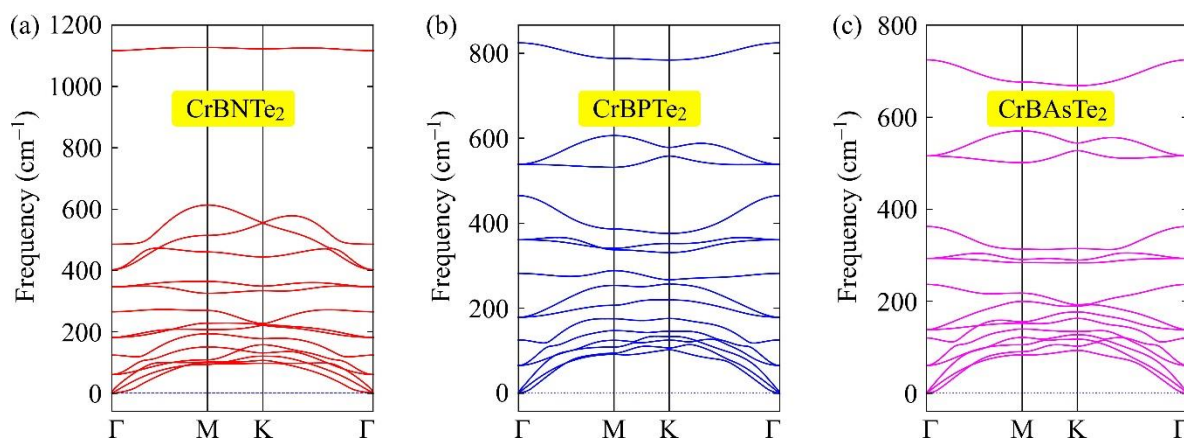


Fig. 2. Phonon spectra of 2D Janus CrBNTe₂ (a), CrBPTe₂ (b), and CrBAsTe₂ (c) monolayers

Band structures of Janus CrBZTe₂ monolayers are shown in Fig. 3. It is demonstrated that while the Janus CrBNTe₂ monolayer is a metal, both CrBPTe₂ and CrBAsTe₂ monolayers are semiconductors with indirect band gaps. At the PBE theoretical level, the band gaps of CrBPTe₂ and CrBAsTe₂ monolayers are 0.54 and 0.46 eV, respectively. Clearly, the band gaps of the Janus CrBZTe₂ monolayers are much smaller than those of conventional 2D transition metal dichalcogenides such as MoTe₂ (1.13 eV) [23], as well as Janus transition metal dichalcogenide structures like MoSTe (1.06 eV) [24] and MoSeTe (1.34 eV) [25]. As illustrated in Fig. 3, the

band structures calculated by using the PBE and HSE06 functionals exhibit very similar dispersive features. For both CrBPTe₂ and CrBAsTe₂ monolayers, the valence band maximum and the conduction band minimum are located at the M point of the Brillouin zone. The two approaches differ primarily in their predicted band-gap value. It is well known that the PBE functional tends to underestimate band-gap values because of the intrinsic limitations of the generalised gradient approximation in describing the exchange-correlation interaction. In contrast, the HSE06 hybrid functional partially incorporates exact Hartree-Fock exchange, leading to a more accurate

description of the electronic structure and, consequently, more reliable band-gap predictions. Our calculated results indicate that the HSE06 band gaps of CrBPTe₂ and CrBAsTe₂ monolayers are 0.83 and 0.72 eV, respectively, which are significantly larger than those predicted by the PBE

functional. These moderate band-gap values suggest that both materials may be promising candidates for applications in nanoelectronic and optoelectronic devices.

