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# Dirac Metallic FeB<sub>2</sub>-Induced Low Schottky Barrier and Electrically Tunable Schottky Contact in FeB<sub>2</sub>/MoS<sub>2</sub> van der Waals Heterostructure

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In this work, we employ first-principles density functional theory (DFT) calculations to systematically investigate the interfacial electronic properties and contact behavior of a Dirac-metallic Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> van der Waals (vdW) heterostructure. The Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> system is found to be energetically, mechanically, thermally, and dynamically stable, indicating its potential experimental feasibility. Notably, the heterostructure forms an n-type Schottky contact with an ultralow electron barrier height of 0.125 eV and a low tunneling resistance of  $1.82 \times 10^{-9} \Omega \cdot \text{cm}^2$ . This superior contact performance is attributed to the delocalized Dirac electrons and the weak Fermi-level pinning at the interface, providing key insight into the role of Dirac metals in contact engineering. Furthermore, the Schottky barrier can be effectively tuned by an external electric field, enabling a reversible transition from Schottky to Ohmic contact. These findings highlight the promise of Dirac metallic FeB<sub>2</sub> as an efficient electrode material and offer practical guidance for the design of high-performance 2D nanoelectronic and optoelectronic devices with reduced contact resistance.

## 1 Introduction

In recent decades, two-dimensional (2D) materials have become a cornerstone of condensed matter physics and materials science owing to their unique and versatile properties<sup>1–4</sup>. The confinement of charge carriers within atomically thin layers gives rise to electronic, optical, and mechanical characteristics that markedly differ from their bulk counterparts. Prominent examples include graphene<sup>5</sup>, phosphorene<sup>6</sup>, transition metal dichalcogenides (TMDs)<sup>7</sup>, and MXenes<sup>8</sup>, which have all attracted intensive attention. These materials are not only scientifically intriguing but also hold transformative potential for applications ranging from flexible electronics and photodetectors to quantum computing and energy harvesting. Despite their promise, the functionalities of individual 2D materials remain limited, often constraining their application in advanced device architectures. For example, the absence of a sizable band gap in graphene significantly ham-

pers its use in logic devices requiring a high on/off current ratio<sup>9</sup>. Similarly, although phosphorene exhibits a tunable direct band gap and high carrier mobility<sup>10</sup>, its intrinsic instability under ambient conditions severely limits practical applications<sup>11</sup>. In the case of MoS<sub>2</sub>, while the presence of a sizable band gap makes it attractive for field-effect transistors and optoelectronic devices<sup>12</sup>, its relatively low carrier mobility remains a critical bottleneck for high-performance applications<sup>13</sup>.

To overcome these limitations and unlock new functionalities, the creation of van der Waals (vdW) heterostructures by stacking<sup>14,15</sup> or integrating<sup>16,17</sup> different 2D materials has become a major research focus. Vertical heterostructures, formed by stacking individual layers, are particularly advantageous for investigating interfacial charge transfer, band alignment, and Schottky barrier formation across atomically sharp interfaces. In contrast, lateral heterostructures, where different materials are seamlessly joined within the same plane, are more suitable for studying in-plane transport and junction properties but typically require more complex structural modeling and fabrication considerations. By suitable selecting and combining different layers, researchers can tailor the physical properties and induce interfacial phenomena that are absent in the individual constituents. With continuous advances in fabrication techniques and increasingly accurate computational models, the rational design of vdW heterostructures is expected to enable multifunctional devices. Among various configurations, metal-semiconductor vdW heterostructures

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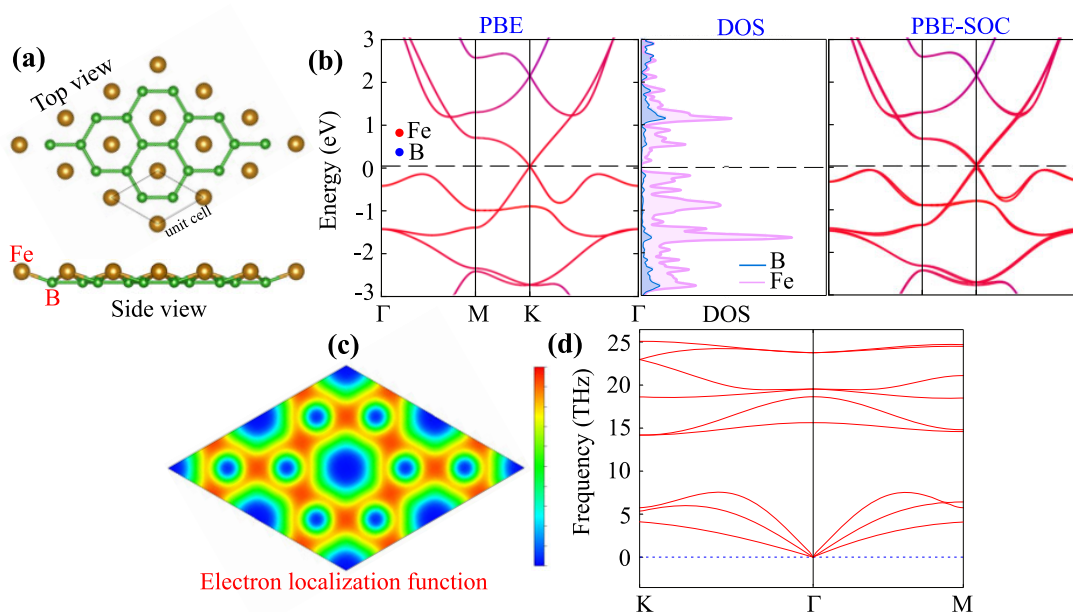
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**Fig. 1** (a) Optimized geometry, (b) projected band structures without and with the presence of SOC effect and the projected density of states, (c) electron localization function and (d) phonon spectrum of FeB<sub>2</sub> monolayer.

are of particular interest due to their crucial role in tuning contact resistance, band alignment, and carrier injection in next-generation electronic and optoelectronic devices<sup>18,19</sup>.

