

Designing one-dimensional well-isolated flat bands in untwisted bilayer black phosphorus by asymmetric uniaxial strain

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One-dimensional (1D) flat bands in low-dimensional materials enable the study of exotic correlated phases like bond density waves, Luttinger liquids, and Mott insulators. However, the underlying mechanisms driving their formation remain elusive, and achieving well-isolated 1D flat bands in readily achievable systems remains a significant challenge. Here we present a versatile method for engineering tunable 1D flat bands in untwisted bilayer black phosphorus using asymmetric uniaxial strain to achieve differential strain in each layer. Our first-principles calculations reveal that both the highly anisotropic stacking pattern effect and the anisotropic intralayer orbital hybridization between moiré impurities (i.e., local stacking configurations) play critical roles in the formation of 1D flat bands. Notably, asymmetric armchair strain can generate 1D well-isolated flat bands at experimentally accessible strains owing to its pronounced stacking pattern effect. This configuration provides an opportunity to directly observe 1D flat band dispersion using angle-resolved photoemission spectroscopy. Furthermore, we demonstrate that transitioning from 1D to 2D flat bands is possible by applying asymmetric biaxial strain. Our work establishes asymmetric strain as a powerful tool for engineering flat bands in bilayer systems and opens new avenues for exploring 1D strongly correlated electron systems.

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I. INTRODUCTION

In the field of low-dimensional materials research, the study of two-dimensional (2D) and one-dimensional (1D) flat-band physics has become a significant direction [1–3]. The wave functions of 2D flat bands exhibit localization characteristics in all directions in real space, significantly restricting the kinetic energy of electrons. This restriction enhances the correlation interactions between electrons, which play a crucial role in various exotic quantum states, such as superconductivity [4–7], correlated insulators [4–6], ferromagnetism [8], fragile topology [9–11], and Chern insulators [12]. Creating moiré superlattices by twisting small angles is one method to produce 2D flat bands. Typical systems include twisted bilayer graphene [4,5], twisted bilayer transition metal dichalcogenides (TMDCs) [13–16], and twisted bilayer hexagonal boron nitride (h-BN) [17,18]. Unlike 2D flat bands, 1D flat bands possess tiny band dispersion only in one direction, while maintaining strong band dispersion in other directions. Correspondingly, their wave functions are

localized in one direction and delocalized in others. Consequently, such 1D flat bands exhibit different electron correlation characteristics from 2D flat bands [19–21]. Systems with 1D flat bands can demonstrate exotic phenomena like bond density waves, Luttinger liquids, and Mott insulators, and they can host Ising and Kosterlitz–Thouless quantum phase transitions, providing an ideal platform for studying 1D quantum systems [22–25]. In the twisted moiré structures, the formation of 2D flat bands can be attributed to the magic angle mechanism [26–29] or stacking pattern mechanism [17,30,31]. However, the driving force of 1D flat bands is not well understood.

An *isolated* flat band refers to a single, well-separated flat band near the Fermi level, distinctly detached from adjacent bands by a finite energy gap [Fig. 1(a)]. In contrast, an *entangled* flat band comprises multiple energetically proximate flat bands that are intertwined with each other, making it difficult to distinguish them individually, even though the group may still be separated from other bands by energy gaps [Fig. 1(b)]. In monolayer lattices such as Kagome [32–34], Lieb lattices [35–37], or coloring-triangle lattices [38,39], the formation of 2D entangled flat (often nontrivial) bands typically rely on special lattice symmetries and interference effects [40,41]. In some specific models (e.g., interlocking-circles lattices), the 2D isolated flat bands can emerge from constructive interference patterns [42]. For bilayers, theoretical predictions suggest that small-angle twisting in the bilayer black phosphorus (t-BP) or GeSe can achieve 1D isolated flat bands along

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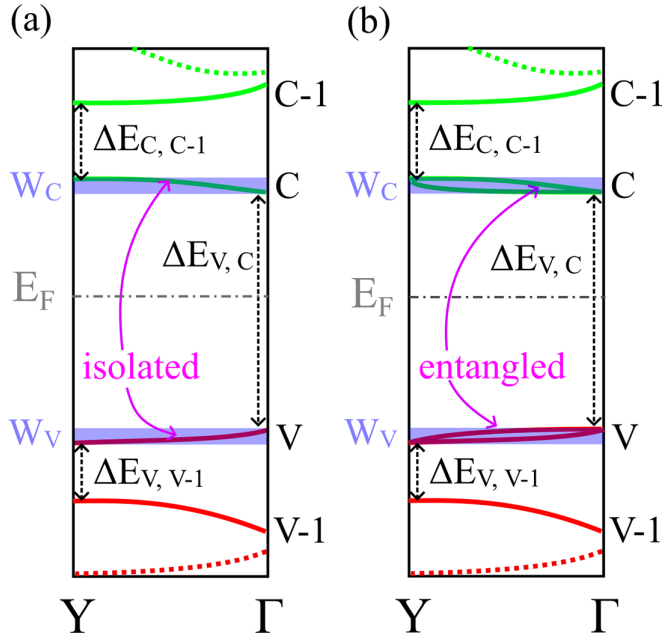


FIG. 1. Comparison between isolated and entangled flat bands. (a) An isolated flat band is a single, well-separated flat band near the Fermi level, clearly detached from adjacent bands by a finite energy gap. (b) An entangled flat band consists of multiple energetically close and intertwined flat bands, which are difficult to distinguish individually, although the group may still be isolated from other bands by energy gaps. The blue shaded region highlights the location of the flat band, with its vertical extent representing the bandwidth W_V or W_C of the flat band in the HVB or LCB, respectively. $\Delta E_{V,C}$ denotes the band gap, while $\Delta E_{V,V-1}$ ($\Delta E_{C,C-1}$) represents the energy separations between the flat band V (C) and its adjacent band V-1 (C-1). E_F indicates the Fermi level.

the zigzag direction [22,43,44]. However, the isolated energy of such flat bands (defined as the smallest energy separation between the flat band μ and its nearest band ν , denoted as $\Delta E_{\mu,\nu}$) corresponding to the highest valence band (HVB) is relatively small (<5 meV). Specifically, $\Delta E_{V,V-1}$ refers to the energy gap between the highest valence band (V, i.e., HVB) and the second-highest valence band (V-1), while $\Delta E_{C,C-1}$ represents the energy gap between the lowest conduction band (C, i.e., LCB) and the second-lowest conduction band (C-1), as illustrated in Fig. 1(a). Moreover, achieving 1D isolated flat bands along the armchair direction in these systems is more difficult because of the strong band dispersion in this direction, which might require extremely small twist angles, posing experimental challenges. Although the 1D isolated flat band signals might be indirectly detected through electron transport [4–6] or tunneling spectroscopy [45–49], the small $\Delta E_{\mu,\nu}$ (which refers to $\Delta E_{V,V-1}$ and $\Delta E_{C,C-1}$ and will be used consistently throughout unless specified otherwise) makes it challenging to directly observe their dispersion features in momentum space due to the energy resolution limit (generally greater than 34 meV) of nanoARPES [50]. Therefore, effectively increasing the $\Delta E_{\mu,\nu}$ values in a bilayer system using a simple approach is crucial for achieving 1D flat bands that are well isolated near the Fermi level. Such a design confers several key advantages, including enhanced feasibility

for direct experimental observation, simplified electrostatic gating, and effective suppression of interference from adjacent bands, which collectively constitute essential prerequisites for a wide range of advanced applications [51,52].