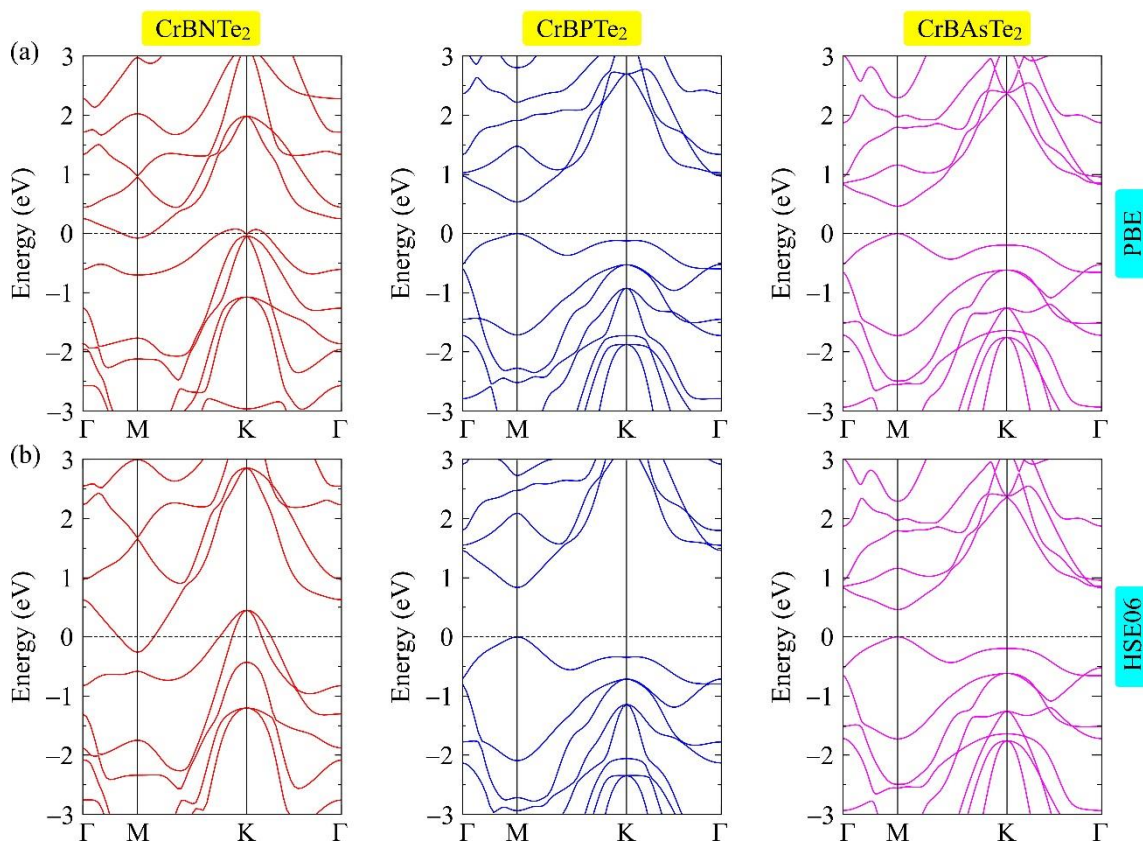


Fig. 3. Band structures of Janus CrBZTe₂ monolayers calculated by using the PBE (a) and HSE06 (b) functionals

To characterise the surface electronics of the proposed 2D materials, we calculated their work function based on the electrostatic potential distribution. It is a fundamental parameter that dictates charge injection and surface sensitivity, and it is also critical for determining the Schottky barrier height and the alignment of energy levels in van der Waals heterostructures. The work function Φ is determined by the difference between the vacuum energy level E_{vac} and the Fermi level E_F as $\Phi = E_{\text{vac}} - E_F$. This parameter provides an insight into the chemical stability of the materials and their potential performance in optoelectronic applications. The planar-averaged electrostatic