Recently, a novel boron-based 2D Dirac FeB<sub>2</sub> material has been reported, in which planar hexacoordinate iron (Fe) atoms are embedded within a boron honeycomb lattice structure<sup>20</sup>. Monolayer FeB<sub>2</sub> hosts a Dirac cone near the Fermi level, giving rise to massless Dirac fermions with a remarkable Fermi velocity of  $6.54 \times 10^5$  m/s, thereby enabling ultrafast charge transport<sup>20</sup>. In addition, monolayer FeB<sub>2</sub> exhibits metallic behavior with excellent electrical conductivity and ultrahigh carrier mobility on the order of  $10^5$  cm<sup>2</sup>/Vs, which is comparable to that of graphene<sup>21</sup>. Notably, nanosheet FeB<sub>2</sub> can also be synthesized in recent experiment<sup>22</sup> and it has been predicted to serve as a promising electrode material for metal-ion batteries<sup>23</sup>. All these findings suggest that FeB<sub>2</sub> is not only of fundamental interest as a novel 2D Dirac metal but also holds great promise as a metallic building block for integration into 2D metal–semiconductor heterostructures.

Currently, the integration of 2D metals with TMDs semiconductors has attracted considerable attention owing to the unique electronic and optical properties of TMDs as well as their relatively stable and scalable synthesis<sup>24–26</sup>. Such metal–semiconductor heterostructures provide a versatile platform for exploring interfacial physics and developing high-performance electronic and optoelectronic devices. Among the family of 2D TMD semiconductors, MoS<sub>2</sub> is the most widely studied due to its sizable band gap<sup>27</sup> and outstanding mechanical behavior<sup>28</sup>. Recently, heterostructures combining two-dimensional (2D) metals with MoS<sub>2</sub> semiconductors have been successfully fabricated and investigated<sup>29,30</sup>. These studies demonstrated that MoS<sub>2</sub> serves as an efficient channel material for integration with 2D metallic lay-

ers. Therefore, in this work, we design the integration of metal–semiconductor heterostructure between 2D metallic FeB<sub>2</sub> and 2D semiconductor MoS<sub>2</sub> using first-principles calculations.

## 2 Computational details

First-principles calculations based on density functional theory (DFT) were performed using the PWscf package within the Quantum ESPRESSO distribution<sup>31,32</sup>. The exchange–correlation interaction was treated within the generalized gradient approximation (GGA) using the Perdew–Burke–Ernzerhof (PBE) functional<sup>33</sup>. The electron–ion interactions were described by projector augmented wave (PAW) pseudopotentials. A plane-wave basis set with a kinetic energy cutoff of 510 eV was employed to ensure convergence of total energies. Brillouin zone integrations were carried out using a Monkhorst–Pack  $k$ -point mesh of  $15 \times 15 \times 1$ . A vacuum spacing of 30 Å was introduced along the out-of-plane direction to avoid spurious interactions between periodic images. All structures were fully relaxed until the residual force on each atom was less than 0.01 eV/Å, and the total energy convergence criterion was set to  $10^{-8}$  eV. Spin-orbit coupling (SOC) effects were also included in the calculations to account for relativistic interactions, which are known to play a crucial role in transition metals. To investigate vibrational properties and dynamical stability, phonon spectra were calculated within density functional perturbation theory (DFPT)<sup>34,35</sup>. Phonon dispersions were obtained using a  $3 \times 3 \times 1$   $q$ -point mesh.

## 3 Results and Discussion

We first investigate the structural, electronic, and dynamical stability of monolayer FeB<sub>2</sub> as a prerequisite for constructing the FeB<sub>2</sub>/MoS<sub>2</sub> heterostructure. Upon full structural optimization, Fe atoms remain embedded within the boron honeycomb lat-



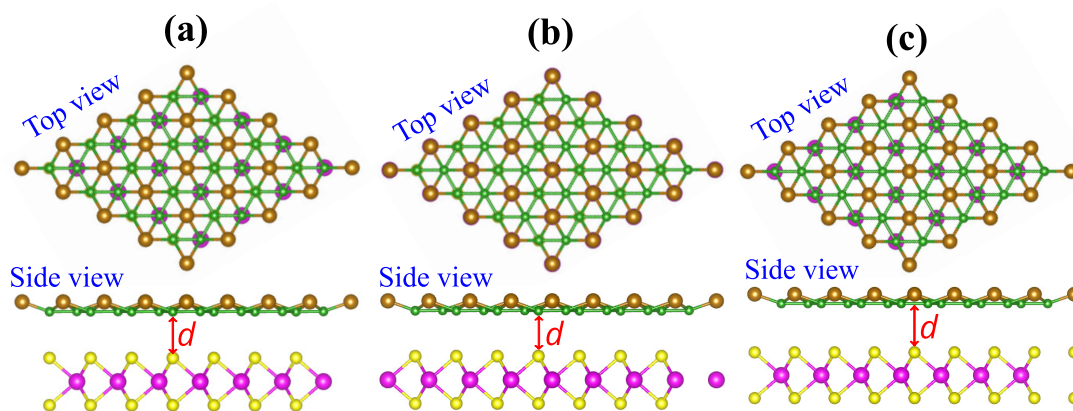


Fig. 2 Optimized atomic structures of Dirac states metal  $\text{FeB}_2/\text{MoS}_2$  heterostructures