Moiré superlattices can be achieved not only by twisting but also through lattice mismatch [53] or external periodic strain [54]. However, the resulting 1D flat bands—whether narrowly isolated or entangled—typically require complex and technically demanding fabrication processes. Besides, asymmetric strain methods (heterostrain) [55–62] can be easily utilized to create 1D or 2D moiré superlattices by inducing lattice mismatch through controlled strain magnitudes and directions in each layer. This method enables tunable moiré patterns, enhanced flat band formation, and broad material compatibility, making it a promising alternative to twist-induced strategies for exploring novel electronic phenomena. A detailed comparison with other methods is provided in Table S1 of the Supplemental Material [63]. In 2023, Efthimios Kaxiras *et al.* investigated the 1D moiré physics and chemistry in heterostrained bilayer graphene, demonstrating that uniaxial zigzag heterostrain can induce 1D isolated flat electronic bands around the Fermi level. However, these 1D flat bands are entangled and exhibit only narrowly isolated energy gaps [60]. The emergence of entangled flat bands in twisted bilayer graphene is likely related to electronic interference effects [26–29]. In contrast, many 2D semiconductor materials exhibit significant stacking effects [17,30,31], making them more prone to forming 1D isolated flat bands under asymmetric strain. This is particularly true for black phosphorus-like systems, which are strongly anisotropic semiconductors. The 1D isolated flat band physics in such materials under asymmetric strain is especially important and warrants urgent exploration, as it may enable the realization of strained bilayer black phosphorus (BP) with large $\Delta E_{\mu,\nu}$, along with a distinct underlying mechanism.

In this study, we delve into the potential of utilizing small asymmetric armchair/zigzag strain in bilayer systems, exemplified by bilayer BP, to achieve tunable 1D moiré superlattices and associated 1D well-isolated flat bands. We demonstrate that the formation of 1D isolated flat bands results from a delicate interplay between the highly anisotropic stacking pattern effect (i.e., band-edge differences along two directions) and the direction-dependent intralayer orbital hybridization interactions between moiré impurities. Compared to the asymmetric zigzag strain (AZS) bilayer BP, the asymmetric armchair strain (AAS) bilayer BP exhibits the remarkable ability to induce 1D well-isolated flat bands with a relatively small strain ranging from 3% to 5%, due to its distinctive stacking pattern effect. Our findings indicate that AAS bilayer BP could potentially enable the direct observation of 1D flat band dispersion using nanoARPES, positioning it as an ideal platform for realizing 1D strongly correlated systems and providing a promising avenue for experimental verification. On the other hand, by manipulating asymmetric biaxial strain (ABS), transitions between 1D and 2D flat bands can be realized. Beyond the specific case of strained bilayer BP, this work envisions the potential of this mechanical approach to broaden the horizons of low-dimensional flat-band physics in other bilayer 2D materials with strong stacking pattern effect. Hence, our research endeavors to provide novel

insights and applications for 1D well-isolated flat band phenomena in 2D materials, ultimately propelling advancements in this burgeoning field.

II. COMPUTATIONAL METHODS

A. Density functional theory computational details

First-principles calculations based on density functional theory (DFT) were employed to investigate the structural optimization and electronic properties of the small bilayer BP systems, including four high-symmetry stacking patterns and 5% AAS bilayer BP. The projector augmented-wave method [64] was implemented within the plane-wave-based Vienna *Ab initio* Simulation Package (VASP) [65,66] to handle the electron-ion interactions. The vdW interactions between layers were accounted for using the semiempirical D3 method [67]. The exchange-correlation energy of electrons was treated within the generalized gradient approximation using the Perdew-Burke-Ernzerhof functional [68]. The plane-wave cutoff energy was set to 500 eV. To efficiently model the geometric structures of large moiré superlattices, we leveraged VASP's built-in machine learning (ML) capabilities. VASP employs on-the-fly machine learning [69–71] using Bayesian linear regression [70] to dynamically fit force field parameters during *ab initio* molecular dynamics (AIMD) simulations, reducing computational costs compared to traditional AIMD methods while maintaining prediction accuracy. In AIMD simulations, a time step of 2 fs was employed with a Langevin thermostat [72,73] for constant temperature control (NVT ensemble). The training utilized 10 000 steps with a self-consistent field (SCF) energy convergence criterion of 10^{-5} eV. The efficacy of the ML approach is exemplified by the case of the 5% AAS bilayer BP moiré superstructure. Based on ML predictions, the maximum error in atomic positions compared to full DFT calculations is a mere 0.03 Å for the z coordinate, with negligible errors in the x and y coordinates. This translates to a band-gap error of only 0.04 eV (Fig. S1 of the Supplemental Material [63]). A comparative analysis of VASP and RESCU [74] calculations can be found in the Note S1 of the Supplemental Material [63].

To investigate the electronic structure properties of large moiré superlattices, we employed the RESCU software package [74]. RESCU utilizes the Chebyshev filtering technique [75] for efficient eigenvalue problem solutions. This technique enables parallel computing, making RESCU well suited for handling the demanding calculations associated with large-scale electronic structures. The study focuses on 1D moiré superlattices with pronounced anisotropy in lattice constants along the x and y directions. For large moiré periods larger than 49 Å, calculations were performed using a single k -point to sample the moiré Brillouin zone. For shorter moiré periods of 3.3 and 4.6 Å, a denser k -point mesh of 12 points was adopted, corresponding to a sampling density of approximately $0.03 \times 2\pi/\text{Å}$. Optimized norm-conserving Vanderbilt pseudopotentials [76] were employed to represent the electron-ion interactions efficiently. Kohn-Sham states were described using a double- ζ plus polarization function basis set, balancing accuracy and computational cost well. The real-space grid resolution was set to 0.30 bohr for optimal

convergence. To accelerate the SCF calculations, a wave-function mixing coefficient of 0.05 was used.

B. Relationship between 1D moiré superlattice length and uniaxial strain

Moiré superlattices typically arise from lattice mismatch and/or relative rotation between two stacked monolayer 2D materials [77], although more complex multilayer configurations are also possible [78,79]. We obtained a generalized expression that describes the relationship between the moiré wavelength and the twist angle, lattice mismatch, and atomic lattice constants for orthorhombic systems. Specifically, for bilayer orthorhombic lattices, the moiré wavelength λ_x and λ_y are given by the following generalized formulas (the derivation can be found in Note S2 of the Supplemental Material):

$$\lambda_x = \frac{(1 + \delta_x)a_{x1}}{\sqrt{(1 + \delta_x - \cos\phi)^2 + \sin^2\phi}}, \quad (1)$$

$$\lambda_y = \frac{(1 + \delta_y)b_{y1}}{\sqrt{(1 + \delta_y - \cos\phi)^2 + \sin^2\phi}}, \quad (2)$$

where δ_x and δ_y represent the lattice mismatch between the top and bottom atomic layers along the x and y directions, respectively. a_{x1} and b_{y1} denote the lattice constants of the unstrained atomic unit cell in the x and y directions, respectively. Note that the x and y directions are orthogonal.

When the atomic lattices of the top and bottom layers exhibit lattice mismatch along the x direction but are matched along the y direction, a 1D moiré structure forms along the x axis. According to Eqs. (1) and (2), the moiré wavelength in the x and y directions are given by (the derivation can be found in Note S2 of the Supplemental Material):

$$\lambda_x = \frac{(1 + \delta_x)a_{x1}}{\delta_x}, \quad (3)$$

$$\lambda_y = b_{y1}. \quad (4)$$

III. RESULTS AND DISCUSSIONS

A. Structural models

Figure 2 illustrates the schematic construction and device model of a 1D moiré superlattice induced by asymmetric uniaxial strain. Figure 2(a) displays the top layer of the bilayer BP that remains largely unaffected by the substrate strain due to the interlayer vdW interaction between the top and the bottom layers of BP. The top layer consists of an unstrained atomic lattice with lattice constants a_{x1} and b_{y1} , which is periodically extended along the x direction by a factor of m_1 to form a supercell with a length of $\lambda_{x1} = m_1 a_{x1}$. Figure 2(b) shows the bottom layer of the bilayer BP that is in direct contact with the substrate, which is significantly modulated by the applied substrate strain. The bottom layer is subjected to uniaxial tensile strain along the x direction, resulting in modified lattice constants a_{x2} , and a corresponding supercell length $\lambda_{x2} = m_2 a_{x2}$. The asymmetric lattice mismatch is introduced through the strain, defined as $\delta_x = (a_{x2} - a_{x1})/a_{x1}$, while $\delta_y = 0$, since $b_{y1} = b_{y2}$. When the supercells of the above two layers are stacked with matched periodicities along the x direction, a commensurate 1D moiré superlattice is