potentials of CrBZTe₂ materials are shown in Fig. 4. Owing to the intrinsic out-of-plane structural asymmetry of Janus materials, the two opposite surfaces of the monolayers experience different electrostatic environments, resulting in a noticeable difference in the vacuum energy levels. This vertical asymmetry gives rise to an internal electric field across the monolayer, which can significantly influence the electronic and surface properties of the materials. Our calculations indicate that the vacuum level difference $\Delta\Phi$ in the Janus CrBNTe₂ monolayer is relatively small, suggesting a weak built-in potential across the layer. In contrast, CrBPTe₂ and CrBAsTe₂ exhibit

much larger vacuum-level differences between their two surfaces, reaching 0.82 and 0.66 eV, respectively (Table 1). Such large potential differences imply the presence of a strong intrinsic dipole moment and a built-in electric field in these Janus monolayers, which may play an essential role in modulating charge separation and enhancing their potential for applications in electronic and optoelectronic nanodevices. The calculated work functions at the bottom Te surface (where Te is bonded to Cr) of Φ_1 and at the top Te surface (where Te is bonded to B) of Φ_2 for the

Janus CrBZTe₂ monolayers (Fig. 1) are summarised in Table 1. It is indicated that, in the CrBPTe₂ and CrBAsTe₂ semiconductors, the work function Φ_1 on the bottom side of the Te layer is higher than the work function Φ_2 on the top one, suggesting that the top surface facilitates electron emission more effectively. In contrast, the metallic CrBNTe₂ monolayer shows the opposite trend ($\Phi_1 < \Phi_2$), although the difference between the two work functions is relatively small.

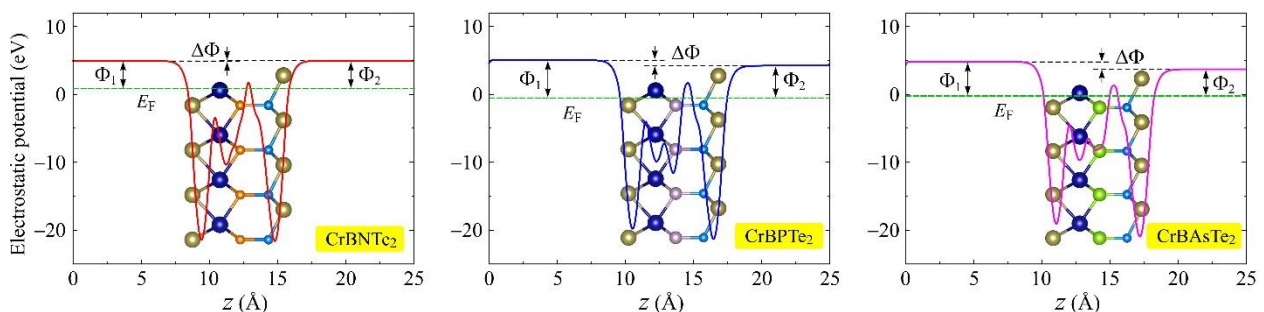


Fig. 4. Planar-averaged electrostatic potentials of Janus CrBZTe₂ monolayers. The Fermi level E_F is indicated by the horizontal dotted line

In the last part, we explore the carrier mobility of the studied materials. Our analysis focuses on CrBPTe₂ and CrBAsTe₂, while the CrBNTe₂ monolayer is not considered because of its metallic nature, which makes the evaluation of conventional carrier mobility less meaningful. Carrier mobility is strongly affected by the scattering processes experienced by charge carriers as they move through the crystal lattice. In semiconductors, these scattering events can significantly limit the transport of electrons and holes. To obtain reliable and quantitatively accurate mobility values, it is therefore essential to account for the dominant phonon-related scattering mechanisms. In this work, carrier mobility was evaluated by using the AMSET package. This approach provides a comprehensive treatment of transport by explicitly integrating ADP, IMP, PIE, and POP scattering within a unified framework. Such a treatment is essential