tice, forming a planar hexacoordinate geometry in good agreement with previous reports<sup>20,22</sup>. The optimized lattice constant is determined to be 3.18 Å, consistent with earlier theoretical predictions<sup>20,22</sup>. The  $\text{FeB}_2$  monolayer crystallizes in the  $P6/3m$  space group. Its unit cell consists of one Fe atom embedded within a two-dimensional hexagonal boron lattice, as illustrated in Fig. 1(a). The vertical distance between the Fe atom and the boron hexagonal plane is calculated to be 0.63 Å, which is in excellent agreement with previous theoretical predictions<sup>20</sup>, thereby validating the reliability of our computational approach. The electronic band structures of  $\text{FeB}_2$  monolayer without and within the presence of SOC effect are illustrated in Fig. 1(b). Both PBE and PBE-SOC reveal that  $\text{FeB}_2$  monolayer exhibits a metallic behavior with a Dirac cone located near Fermi level at the K point. When SOC effect is included, a band splitting emerges near the Dirac point, but the metallic nature of the system remains intact. The projected density of states (PDOS) of  $\text{FeB}_2$  monolayer indicate that its Dirac states near the Fermi level is mainly contributed by the Fe- $d$  orbital states. To further understand the physical origin of the  $\text{FeB}_2$  monolayer, we analyzed its electron localization function (ELF), as shown in Fig. 1(c). The results reveal that the  $\text{FeB}_2$  monolayer is characterized by strong covalent bonding within the hexagonal boron plane, while the Fe atom exhibits delocalized electron distribution with weak interaction with the surrounding boron atoms. Furthermore, to further evaluate the dynamical stability of  $\text{FeB}_2$ , phonon dispersion calculations were carried out within the framework of DFPT, as displayed in Fig. 1(d). The absence of imaginary frequencies across the entire Brillouin zone confirms that monolayer  $\text{FeB}_2$  is dynamically stable and, in principle, experimentally realizable.

We further design a metal-semiconductor  $\text{FeB}_2/\text{MoS}_2$  heterostructure by vertically stacking the Dirac metallic  $\text{FeB}_2$  monolayer on top of semiconducting  $\text{MoS}_2$ . Three possible stacking configurations of the  $\text{FeB}_2/\text{MoS}_2$  heterostructure are illustrated in Fig. 2. In these models, the Fe atoms are positioned at different high-symmetry sites relative to the Mo and S atoms of the  $\text{MoS}_2$  layer, namely FM-1, FM-2 and FM-3. After full structural relaxation, the interlayer distances ( $d$ ) between the topmost S layer of  $\text{MoS}_2$  and the bottom B layer of  $\text{FeB}_2$  in the Dirac- $\text{FeB}_2/\text{MoS}_2$  heterostructure are found to be 3.06, 3.00, and 3.34 Å for the

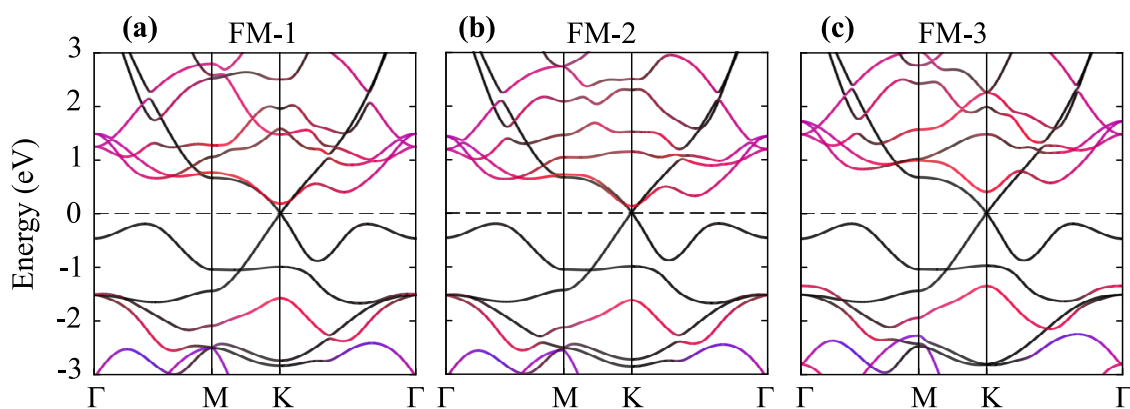
FM-1, FM-2, and FM-3 stacking configurations, respectively. It is evident that among these configurations, the FM-2 stacking exhibits the shortest interlayer spacing. Moreover, the obtained interlayer spacing for all configurations fall within the typical range of vdW interactions, confirming the weakly bonded nature of the Dirac- $\text{FeB}_2/\text{MoS}_2$  heterostructure. Furthermore, to quantitatively evaluate the interlayer coupling and relative stability, we calculated the binding energies ( $E_b$ ) of these stacking configurations using the expression:

$$E_b = \frac{E_H - E_{\text{FeB}_2} - E_{\text{MoS}_2}}{A} \quad (1)$$

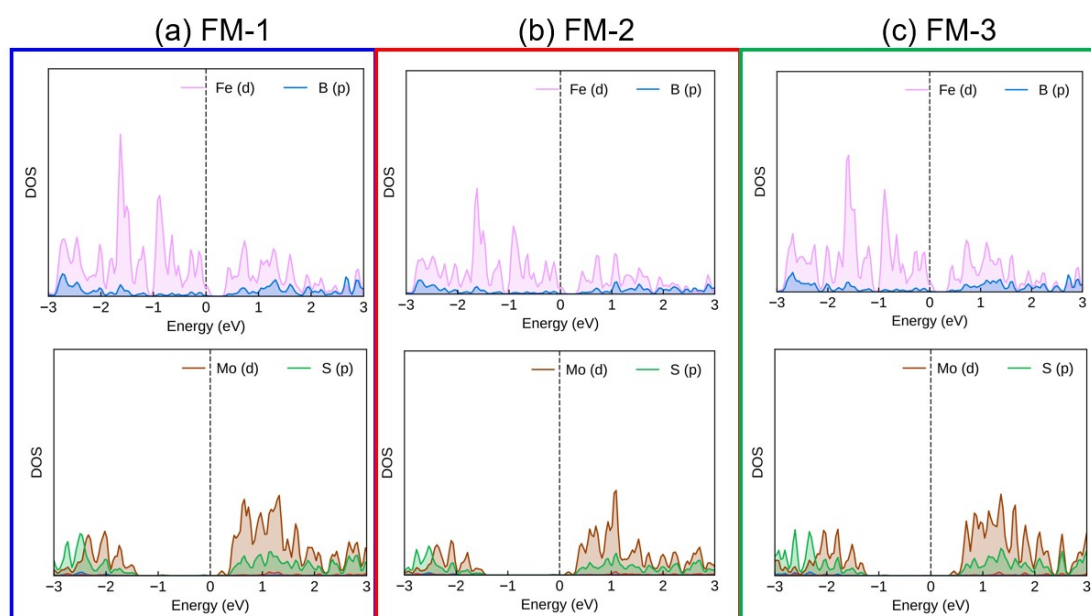
Here,  $E_H$ ,  $E_{\text{FeB}_2}$ , and  $E_{\text{MoS}_2}$  represent the total energies of the Dirac- $\text{FeB}_2/\text{MoS}_2$  heterostructure, and the isolated  $\text{FeB}_2$  and  $\text{MoS}_2$  monolayers, respectively. The calculated binding energies of the Dirac- $\text{FeB}_2/\text{MoS}_2$  heterostructure for the FM-1, FM-2, and FM-3 stacking configurations are found to be -25.83, -27.66, and -21.41 meV/Å<sup>2</sup>, respectively. The negative values of the binding energies indicate that all the stacking configurations are energetically favorable and stable. Among them, the FM-2 configuration exhibits the lowest binding energy, confirming that it is the most energetically preferred stacking arrangement for the Dirac- $\text{FeB}_2/\text{MoS}_2$  heterostructure. In addition, these values are comparable to those obtained in other typical vdW heterostructures, such as  $\text{PbN}/\text{CdO}$ <sup>36</sup>,  $\text{NbSe}_2/\text{MoS}_2$ <sup>37</sup>,  $\text{SiC}/\text{Borophene}$ <sup>38</sup>,  $\text{AlN}/\text{Zr}_2\text{CO}_2$ <sup>39</sup> and  $\text{Ti}_2\text{C}/\text{MoS}_2$ <sup>40</sup>, confirming that the interaction between  $\text{FeB}_2$  and  $\text{MoS}_2$  layers is dominated by weak vdW forces rather than chemical bonding.

We further investigate the electronic properties of the Dirac- $\text{FeB}_2/\text{MoS}_2$  heterostructures under different stacking configurations by analyzing their projected band structures and atom-resolved density of states (DOS), as illustrated in Fig. 3 and Fig. 4. It is evident that all stacking configurations preserve the metallic character of the heterostructure, with a distinct Dirac cone located at the K point. The Dirac cone originates predominantly from the  $\text{FeB}_2$  layer, indicating that the intrinsic Dirac feature of  $\text{FeB}_2$  is well retained upon interfacing with the  $\text{MoS}_2$  monolayer. The similar preservation was also observed in other vdW metal-semiconductor heterostructures, such as  $\text{graphene}/\text{GaN}$ <sup>41</sup>. Likewise, the semiconducting nature of the  $\text{MoS}_2$  layer remains al-





**Fig. 3** Projected band structures of the Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> heterostructure for (a) FM-1, (b) FM-2 and (c) FM-3 stacking configurations. The contributions of the Dirac-FeB<sub>2</sub> and MoS<sub>2</sub> layers are marked by black and red-blue lines, respectively. The Fermi level is set to be zero and marked by the dashed black line.



**Fig. 4** PDOS of all atoms in the Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> heterostructure for (a) FM-1, (b) FM-2 and (c) FM-3 stacking configurations.

most unaffected. This preservation of the intrinsic electronic characteristics of both components can be attributed to the weak van der Waals interaction at the Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> interface, which prevents significant orbital hybridization between the two layers.

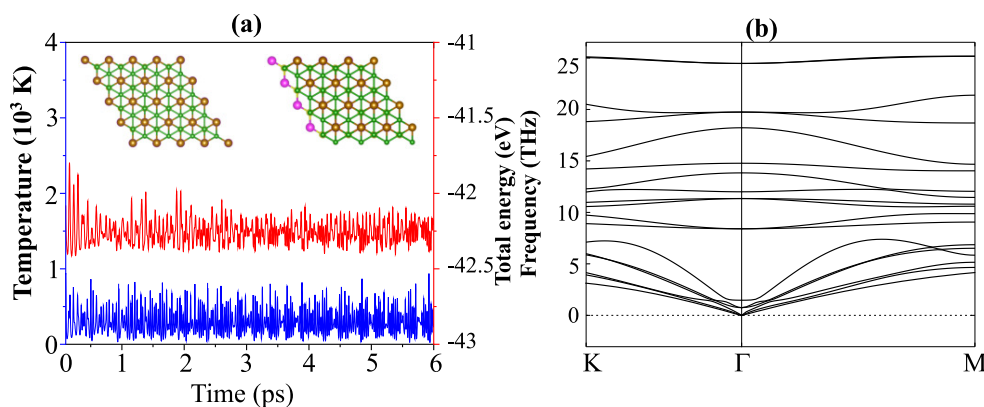
Interestingly, a metal–semiconductor junction is naturally formed at the Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> interface, which plays a vital role in tailoring the charge transport characteristics and designing next-generation nanoelectronic and optoelectronic devices. At the Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> interface, Schottky-type contacts with narrow barrier heights are formed in all stacking configurations. This behavior arises because the Fermi level of the metallic Dirac-FeB<sub>2</sub> layer lies between the conduction and valence band edges of the semiconducting MoS<sub>2</sub> layer. The Schottky barriers at the metal–semiconductor interface are defined as follows:

$$\Phi_{\text{SB}}^{\text{e}} = E_{\text{C}} - E_{\text{F}}, \quad \Phi_{\text{SB}}^{\text{h}} = E_{\text{F}} - E_{\text{V}}, \quad (2)$$

where  $\Phi_{\text{SB}}^{\text{e}}$  and  $\Phi_{\text{SB}}^{\text{h}}$  represent the electron and hole Schottky barrier heights, respectively. Here,  $E_{\text{C}}$  and  $E_{\text{V}}$  denote the energies of the conduction band minimum (CBM) and valence band maximum (VBM) of the MoS<sub>2</sub> layer, while  $E_{\text{F}}$  is the Fermi level of the Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> heterostructure. The calculated Schottky barriers  $\Phi_{\text{SB}}^{\text{e}}$  ( $\Phi_{\text{SB}}^{\text{h}}$ ) for the FM-1, FM-2, and FM-3 configurations are found to be 0.179 (1.679), 0.125 (1.665) and 0.404 (1.754) eV, respectively. It is obvious that the Schottky barriers  $\Phi_{\text{SB}}^{\text{e}}$  is significantly smaller than the  $\Phi_{\text{SB}}^{\text{h}}$ , specifying that the Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> heterostructure possesses the *n*-type Schottky contact for all stacking configurations. Among those configurations, the FM-2 configuration exhibits the smallest  $\Phi_{\text{SB}}^{\text{e}}$ , suggesting more efficient charge injection across the interface.

To gain deeper insights into the interfacial electronic coupling and the origin of the Schottky barriers, it is essential to analyze the projected density of states (PDOS) of the individual atoms in the Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> heterostructure. The PDOS provides valu-





**Fig. 5** (a) The fluctuations of the temperature and total energy and (b) phonon spectra of the Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> heterostructure. The insets present the atomic structures of the Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> heterostructure before and after performing the AIMD simulation of 6 ps.

able information on the orbital hybridization between the metallic FeB<sub>2</sub> layer and the semiconducting MoS<sub>2</sub> layer, as well as the alignment of the Fermi level relative to the band edges of MoS<sub>2</sub>. In particular, the interaction at the metal–semiconductor interface can induce metal-induced gap states (MIGS) within the band gap of MoS<sub>2</sub>, which play a crucial role in determining the Schottky barrier height and may lead to Fermi-level pinning (FLP). Therefore, a careful examination of the PDOS allows us to identify the degree of hybridization, the presence of MIGS, and the extent to which FLP influences the electronic properties of the Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> interface. The PDOS of the Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> heterostructure for all stacking configurations are shown in Fig. 4. It is evident that the electronic states crossing the Fermi level are mainly contributed by the metallic Dirac-FeB<sub>2</sub> layer, while the MoS<sub>2</sub> layer contributes negligible states near the Fermi level. Additionally, this finding confirms the absence of noticeable MIGS at the Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> interface, indicating that the electronic coupling between the two layers is weak and that the FLP is negligible.

Furthermore, to examine the feasibility of experimentally synthesizing the Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> heterostructure, we evaluated its structural stability by performing mechanical response analysis, AIMD simulations, and phonon dispersion calculations, as illustrated in Fig. 5. The mechanical stability of the heterostructure can be examined by analyzing the in-plane elastic constants  $C_{ij}$  by fitting the strain–energy relationship within the small strain range ( $\pm 1.5\%$ ). For a 2D hexagonal lattice, there are three relevant independent elastic constants, namely  $C_{11}$ ,  $C_{12}$ , and  $C_{66} = [C_{11} - C_{12}]/2$ . According to the Born-Huang stability criteria for a hexagonal system<sup>42</sup>, the mechanical stability is guaranteed when:  $C_{11} > 0$ ,  $C_{66} > 0$  and  $C_{11} > |C_{12}|$ . Our results show that the elastic constants  $C_{11}$ ,  $C_{12}$ , and  $C_{66}$  are obtained to be 293.84, 113.46 and 90.19 N/m, respectively. All these values satisfy the above criteria, confirming the mechanical robustness of the heterostructure. Additionally, Furthermore, the in-plane Young's modulus ( $Y$ ) and Poisson's ratio ( $\nu$ ) are derived from the elastic constants as:

$$Y = \frac{C_{11}^2 - C_{12}^2}{C_{11}}, \quad \nu = \frac{C_{12}}{C_{11}}. \quad (3)$$

The Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> heterostructure exhibits a Young's modulus of  $Y = 250.02$  N/m and a Poisson's ratio of  $\nu = 0.39$ . The relatively large  $Y$  value indicates a strong in-plane stiffness and robust covalent bonding within the heterostructure, while the moderate Poisson's ratio suggests a reasonable degree of mechanical flexibility. These features confirm that the Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> heterostructure possesses excellent mechanical robustness.