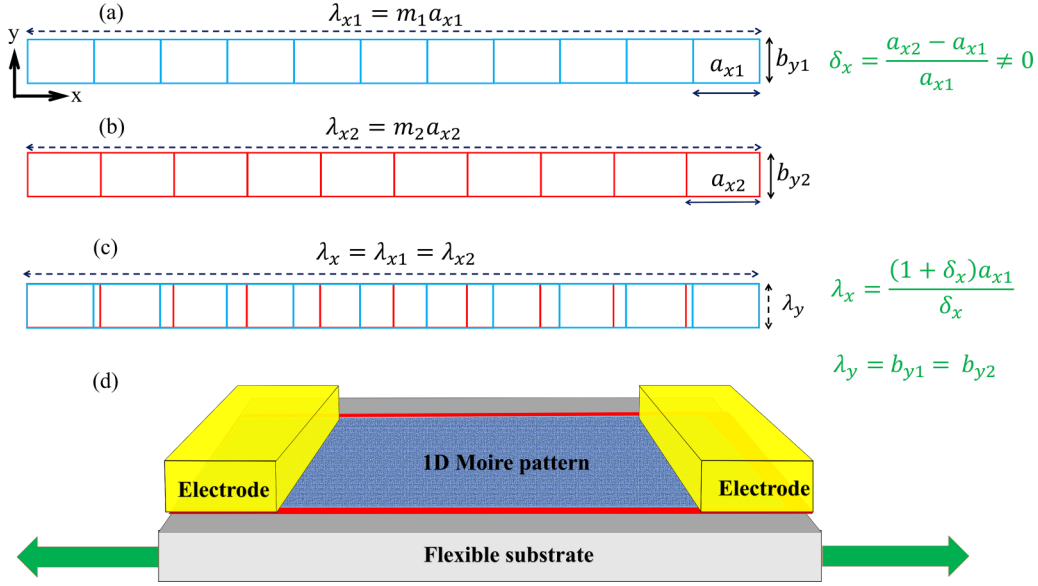


FIG. 2. Schematic and device model of a 1D moiré superlattice induced by asymmetric uniaxial strain. (a) Top-layer unit cell with atomic lattice constants a_{x1} and b_{y1} , periodically extended along the x direction by a factor of m_1 to form a supercell of length $\lambda_{x1} = m_1 a_{x1}$. (b) Bottom-layer unit cell subjected to uniaxial tensile strain along the x direction, resulting in new atomic lattice constants a_{x2} and b_{y2} and a corresponding supercell length $\lambda_{x2} = m_2 a_{x2}$. The lattice mismatch by asymmetric uniaxial strain is defined as $\delta_x = (a_{x2} - a_{x1})/a_{x1}$ and $\delta_y = 0$. m_1 and m_2 are positive integers. (c) One-dimensional bilayer moiré superlattice formed by stacking the unstrained top and strained bottom supercells with matched periodicities, resulting in a commensurate configuration. The moiré wavelength along x and y directions are given by $\lambda_x = (1 + \delta_x)a_{x1}/\delta_x$ and $\lambda_y = b_{y1} = b_{y2}$. (d) Device model showing the bilayer BP moiré structure placed on a flexible substrate beneath two electrodes. Green arrows indicate the direction of applied strain.

formed [Fig. 2(c)]. The resulting moiré wavelength are given by $\lambda_x = (1 + \delta_x)a_{x1}/\delta_x$ and $\lambda_y = b_{y1} = b_{y2}$. Figure 2(d) illustrates the layout of the asymmetrically contacted bilayer BP device and the strategy for applying uniaxial strain. The device configuration allows for the application of strain in a specific direction, enabling the formation of 1D moiré superlattices along the desired axis.

This study primarily focuses on two types of asymmetric uniaxial layer strains along high-symmetry directions: AAS and AZS. This approach can also be extended to apply ABS, including equal or unequal strain intensities, providing further control over the moiré patterns and their associated electronic properties. Considering the limitations of experimentally achievable maximum strain ($\sim 10\%$) and computational cost constraints, we mainly explore uniaxial strain magnitudes of 1.10%, 1.81%, 2.857%, and 5.00%.

B. Electronic structures of AAS and AZS bilayer BP

Applying AAS to bilayer BP exhibits a fascinating interplay between strain intensity and electronic band structure. Our calculations reveal that small strains (up to 5%) in AAS bilayer BP have a minimal impact on the band gap, which consistently remains around 0.50 eV (Fig. 3). Notably, along the Γ -Y (armchair or y) direction, both the HVB and the LCB exhibit the character of flat bands (Fig. 3). However, significant band dispersion persists along the Γ -X (zigzag or x) direction. Table I summarizes the structural information and key physical properties of AAS bilayer BP under various strain conditions. These properties include bandwidth (W_C and W_V) and isolated energy ($\Delta E_{C,C-1}$ and $\Delta E_{V,V-1}$) of the LCB

and HVB flat bands. In the strain range of 1.00% to 5.00%, both LCB and HVB exhibit narrow bandwidth ranging from 0 to 4 meV. Interestingly, when the strain is increased to 10%, W_C expands to 40 meV, while W_V remains narrow at 4 meV. We further analyzed the variation of $\Delta E_{C,C-1}$ and $\Delta E_{V,V-1}$ with the strains. Within the 1.0% to 5.0% strain range, the average $\Delta E_{C,C-1}$ and $\Delta E_{V,V-1}$ is approximately 160 and 56 meV, respectively. In the LCB, $\Delta E_{C,C-1}$ exhibits an increasing trend from 1.1% to 2.857% strain, followed by a decrease at 5% and 10%. For the HVB, a minimum occurs at 1.81%, after which $\Delta E_{V,V-1}$ rises with further strain. We

TABLE I. Structural information and physical parameters for bilayer BP in the AAS configuration under various uniaxial strains. λ_Z and λ_A denote the moiré superlattice constants along the zigzag and armchair directions, respectively. N indicates the total number of atoms within the moiré superlattice unit cell. W_C and W_V represents the bandwidth of the LCB or HVB in the armchair direction. $\Delta E_{C,C-1}$ and $\Delta E_{V,V-1}$ represent the isolated energy of the LCB or HVB flat bands.

Armchair strain	1.10%	1.81%	2.857%	5.00%	10.00%
λ_Z (Å)	3.30	3.30	3.30	3.30	3.30
λ_A (Å)	415.04	252.63	162.41	94.73	49.62
N	732	444	284	164	84
W_C (meV)	0	0	0	2	40
W_V (meV)	0	0	1	4	4
$\Delta E_{C,C-1}$ (meV)	120	150	200	180	130
$\Delta E_{V,V-1}$ (meV)	40	25	60	100	200