for 2D Janus materials, where intrinsic structural asymmetry and polarity often elevate long-range scattering processes to a dominant role. In contrast, the standard Bardeen-Shockley deformation potential model [26], while simple and computationally efficient, accounts exclusively for acoustic phonon scattering. By neglecting other relevant mechanisms, such as polar optical phonons or ionised impurities, this approach may significantly overestimate carrier mobility, particularly in asymmetric structures. The total carrier mobility was estimated by combining the contributions of the different scattering channels according to Matthiessen's rule, which assumes that the inverse of the total mobility equals the sum of the inverses of the mobilities limited by each scattering process as [11]

$$\frac{1}{\mu_{\text{tot}}} = \frac{1}{\mu_{\text{ADP}}} + \frac{1}{\mu_{\text{IMP}}} + \frac{1}{\mu_{\text{PIE}}} + \frac{1}{\mu_{\text{POP}}}, \quad (2)$$

where μ_{tot} is the total carrier mobility; μ_{ADP} , μ_{IMP} , μ_{PIE} , and μ_{POP} refer to the carrier mobilities governed by ADP, IMP, PIE, and POP scattering, respectively.

Fig. 5 illustrates the temperature dependence of the total electron mobility and its individual scattering-limited components. Two representative carrier concentrations n_c are considered, including a low concentration of $1 \times 10^{16} \text{ cm}^{-3}$ and a high concentration of $1 \times 10^{20} \text{ cm}^{-3}$. It is observed that the ADP scattering mechanism is the dominant factor governing the total electron mobility across both carrier concentration regimes. Additionally, PIE

scattering plays a more significant role than the IMP and POP scattering mechanisms, particularly in low carrier concentrations. The dominance of ADP scattering in these materials can be attributed to the strong electron-phonon coupling near the band edges, which enhances interactions between charge carriers and long-wavelength acoustic phonons. In addition, other scattering channels, such as polar optical phonon scattering and ionised impurity scattering, are comparatively weak under the present conditions, further reinforcing the role of ADP scattering as the primary mechanism limiting carrier transport. Generally, the electron mobilities in both structures are relatively low. This behaviour can be attributed to the strong carrier scattering processes.