To further confirm the thermal and dynamical stability of the Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> heterostructure, we performed ab initio molecular dynamics (AIMD) simulations at room temperature of 300 K for 6 ps with a time step of 1 fs. As shown in Fig. 5(a), both the temperature and total energy fluctuate slightly around their equilibrium values throughout the simulation, indicating the absence of any bond breaking or structural distortion during the thermal process. The insets present the atomic configurations of the heterostructure before and after the AIMD simulation, clearly demonstrating that the overall atomic framework remains intact. Moreover, the phonon dispersion spectrum of the Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> heterostructure, shown in Fig. 5(b), exhibits no imaginary frequencies across the Brillouin zone, thereby confirming its dynamical stability. The coexistence of thermal and vibrational stability strongly suggests that the Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> heterostructure is experimentally feasible and can maintain structural integrity under ambient conditions.

Figure 6 summarizes the interfacial charge redistribution and the electrostatic potential profile of the Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> heterostructure. The charge density difference is defined as

$$\Delta\rho(\mathbf{r}) = \rho_{\text{FeB}_2/\text{MoS}_2}(\mathbf{r}) - \rho_{\text{FeB}_2}(\mathbf{r}) - \rho_{\text{MoS}_2}(\mathbf{r}), \quad (4)$$

and its planar average along the direction normal to the interface is given by

$$\Delta\rho(z) = \frac{1}{A} \iint \Delta\rho(x, y, z) dx dy, \quad (5)$$

As shown in Fig. 6(a), the positive and negative values of  $\Delta\rho$  correspond to charge accumulation and depletion regions, respectively. As shown in Fig. 6(a), the charge redistribution occurs mainly at the vdW gap between FeB<sub>2</sub> and MoS<sub>2</sub>, indicating a weak but noticeable interfacial interaction. The electrons are transferred from the MoS<sub>2</sub> layer to the FeB<sub>2</sub> layer, forming an in-



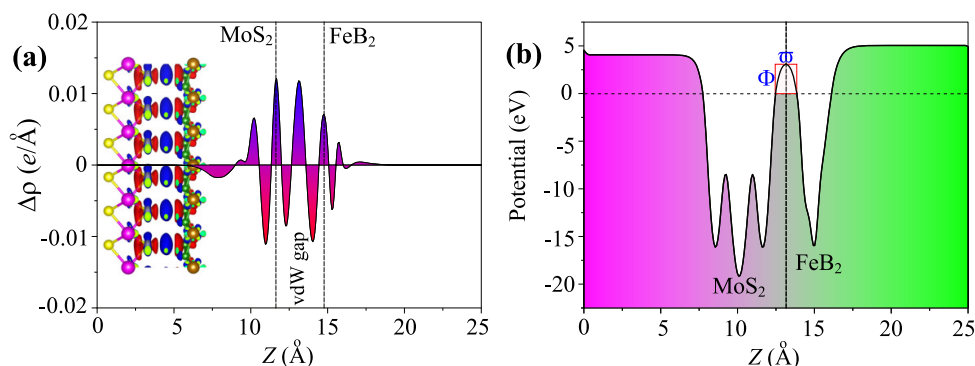


Fig. 6 (a) Planar-averaged charge density difference and (b) electrostatic potential of the Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> heterostructure.

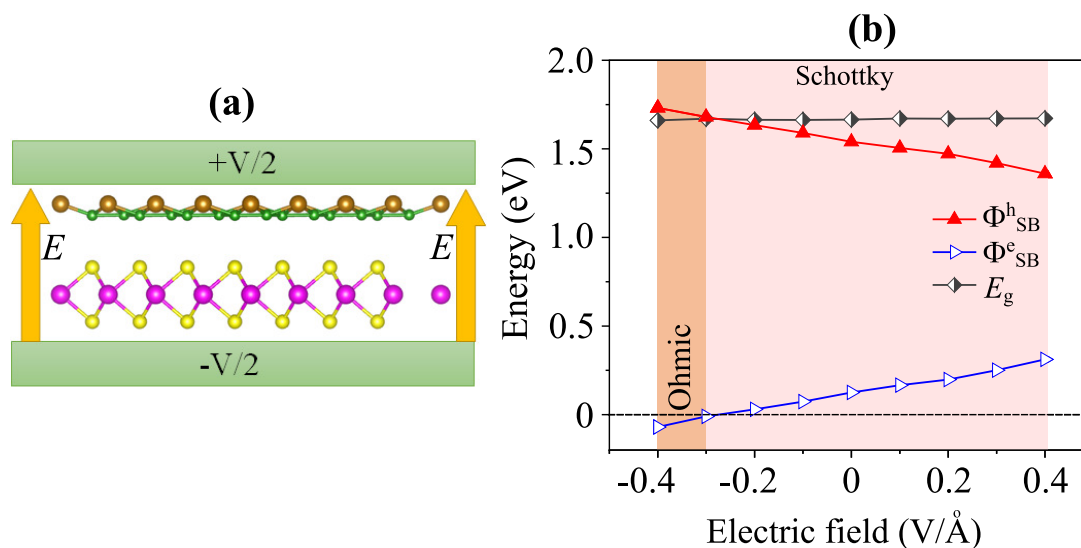


Fig. 7 (a) Schematic model of applied electric field and the variations in the Schottky barriers of the Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> heterostructure as a function of electric fields.

terfacial dipole directed from MoS<sub>2</sub> to FeB<sub>2</sub>. To further elucidate the charge transfer mechanism, the planar-averaged electrostatic potential of the Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> heterostructure was calculated and is presented in Fig. 6(b). The potential difference ( $\Delta\Phi$ ) between the two vacuum levels of FeB<sub>2</sub> and MoS<sub>2</sub> sides represents the built-in potential formed at the interface due to charge redistribution. This built-in electric field can facilitate charge separation and carrier transport across the interface, which is highly desirable for nanoelectronic and optoelectronic device applications.