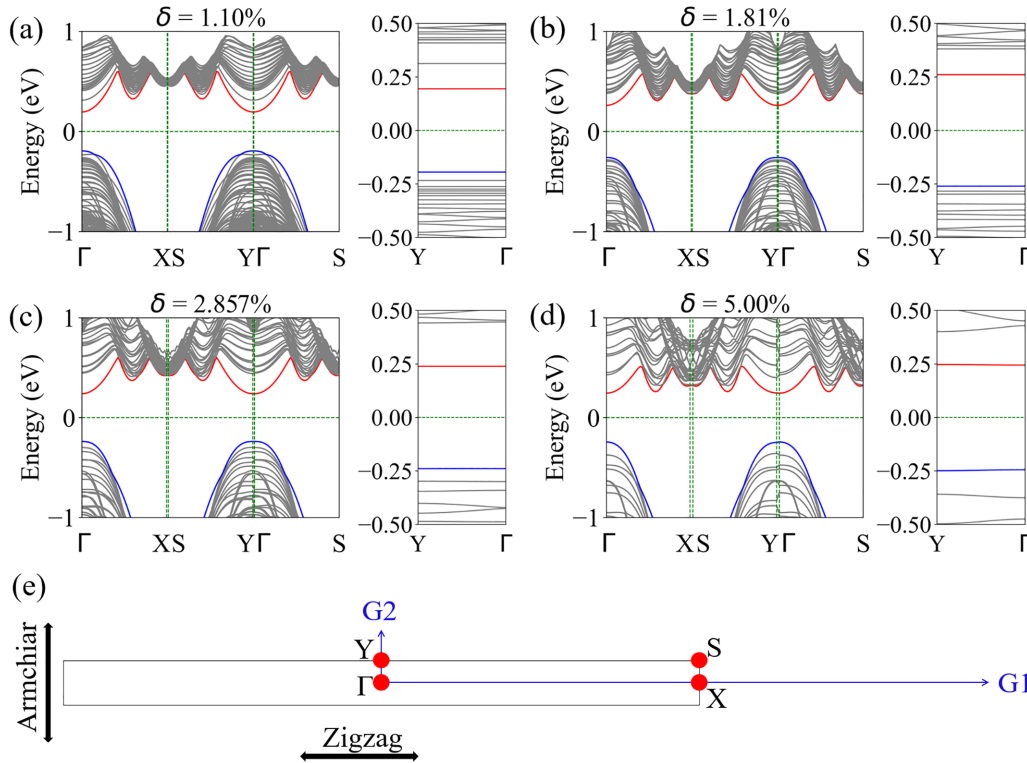


FIG. 3. Band structures in AAS bilayer BP with uniaxial strain magnitudes of (a) 1.10%, (b) 1.81%, (c) 2.857%, and (d) 5.00%. (e) Brillouin zone of AAS bilayer BP and high-symmetry k -points. To enhance clarity, the highest valence band and the lowest conduction band are highlighted in blue and red, respectively. The Fermi level is set at zero. To better visualize the flat band characteristics, the band structure along the Y- Γ direction is presented separately.

attribute the observed nonmonotonic behavior of $\Delta E_{C,C-1}$ and $\Delta E_{V,V-1}$ to the competition between two effects induced by tensile strain: the energy mismatch between layers (E_{diff}) and the orbital spillover effect (η_{orb}), which are discussed in detail later. Notably, under 5% strain conditions, the $\Delta E_{C,C-1}$ and $\Delta E_{V,V-1}$ values for LCB and HVB flat bands reach 180 and 100 meV, respectively [Fig. 3(d)]. These values fall within the energy resolution limits of nanoARPES [50], a powerful technique for probing band structures. These findings suggest the direct detectability of HVB and LCB flat bands using nanoARPES in the range of 2.857 to 5% strain.

Analogously to the AAS bilayer BP, our study reveals the emergence of a 1D moiré superlattice in the zigzag direction within the AZS configuration of bilayer BP when subjected to small strains. This 1D moiré pattern leads to the emergence of flat bands at the HVB and LCB along the Γ -X (zigzag) direction of the Brillouin zone. Notably, within the investigated strain range of 1.0% to 5.0%, both flat bands exhibit zero bandwidth, indicating complete dispersionless character. The corresponding average $\Delta E_{C,C-1}$ and $\Delta E_{V,V-1}$ lies around 7 and 25 meV, with a maximum $\Delta E_{C,C-1}$ reaching 32 meV for the LCB at a strain of 2.857% (Table S2 and Fig. S2 of the Supplemental Material [63]). These relatively low $\Delta E_{C,C-1}$ and $\Delta E_{V,V-1}$ values suggest that directly observing the dispersion of these flat bands in nanoARPES experiments [50] under small strain conditions for the AZS superlattices would be challenging. However, the existence of these flat bands might be measured indirectly with characterization techniques such as electron transport [4–6] or tunneling spectroscopy

[45–49]. The above findings demonstrate that the AAS bilayer BP exhibits a greater propensity for generating 1D flat bands with larger $\Delta E_{C,C-1}$ and $\Delta E_{V,V-1}$ values compared to the AZS bilayer BP, which will be explained later.

Compared to 2D flat bands in twisted moiré superlattices, 1D flat bands in untwisted and strained moiré superlattices exhibit a simpler variety of local stacking pattern types. In the AAS bilayer BP, two primary stacking patterns dominate, including the AA'-like and AB-like stacking patterns (highlighted in gray in Fig. 4). The charge density distribution of the CBM and VBM at the Γ point in this superlattice primarily resides in different regions characterized by AA'-like and AB-like stacking patterns (herein, the two like structures are like AB and AA' stacking patterns but with strain-induced deviation) in real space, respectively. Moreover, those regions with a specific stacking pattern are spatially separated.

Now, we mainly analyze the charge density distribution of the CBM and VBM at the Γ point for the AAS configuration of bilayer BP under 5%. Some key features are revealed as follows. The charge density exhibits extended features along the x (zigzag) direction for CBM [Fig. 4(a)] and VBM [Fig. 4(c)]. Conversely, they show localized features along the y (armchair) direction [Figs. 4(a) and 4(c)]. This anisotropic distribution of charge density reflects the underlying nature of the 1D flat bands. Moreover, the charge density distribution extends across both layers and into the vdW gap [Figs. 4(b) and 4(d)], indicating significant interlayer orbital hybridization for local stacking patterns. The interlayer distance varies for different stacking patterns. The AA'-like configuration

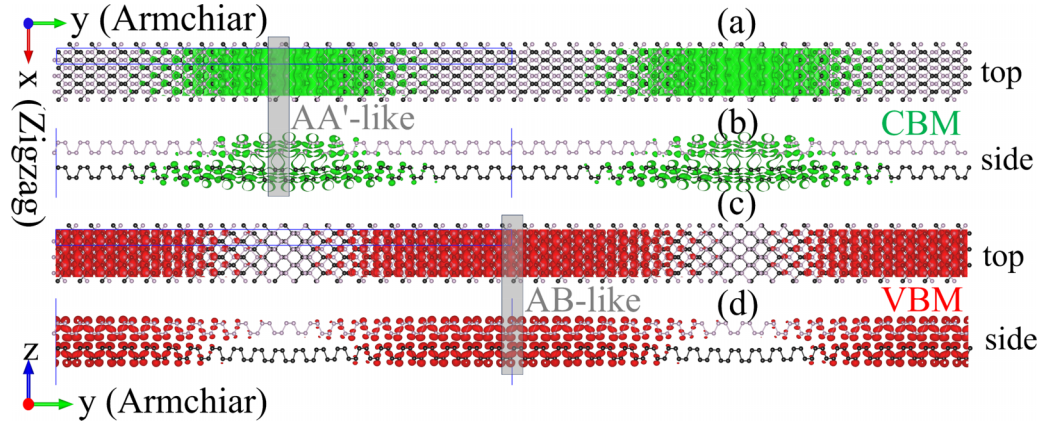


FIG. 4. Charge density distribution of the CBM [(a) and (b)] and VBM [(c) and (d)] at the Γ point in AAS bilayer BP under 5% strain. The gray shaded areas represent local high-symmetry stacking patterns of type AA'-like and type AB-like. Panels (a) and (c) show the top view of the charge density, while panels (b) and (d) show the side view. The isosurface value is set at $1.5 \times 10^{-9} \text{ e}\text{\AA}^{-3}$.

exhibits the largest interlayer spacing, approximately $3.78 \text{ \AA}$, compared to $3.18 \text{ \AA}$ for the AB-like configuration [Fig. 5(a)]. For the AZS configuration of bilayer BP, the emergence of 1D flat bands along the zigzag direction is a notable feature. We also analyzed the charge density distribution of the CBM and VBM at the Γ point (Fig. S3 of the Supplemental Material [63]). It reveals a striking correspondence with the AA-like and AB-like stacking patterns, respectively. The charge density of the CBM and VBM displays localized characteristics along the x (zigzag) direction and delocalized features along the y (armchair) direction. The interlayer distance is largest for the AA-like stacking pattern, approximately $3.50 \text{ \AA}$, while for the AB-like stacking pattern, it is around $3.18 \text{ \AA}$ [Fig. 5(b)].