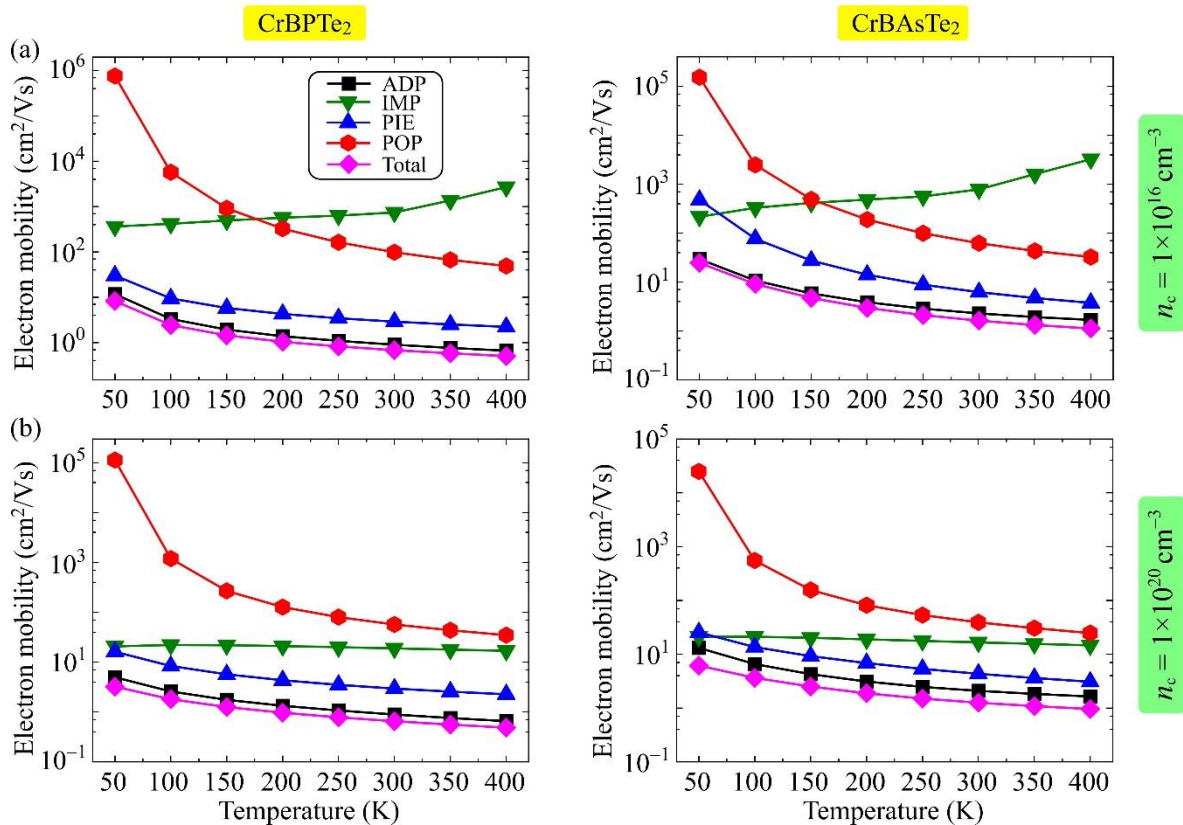


Fig. 5. Temperature-dependent total and phonon-limited electron mobilities of CrBZTe₂ (Z = N, P, and As) materials when $n_c = 1 \times 10^{16} \text{ cm}^{-3}$ (a) and $n_c = 1 \times 10^{20} \text{ cm}^{-3}$ (b)