To quantitatively evaluate the carrier tunneling across the vdW Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> heterostructure, the tunneling probability ( $T_P$ ) and tunneling specific resistivity ( $\rho_t$ ) are estimated using the semi-classical approximation<sup>43</sup>:

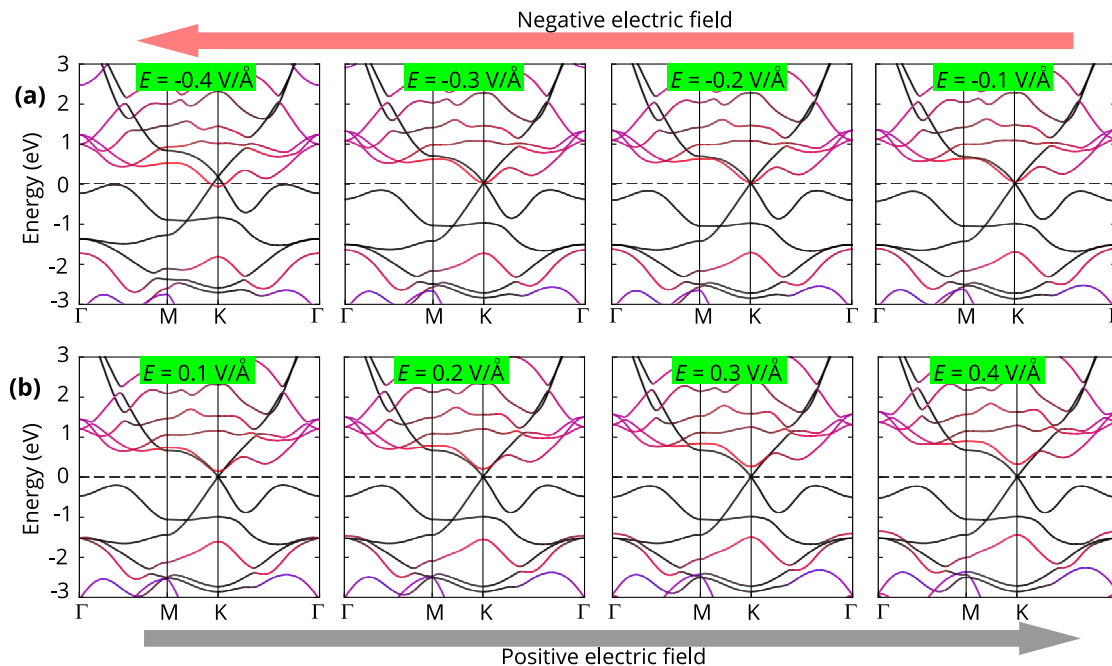
$$T_P = \exp\left(-\frac{4\pi\omega\sqrt{2m_e\Phi}}{\hbar}\right), \quad \rho_t = \frac{2\hbar^2\omega}{3e^2\sqrt{2m_e\Phi}}T_P^{-1},$$

where  $\omega$  and  $\Phi$  represent the tunneling width and barrier height, respectively. Based on the electrostatic potential profile shown in Fig. 6(b),  $\omega \approx 1.37$  Å and  $\Phi \approx 3.06$  eV are obtained, yielding a tunneling probability of  $T_P \approx 9$  % and a tunneling specific resistivity of  $\rho_t \approx 1.82 \times 10^{-9}$  Ω·cm<sup>2</sup>. These results indicate a rel-

atively high tunneling efficiency across the Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> interface. Notably, the obtained  $\rho_t$  value is comparable to those reported for both 3D and 2D (semi-)metal/semiconductor heterostructures<sup>44–47</sup>, demonstrating that the Dirac-FeB<sub>2</sub> layer can serve as an efficient electrode material for electronic device applications.

In practical electronic and optoelectronic devices, the external electric field plays a crucial role in tuning charge transport characteristics, contact resistance, and overall device performance. By modifying the potential landscape at the metal–semiconductor interface, an external field can effectively control carrier injection, Schottky barriers and contact types, thereby offering a powerful means for achieving high-efficiency and low-power device operation<sup>48–50</sup>. To evaluate this effect, we investigated the electronic response of the Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> heterostructure under a perpendicular electric field, as illustrated in Fig. 7(a). The external electric field ( $E$ ) is applied perpendicular to the heterostructure, with its direction defined as positive when pointing from the MoS<sub>2</sub> layer toward the FeB<sub>2</sub> layer. As shown in Fig. 7(b), the Schottky barrier for both electrons ( $\Phi_{SB}^e$ ) and holes ( $\Phi_{SB}^h$ ) exhibit a nearly linear dependence on the applied electric field. A negative

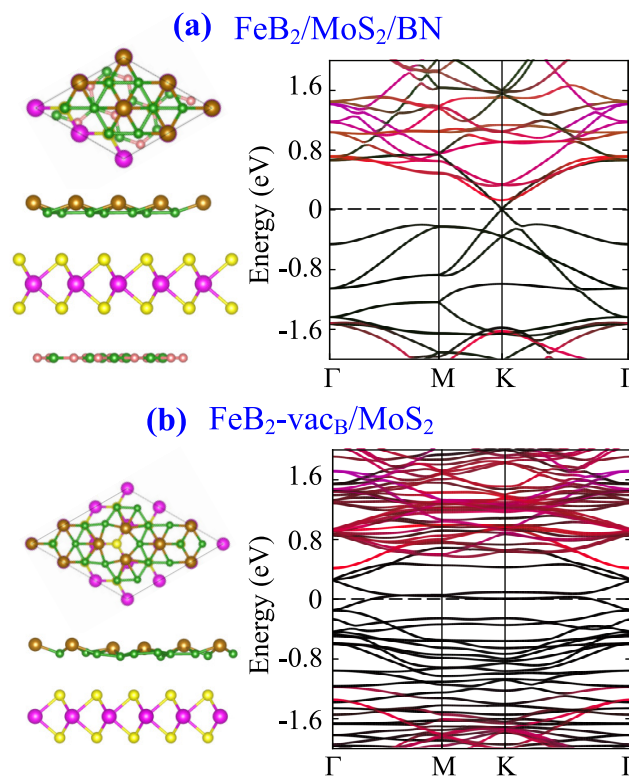




**Fig. 8** The projected band structures of the Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> heterostructure under (a) negative and (b) positive electric fields. The black and red lines represent the contributions of the Dirac-FeB<sub>2</sub> and MoS<sub>2</sub> layers, respectively.