Overall, our study shows that in AAS and AZS bilayer BP, interlayer stacking configurations and strain critically influence the electronic structure and the emergence of 1D flat bands. Specifically, variations in interlayer orbital

hybridization under different stacking patterns affect band-edge ordering and energy band dispersion. These findings highlight the importance of the stacking pattern effect and strain effect in tuning the properties of 1D flat bands. To deepen our understanding of how these factors impact the formation and characteristics of these bands, we will further discuss the band-edge ordering for various local stacking configurations (i.e., stacking pattern effect without strain) and the strain effect on the formation of the 1D isolated flat bands in AAS and AZS bilayer BP.

C. Formation and isolation of 1D flat bands: Role of stacking and strain effects

First, the stacking pattern effect without strain is crucial in determining the formation (narrow bandwidth) of flat bands and which stacking pattern is located at the band edge of the moiré superlattice. The energy differences at the band edges relative to the stacking pattern effect can create an energy barrier (or a potential well) that confines the states within the moiré superlattice. This phenomenon, akin to introducing “moiré impurities” (local stacking configuration), can potentially lead to the formation of isolated 2D flat bands within the band gap of isotropic hexagonal systems such as h-BN and TMDCs [13–18,31]. Although the BP system we investigated is anisotropic, the formation of 1D flat bands can still be attributed to interlayer stacking pattern effects, with a strong emphasis on the directional nature of the system. We can use the VBM of AAS bilayer BP as a case study to elucidate the formation mechanism of its 1D flat bands.

In the armchair direction of AAS bilayer BP, there are two stacking patterns: AB-like and AA'-like. The local environment alternates between AB-like and AA'-like along the y (armchair) direction. However, along the x (zigzag) direction, the configuration is uniformly AB-like or AA'-like depending on the y coordinate, showing no such alternation. Bilayer BP have four stacking configurations: AA, AB, AB', and AA' [Fig. 6(a)]. All of them are semiconductors with direct band gaps (Fig. S4). The AB stacking has a higher energy at the VBM [Fig. 6(b)] than AA' stacking, making AB-like more likely to appear at the VBM of moiré superlattice. Due to an

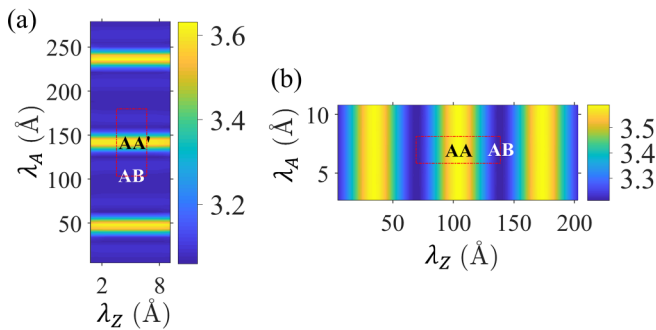


FIG. 5. (a) Contour plot of interlayer vertical distances in a 1D Moiré lattice formed under 5% asymmetric armchair strain. (b) Contour plot of interlayer vertical distances in a 1D Moiré lattice formed under 5% asymmetric uniaxial strain in the zigzag direction. In the figures, λ_Z and λ_A represent the Moiré lattice length along the zigzag and armchair directions, respectively. The red boxes indicate the size of the Moiré lattice unit cell. The ratio of the Moiré lattice lengths in the two directions, λ_Z/λ_A , does not correspond to the aspect ratio of the images. For better viewing, the short edges of figures (a) and (b) have been enlarged. The highly symmetrical stacking structures in the Moiré lattice are marked in the figures.

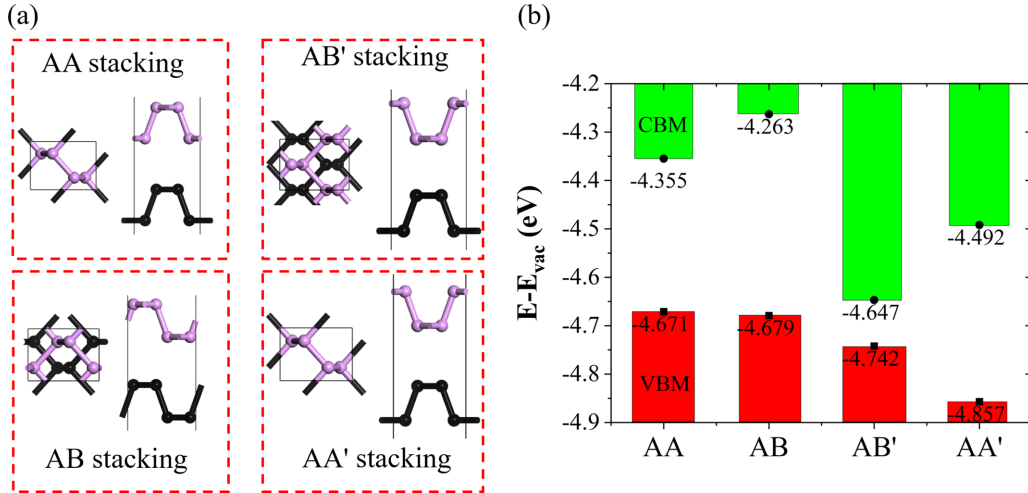


FIG. 6. (a) Schematic illustrations of four high-symmetry stacking configurations of bilayer black phosphorus. (b) Band-edge ordering (relative to the vacuum level) of VBM and CBM for the four high-symmetry stacking patterns of bilayer BP.

energy difference (ΔE) of 0.18 eV at the band edge between the AB and AA' stacking patterns [Fig. 6(b)] and a relatively long moiré lattice length of about 100 Å along the y (armchair) direction, the wave function at the VBM corresponding to the AB-like configuration exhibits localization along the y direction [Fig. 4(c)]. However, along the x (zigzag) direction, there is no energy barrier to suppress its wave function, so its wave function remains delocalized. Consequently, the highly anisotropic interlayer stacking pattern effect—with regions exhibiting both negligible and pronounced ΔE —together with the strain-tunable and direction-dependent intralayer orbital hybridization between moiré impurities, characterized by a small moiré periodicity λ_z and a large λ_A along orthogonal directions, collectively facilitates the formation of 1D flat bands with narrow bandwidth in AAS bilayer BP.

Second, small asymmetric uniaxial layer strain is tunable for the stacking pattern effect and then modifies the isolated energy of the 1D flat band in the moiré superlattice. This external strain exerts a dual influence on the stacking pattern effect [Fig. 7(a)]. It increases the atomic orbital energy difference between the upper and lower BP layers (E_{diff}), analogously to modifying on-site energies, thereby weakening the interlayer quasibonding (QB) interaction [Fig. 7(a)]. Concurrently, asymmetric strain enhances the out-of-plane orbital delocalization (e.g., p_z orbitals) in the strained (red) top layer—a phenomenon referred to as the orbital spillover effect—which is characterized by $\eta_{\text{orb}}^{\text{II}}$ and $\eta_{\text{orb}}^{\text{I}}$ for stacking configurations II and I, respectively. This orbital spillover effect is proportional to $E_{\text{QB}}^{\text{II}}$ and E_{QB}^{I} , which represent the VBM shifts from monolayer to bilayer induced by the QB interactions in stacking II and I, respectively [Fig. 7(a)]. Thus, based on the nondegenerate two-orbital interaction model [80], the band-edge difference (ΔE) between stacking configurations II and I in this case arises from the nonlinear modulation of interlayer QB interactions as well as the orbital energy mismatch between layers. ΔE can be approximated as

$$\Delta E \approx \frac{(E_{\text{QB}}^{\text{II}})^2 - (E_{\text{QB}}^{\text{I}})^2}{E_{\text{diff}}} = \frac{(\Delta E_{\text{QB}})^2}{E_{\text{diff}}} \quad (5)$$

where $(\Delta E_{\text{QB}})^2$ is used as a shorthand for $(E_{\text{QB}}^{\text{II}})^2 - (E_{\text{QB}}^{\text{I}})^2$ for simplicity, and $\Delta E_{\text{QB}} \ll E_{\text{diff}}$.