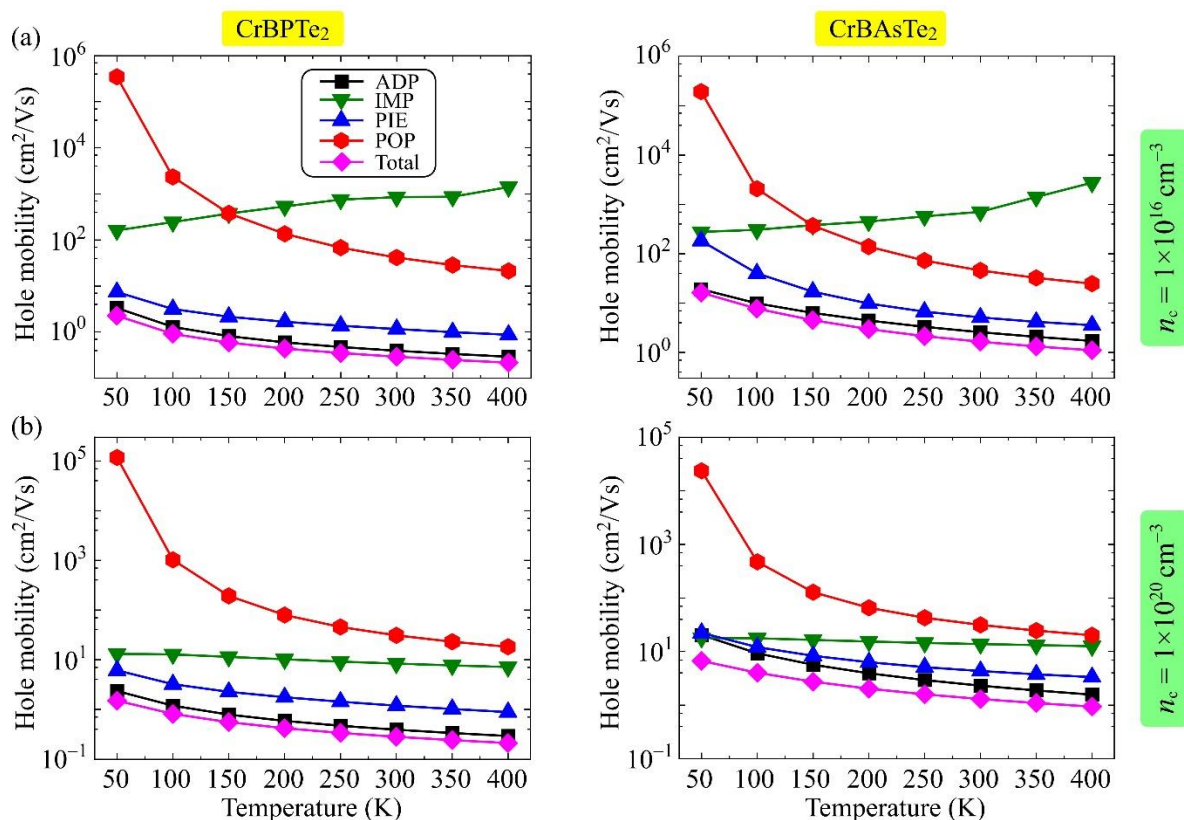


Fig. 6. Temperature-dependent total and phonon-limited hole mobilities of CrBZTe₂ (Z = N, P, and As) materials when $n_c = 1 \times 10^{16} \text{ cm}^{-3}$ (a) and $n_c = 1 \times 10^{20} \text{ cm}^{-3}$ (b)

At ambient temperature (300 K), the total electron mobility of the CrBPTe₂ monolayer is $0.68 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ when $n_c = 1 \times 10^{16} \text{ cm}^{-3}$, decreasing to $0.65 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ when $n_c = 1 \times 10^{20} \text{ cm}^{-3}$. The mobility decreases with increasing carrier concentration because of the dominance of carrier-carrier interactions at high density levels. The total electron mobility in the CrBPTe₂ monolayer at ambient temperature is higher, reaching 1.62 and $1.26 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ for carrier concentrations of 1×10^{16} and $1 \times 10^{20} \text{ cm}^{-3}$, respectively.

The influence of phonon scattering mechanisms on hole mobility is analogous to that observed for electrons. As illustrated in Fig. 6, the hole mobility is primarily governed by the ADP scattering. When $n_c = 1 \times 10^{16} \text{ cm}^{-3}$, the ambient temperature hole mobilities for CrBPTe₂ and CrBAsTe₂ monolayers are 0.29 and $1.65 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$, respectively. Notably, while carrier mobilities governed by phonon scattering typically decrease

with temperature, the IMP-limited mobility exhibits the opposite trend, increasing as the temperature rises, particularly in the low carrier concentration cases, as displayed in Figs. 5a and 6a. The μ_{IMP} increases with temperature in the low carrier concentration regime because higher thermal velocities allow carriers to pass through the electrostatic fields of ionised impurities more rapidly, thereby reducing the deflection probability.

4 Conclusion

In this work, we have performed a comprehensive DFT study of the structural stability, electronic properties, and carrier transport behaviour of Janus CrBZTe₂ monolayers. The calculated results confirm that these materials possess stable crystal structures, indicating their feasibility for experimental realisation. It was demonstrated that

that the CrBPTE₂ monolayer exhibits metallic characteristics, whereas both CrBPTE₂ and CrBAsTe₂ behave as direct band-gap semiconductors. With small band gaps, CrBPTE₂ and CrBAsTe₂ semiconductors are promising for applications in infrared optoelectronic devices, photodetectors, and thermoelectric technologies. The intrinsic out-of-plane structural asymmetry in 2D Janus materials induces a built-in electric field and a vacuum level difference between the two surfaces, which can effectively promote charge separation and thus make these materials promising candidates for photocatalytic applications. By comprehensively evaluating carrier mobility, particularly through identifying

the dominant phonon scattering mechanism governing the mobility values, this study provides valuable insights for tailoring the physical properties of the materials via external perturbations. Such understanding may facilitate the effective optimisation and practical implementation of these materials in technological applications.

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