$E$  reduces  $\Phi_{\text{SB}}^e$  while slightly increasing  $\Phi_{\text{SB}}^h$ , indicating enhanced electron injection from FeB<sub>2</sub> into MoS<sub>2</sub>. When the field strength exceeds approximately  $-0.30 \text{ V/\AA}$ , the  $\Phi_{\text{SB}}^e$  becomes negligible, leading to a transition from a Schottky to an Ohmic contact. A similar behavior has been reported by Wang et al.<sup>48</sup>, where an external electric field of about  $0.3 \text{ V/\AA}$  induces a Schottky-to-Ohmic transition in the graphene/GeC heterostructure. In contrast, a positive electric field increases the  $\Phi_{\text{SB}}^e$  and reduces the  $\Phi_{\text{SB}}^h$ . In this case,  $\Phi_{\text{SB}}^e$  remains considerably smaller than  $\Phi_{\text{SB}}^h$ , indicating that the Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> heterostructure retains its  $n$ -type Schottky contact character.

To further elucidate the underlying mechanism of Schottky barrier modulation, we examined the projected band structures of the Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> heterostructure under different electric fields, as illustrated in Fig. 8. Under a negative electric field, the Dirac point of the FeB<sub>2</sub> layer gradually shifts upward relative to the CBM of MoS<sub>2</sub>, resulting in a smaller electron Schottky barrier ( $\Phi_{\text{SB}}^e$ ). This shift facilitates charge transfer from FeB<sub>2</sub> to MoS<sub>2</sub>, promoting efficient electron injection and eventually leading to an Ohmic contact when  $E < -0.30 \text{ V/\AA}$ . At the negative  $E = -0.4 \text{ V/\AA}$ , the CBM of the MoS<sub>2</sub> layer crosses the Fermi level of the Dirac-FeB<sub>2</sub> layer, signifying the transformation from  $n$ -type Schottky contact to the  $n$ -type Ohmic contact. In contrast, under a positive electric field, the Dirac point of FeB<sub>2</sub> moves downward, increasing  $\Phi_{\text{SB}}^e$  and decreasing the hole barrier  $\Phi_{\text{SB}}^h$ . The opposite band bending in this regime suppresses electron tunneling and weakens the interfacial charge transfer. Despite this modulation, the Fermi level remains closer to the MoS<sub>2</sub> CBM than its VBM, confirming that the Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> heterostructure consistently retains its  $n$ -type Schottky contact nature across the entire field range. All these findings demon-



**Fig. 9** Atomic structures and band structures of FeB<sub>2</sub>/MoS<sub>2</sub> heterostructure with the presence of (a) BN substrate and (b) B vacancy ( $\text{vac}_B$ ).



strate that the Schottky barriers and contact types in the Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> heterostructure can be effectively tuned by an external electric field. The field-induced modulation enables a reversible transition between Schottky and Ohmic contacts, allowing precise control over carrier injection and transport characteristics at the interface. Such tunability provides a promising strategy for designing next-generation field-effect transistors, Schottky diodes, and other nanoelectronic or optoelectronic devices based on the Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> heterostructures with high efficiency and low contact resistance.

In practical device configurations, metal–semiconductor heterostructures are typically supported on a substrate and may also contain intrinsic defects at the interface. Therefore, to assess the robustness of the contact behavior, we further examine the influence of a representative hexagonal BN substrate as well as vacancy defects on the FeB<sub>2</sub>/MoS<sub>2</sub> heterostructure. The atomic structures and band structures of these configurations are depicted in Fig. 9. Our results show that the presence of a BN substrate gives rise to a slight reduction in  $\Phi_{\text{SB}}^e$  to 0.120 eV, while the presence of a B vacancy defect leads to an increase in  $\Phi_{\text{SB}}^e$  to 0.382 eV. These findings indicate that the contact characteristics are relatively robust against substrate effects, whereas defects can significantly modify the Schottky barrier through the introduction of localized states and altered charge transfer at the interface.

## 4 Conclusions

In this work, we have explored the structural, electronic, and interfacial properties of the Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> vdW heterostructure using first-principles calculations. The FeB<sub>2</sub> monolayer exhibits a stable planar hexacoordinate structure with a Dirac-like metallic nature, which is well preserved upon stacking with semiconducting MoS<sub>2</sub>. The Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> heterostructure is energetically, mechanically, thermally and dynamically stable and forms an n-type Schottky contact with a small electron barrier height and high tunneling probability, facilitating efficient carrier injection across the interface. Furthermore, the external electric field provides an efficient way to modulate the Schottky barrier and contact type. A negative field reduces the electron barrier and induces an Ohmic contact, whereas a positive field increases it while preserving the n-type character. These results highlight the Dirac-FeB<sub>2</sub>/MoS<sub>2</sub> heterostructure as a promising candidate for next-generation tunable, low-resistance, and high-efficiency 2D electronic and optoelectronic devices.

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**\* Data Availability Statement**

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