For comparison, Fig. 7(b) shows the stacking pattern effect in the absence of strain. The atomic orbital energy difference between the upper and lower BP layers (E_{diff}) is zero. In this degenerate two-orbital interaction model [80], the band-edge difference ΔE is attributed solely to the difference in interlayer QB interactions between stacking configurations II and I and is expressed as

$$\Delta E \approx E_{\text{QB}}^{\text{II}} - E_{\text{QB}}^{\text{I}}. \quad (6)$$

The interplay between E_{diff} and $(\Delta E_{\text{QB}})^2$ can reduce and enhance the ΔE [see Eq. (5)], respectively, thereby modulating the values of $\Delta E_{C,C-1}$ and $\Delta E_{V,V-1}$ in the moiré superlattice. We next provide a qualitative explanation of how this competition shapes the $\Delta E_{V,V-1}$ and $\Delta E_{C,C-1}$. For the LCB, within the 1.10–2.857% range, we have shown that $\Delta E_{C,C-1}$ increases with the strain (see Table I), which can be explained by that the increase in $(\Delta E_{\text{QB}})^2$ outweighs that of E_{diff} . As the strain increases beyond this range but remains below 5%, the increase in E_{diff} dominates over that of $(\Delta E_{\text{QB}})^2$, leading to a slight decrease in $\Delta E_{C,C-1}$ (see Table I). For the HVB, in the low-strain regime (ranging from 1.1% to $\sim 1.81\%$), the increase in E_{diff} dominates over that of $(\Delta E_{\text{QB}})^2$, leading to a decrease in $\Delta E_{V,V-1}$ (see Table I). As strain exceeds this range, the growth of $(\Delta E_{\text{QB}})^2$ becomes dominant, resulting in a subsequent increase in $\Delta E_{V,V-1}$ (see Table I). The pronounced increase in $(\Delta E_{\text{QB}})^2$ with increasing strain is evidenced by the charge density distributions of the CBM, where the orbital spillover effect across the vdW gap is clearly enhanced [Figs. 8(a), 8(b), and 8(c), left]. In contrast, the orbital spillover of the VBM remains weak under low strain levels [1.1–1.81%; Fig. 8(a) and 8(b), right] but becomes more pronounced at higher strain [Fig. 8(c), right]. Consequently, at small strain the relatively large isolated energy [see Eq. (1)] in the AAS bilayer BP can be attributed to the pronounced interlayer stacking effect, which can be either enhanced or suppressed by strain through the nonlinear term $(\Delta E_{\text{QB}})^2/E_{\text{diff}}$.

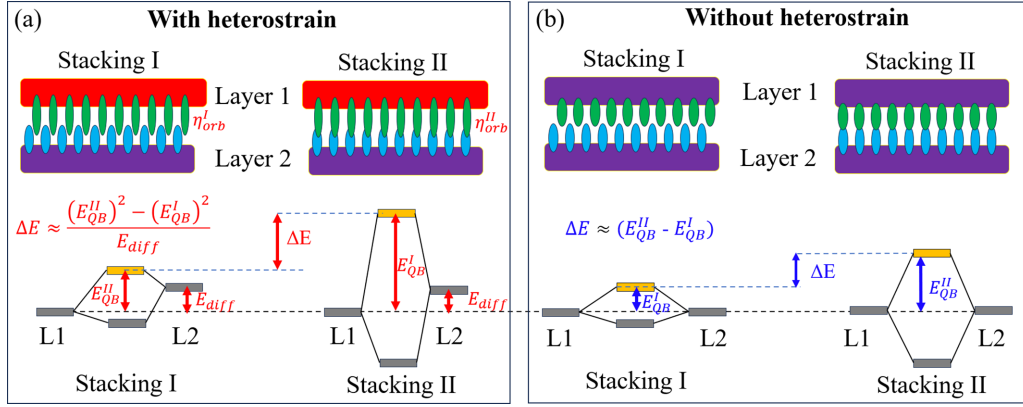


FIG. 7. Evolution of stacking pattern effect (a) with and (b) without asymmetric strain (also known as heterostrain). In figure a, band-edge difference between stacking configurations II and I (ΔE) under asymmetric strain is attributed to the nonlinear modification of interlayer QB interactions and orbital energy mismatch and can be approximated as $\Delta E = ((E_{QB}^{II})^2 - (E_{QB}^I)^2)/E_{diff}$, where E_{QB}^{II} and E_{QB}^I represent the VBM shifts from monolayer to bilayer induced by QB interactions in stacking II and I, respectively. E_{diff} denotes the strain-induced atomic orbital energy difference between the upper and lower BP layers. η_{Orb}^{II} and η_{Orb}^I represent the out-of-plane orbital delocalization induced by asymmetric in the "red" layer and they are proportional to E_{QB}^{II} and E_{QB}^I , respectively. In (b), band-edge difference between stacking configurations II and I (ΔE) in the absence of strain is attributed to the difference in their interlayer QB interactions, expressed as $\Delta E = E_{QB}^{II} - E_{QB}^I$. Band edge is represented with solid lines in gray and yellow. The schematic diagram of the atomic orbital characteristics and distribution is represented using green and blue ellipsoids for upper and lower BP layers. Layer 1 (or namely L1) and Layer 2 (or namely L2) denote monolayer before the interlayer orbital hybridization.

However, as the strain further increases to 10%, the distance between moiré impurities largely decreases, enhancing the intralayer orbital hybridization within the same stacking configuration through the CBM wave-function overlap [Fig. 8(d), left]. This leads to an increased bandwidth ($W_C = 40$ meV) and a corresponding reduction in $\Delta E_{C,C-1}$ to 130 meV. For the HVB, the VBM wave function remains localized [Fig. 8(d), right], resulting in a narrow bandwidth ($W_V = 4$ meV) and a relatively large isolated energy ($\Delta E_{V,V-1} = 200$ meV).

Interestingly, in the unstrained high-symmetry lattices with AA and AB stacking patterns [Fig. 6(a)], their VBM energies are nearly degenerate [Fig. 6(b)]. This degeneracy implies that VBM flat bands along the zigzag direction would not easily form within the moiré superlattice [30,31]. However, the application of AZS disrupts this degeneracy [Fig. 7(b)], leading to a higher VBM for the AB-like stacking pattern relative to the AA-like stacking pattern. This observation underscores the significant contribution of the AB-like stacking pattern

to the VBM, as illustrated in Fig. S3 of the Supplemental Material [63]. As a result, 1D flat bands also emerge in AZS superlattices through the same mechanism as in the AAS bilayer BP. While the AZS bilayer BP exhibits similar strain-dependent trends in the $\Delta E_{V,V-1}$ and $\Delta E_{C,C-1}$ (Table S2), it shows a narrower $\Delta E_{\mu,v}$ compared to the AAS counterpart. The relatively small isolated energy in the AZS bilayer BP is primarily attributed to the weak interlayer stacking effect [Fig. 6(b)].

D. Transitions between 1D and 2D flat bands by asymmetric biaxial strain

Having established a detailed understanding of the factors that govern the emergence of 1D flat bands in AAS and AZS bilayer BP, we recognize the potential to manipulate these electronic states through other strategies. In particular, the application of ABS presents an intriguing method (Fig. S5 of the Supplemental Material [63]) to modulate the band structure further. In the following, we investigate how such strain can drive transitions between 1D and 2D flat bands, thereby enhancing our ability to tailor the electronic properties of bilayer black phosphorus for potential applications in nanoelectronics and quantum materials

The ABS superlattice with 5% biaxial strain involves 3364 phosphorus atoms. It includes four local stacking patterns: AA-like, AB-like, AA'-like, and AB'-like [Fig. 9(a)]. Figure 9(a) shows a contour plot of the interlayer vertical distances in ABS bilayer BP at 5% strain. The interlayer vertical distance varies significantly across the stacking configurations. The AA'-like stacking pattern exhibits the largest distance (3.69 Å), while the AB-like stacking pattern has the smallest (2.96 Å). The AB'-like and AA-like stacking patterns fall in between, with distances of 3.40 and 3.50 Å, respectively. Compared to the AZS case, the difference in interlayer

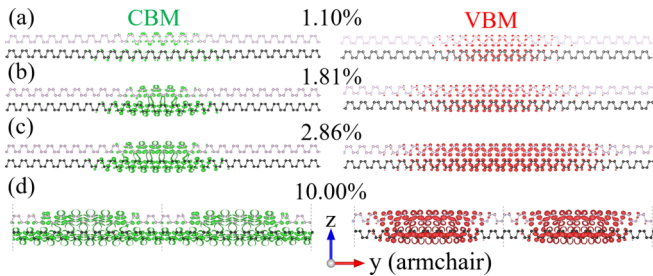


FIG. 8. Charge density distributions of the CBM (left panel) and VBM (right panel) at the Γ point in AAS moiré superlattices under (a) 1.10%, (b) 1.81%, (c) 2.86%, and 10.00% strain. The isosurface value is set at $1.5 \times 10^{-9} \text{ e}\text{\AA}^{-3}$.

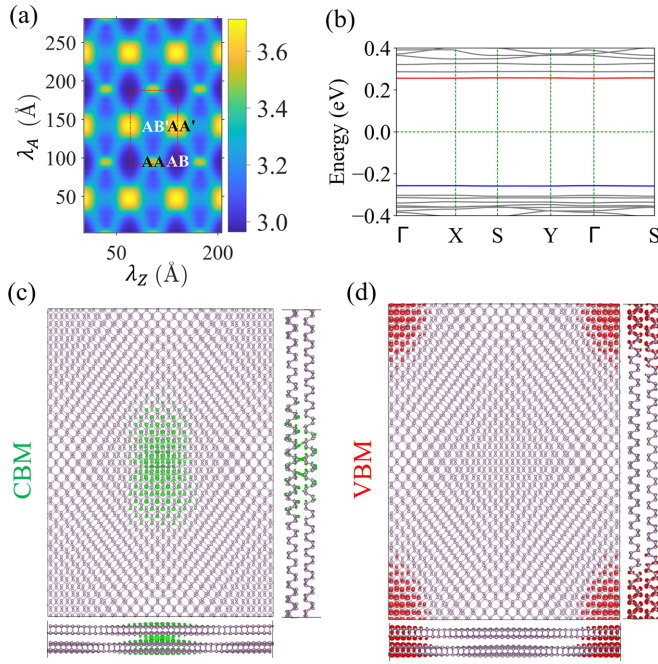


FIG. 9. The formation of 2D flat bands and their corresponding charge density distribution under a 5% biaxial strain. (a) Contour plot of the interlayer vertical distance between two constituent layers of ABS bilayer BP superlattice with 5% biaxial strain. The distribution of four stacking patterns in ABS bilayer BP is highlighted inset. (b) Band structure in ABS bilayer BP with biaxial strain magnitudes of 5.0%. Charge density distributions of the CBM (c) and VBM (d) at the Γ point in a 2D moiré superlattice under 5% biaxial strain. The isosurface value is set at $5 \times 10^{-11} \text{ e}\text{\AA}^{-3}$.

vertical distance between the AB-like and AA-like stacking patterns along the zigzag direction is larger by $0.22 \text{ \AA}$. This can be attributed to a release of internal stress in the arm-chair direction due to its lower elastic constant. Our study reveals a synergistic effect of the anisotropic mechanical properties on the interlayer orbital interactions in ABS bilayer BP. This interplay can modify the $\Delta E_{C,C-1}$ and $\Delta E_{V,V-1}$ values. Notably, the ABS superlattice exhibits a significantly larger $\Delta E_{V,V-1}$ ($\sim 50 \text{ meV}$) for the HVB flat band compared to the pure AZS case (10 meV at 5%). However, this $\Delta E_{V,V-1}$ value in the ABS superlattice remains lower than that observed in the pure AAS case (100 meV at 5%).

Our band structure analysis [Fig. 9(b)] reveals the formation of remarkable 2D flat bands for both the HVB and LCB across the entire Brillouin zone. These 2D flat bands exhibit zero bandwidth, which can also be well understood by anisotropic stacking pattern effect and strain effect on the intralayer interaction between moiré impurities. The charge density distributions of the VBM and CBM at the Γ point [Figs. 9(c) and 9(d)] exhibit pronounced localization in all spatial dimensions. This localization mirrors the behavior observed in other established 2D flat band systems, such as twisted graphene [4,5], transition metal dichalcogenides [13–16], and h-BN [17,18]. In contrast to the previously observed 1D flat bands in AAS and AZS superlattices, the ABS approach leads to the formation of 2D flat bands. This finding highlights the unique capability of the ABS approach

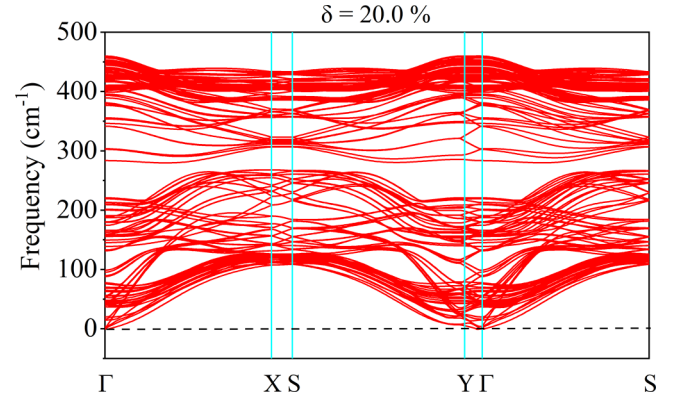


FIG. 10. Phonon dispersion of the moiré structure of AAS bilayer BP under 20% strain.

to manipulate the dimensionality of flat bands, offering greater control over their electronic properties.

Furthermore, the $\Delta E_{C,C-1}$ and $\Delta E_{V,V-1}$ values in the ABS superlattice are 50 and 40 meV, respectively. This implies that the 2D HVB flat band in bilayer BP under 5% asymmetric biaxial strain should be directly observable in nanoARPES experiments. The ABS method offers a powerful tool to manipulate the flat bands. It can induce a transition from 1D to 2D character and simultaneously tune the $\Delta E_{C,C-1}$ and $\Delta E_{V,V-1}$ through synergistic effects. Additionally, configurations with a higher number of local stacking types, such as ABS and twisted bilayer BP, generally exhibit lower $\Delta E_{C,C-1}$ and $\Delta E_{V,V-1}$ for their flat bands because of numerous competitive factors stemming from ΔE , d and synergistic strain effect.

E. Stability

It is well known that 2D materials generally exhibit high mechanical flexibility [81–83], with BP being particularly notable in this regard. Both monolayer and bilayer BP have been reported to withstand tensile strains as high as 30–32% [84–86]. The phonon dispersion analysis is essential for evaluating the dynamical stability of strained structures. However, such calculations are typically prohibitive for moiré superlattices due to the large number of atoms involved—often several hundred. In our study, the moiré superlattice is generated by applying an asymmetric uniaxial strain, which leads to the formation of a structurally simplified 1D moiré pattern. This approach significantly reduces the number of atoms compared to twist-induced moiré systems. This reduction in structural complexity enables us to feasibly perform phonon calculations to assess stability.

Using VASP in combination with the PHONOPY package [87], we computed force constants via the finite displacement method. As a preliminary step, we tested the convergence of the phonon dispersion of monolayer BP with different supercell sizes and found that a 6×6 supercell yields well-converged results without any imaginary frequencies. Based on this benchmark, we calculated the phonon dispersion of the AAS bilayer BP structure under 20% strain (with 44 P atoms in unit cell), using a 1×6 supercell (containing 264 P atoms) and 176 displaced configurations. As shown in Fig. 10, no

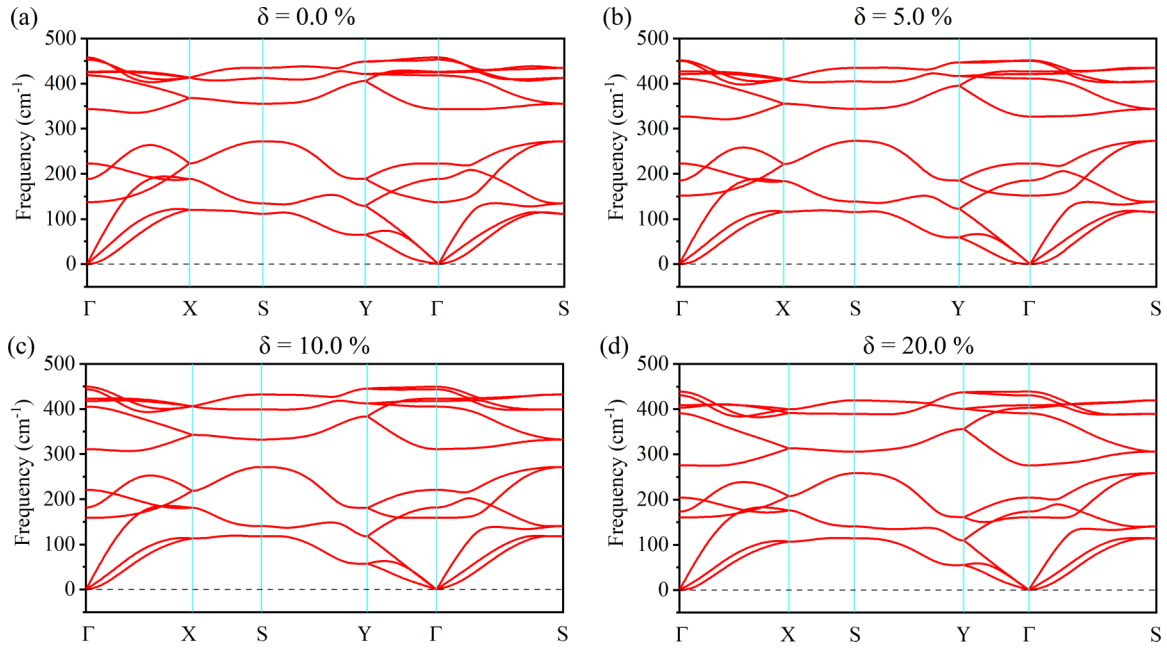


FIG. 11. Phonon dispersion of monolayer BP under tensile strain.

imaginary frequencies are observed across the Brillouin zone, confirming that the AAS bilayer BP structure is dynamically stable under 20% strain. Therefore, we expect that the system remains stable under smaller strains as well.

To further validate the dynamical stability of the AAS bilayer BP moiré structure, we adopted an alternative approach. In our structural model, only the bottom BP layer is subjected to tensile strain, while the top layer remains unstrained. The two layers are primarily coupled through vdW interactions, which may enhance and contribute slightly to the overall structural stability. Given this configuration, it is reasonable to assess the dynamical stability of the system by calculating the phonon dispersion of the strained bottom monolayer BP alone. As shown in Fig. 11, we computed phonon spectra of monolayer BP under various tensile strains along the armchair direction (with the zigzag direction fixed, consistent with our device configuration). The results show no imaginary frequencies in the 0–20% strain range, indicating good dynamical stability of the strained monolayer BP.

In summary, the phonon dispersion calculations of the AAS bilayer BP moiré structure under 20% strain, along with those of the strained monolayer BP over a range of strains, confirm that our proposed system is dynamically stable under the small strain conditions considered.

IV. CONCLUSION AND OUTLOOK

In summary, we demonstrate the underlying physical mechanism governing the bandwidth and isolated energy of 1D flat bands in AAS and AZS bilayer BP—namely, the interplay between the highly anisotropic stacking pattern effect (i.e., band-edge differences along two directions) and the heterostrain (or asymmetric uniaxial strain) effect, which encompasses energy mismatch and orbital spillover, and intralayer orbital hybridization. Below, we summarize the roles of asymmetric uniaxial strain, the formation mechanisms of

1D flat bands, and the strength of the $\Delta E_{C,C-1}$ and $\Delta E_{V,V-1}$ values as three principles:

First, the roles of asymmetric uniaxial strain are multifaceted: (1) It can form a 1D moiré pattern and controls the highly anisotropic moiré superlattice length. (2) It can tune the stacking pattern effect through interlayer orbital hybridization related to the competition between energy mismatch (E_{diff}) and orbital spillover effect. (3) It can influence the direction-dependent intralayer orbital hybridization interactions between moiré impurities.

Second, the mechanism of 1D flat band formation includes the following: (1) Both monolayers and bilayers must be semiconductors, and the outer atoms of the monolayer should exhibit out-of-plane anisotropic orbital characteristics. (2) The highly anisotropic stacking pattern effect (i.e., zero and large ΔE along two directions) is a crucial factor in the formation of 1D flat bands. (3) The direction-dependent intralayer orbital hybridization between moiré impurities, characterized by a small moiré periodicity λ_Z and a large λ_A along orthogonal directions, facilitates the formation of 1D flat bands with narrow bandwidth.

Last, the strength of $\Delta E_{C,C-1}$ and $\Delta E_{V,V-1}$ is related to the interlayer stacking effect (ΔE), which can be either enhanced or suppressed by strain through the nonlinear term $(\Delta E_{\text{QB}})^2/E_{\text{diff}}$. A small strain ($\sim 5\%$) is beneficial for achieving large values of $\Delta E_{C,C-1}$ and $\Delta E_{V,V-1}$.

Therefore, by applying asymmetric layer strain in designed device structures, the direction and magnitude of the strain can be freely controlled, allowing for precise control over the type of flat bands and the magnitude of $\Delta E_{C,C-1}$ and $\Delta E_{V,V-1}$ values to achieve experimentally observable 1D and 2D band physical phenomena, respectively. Our conclusions are expected to apply to other 2D systems (including homostructures, heterostructures, and isotropic materials) that meet the above three principles mentioned. Ultimately, these findings could lead to significant advancements in 1D strongly

correlated electron systems and the development of innovative device functionalities.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [88].

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- [63] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/xkwq-k2gp> for Notes S1-S2, Figs. S1-S5, and Tables S1 and S2. Note S1: Comparative analysis of VASP and RESCU calculations; Note S2: Derivation of moiré wavelength for orthorhombic lattices with lattice mismatch and rotation. Figure

- S1: Band structure of the optimized structure obtained using VASP after applying 5% asymmetrical armchair strain; Fig. S2: Band structures in AZS bilayer BP with various magnitudes; Fig. S3: Charge density distributions of the CBM and VBM at the Γ point in AZS moiré superlattices under 1.10% and 2.86% strain; Fig. S4: Band structures of four high-symmetry bilayer black phosphorus configurations; Fig. S5: Schematic illustration and device model of 2D Moiré superlattice formed by asymmetrical biaxial strain. Table S1: An analysis of the advantages of the asymmetric strain method for creating moiré superlattices and its comparison with other methods; Table S2: Structural information and physical parameters for bilayer BP in the AZS superlattice under various uniaxial strains.
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