

# Asymmetric strain distribution in ferroelectric/paraelectric SnTe-PbTe monolayer lateral heterostructures

Zi'Ang Gao<sup>1</sup>, Jing-Rong Ji<sup>2</sup>, Shiva Prasad Poudel<sup>3</sup>, Jose D. Mella<sup>3</sup>, Wen-Lin Wang<sup>1</sup>, Chengguang Yue<sup>1</sup>, Chong Liu<sup>1</sup>, Stuart S. P. Parkin<sup>2</sup>, Salvador Barraza-Lopez<sup>3,4</sup> (✉), Kai Chang<sup>1</sup> (✉)

<sup>1</sup> Beijing Key Laboratory of Fault-Tolerant Quantum Computing, Beijing Academy of Quantum Information Sciences, Beijing 100193, China

<sup>2</sup> Max Planck Institute for Microstructure Physics, Weinberg 2, Halle 06120, Germany

<sup>3</sup> Department of Physics, University of Arkansas, Fayetteville, Arkansas 72701, USA and MonArk NSF Quantum Foundry, University of Arkansas, Fayetteville, Arkansas 72701, USA

<sup>4</sup> Institute for Solid State Physics, University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa, Chiba 277-8581, Japan

*Nano Res.*, **Just Accepted Manuscript** • <https://doi.org/10.26599/NR.2026.94909142>

<https://www.sciopen.com/journal/1998-0124> on Aug. 24, 2026

© The Authors(s)

## Just Accepted

This is a "Just Accepted" manuscript, which has been examined by the peer-review process and has been accepted for publication. A "Just Accepted" manuscript is published online shortly after its acceptance, which is prior to technical editing and formatting and author proofing. Tsinghua University Press (TUP) provides "Just Accepted" as an optional and free service which allows authors to make their results available to the research community as soon as possible after acceptance. After a manuscript has been technically edited and formatted, and the page proofs have been corrected, it will be removed from the "Just Accepted" web site and published officially with volume and article number (e.g., *Nano Research*, **2025**, *18*, 94906990). Please note that technical editing may introduce minor changes to the manuscript text and/or graphics which may affect the content, and all legal disclaimers that apply to the journal pertain. In no event shall TUP be held responsible for errors or consequences arising from the use of any information contained in these "Just Accepted" manuscripts. To cite this manuscript please use its Digital Object Identifier (DOI®), which is identical for all formats of publication.

## Research Article

# Asymmetric strain distribution in ferroelectric/paraelectric SnTe-PbTe monolayer lateral heterostructures

Zi'Ang Gao<sup>1</sup>, Jing-Rong Ji<sup>2</sup>, Shiva Prasad Poudel<sup>3</sup>, Jose D. Mella<sup>3</sup>, Wen-Lin Wang<sup>1</sup>, Chengguang Yue<sup>1</sup>, Chong Liu<sup>1</sup>, Stuart S. P. Parkin<sup>2</sup>, Salvador Barraza-Lopez<sup>3,4,\*</sup> and Kai Chang<sup>1,\*</sup>

<sup>1</sup>Beijing Key Laboratory of Fault-Tolerant Quantum Computing, Beijing Academy of Quantum Information Sciences, Beijing 100193, China

<sup>2</sup>Max Planck Institute for Microstructure Physics, Weinberg 2, Halle 06120, Germany

<sup>3</sup>Department of Physics, University of Arkansas, Fayetteville, Arkansas 72701, USA and MonArk NSF Quantum Foundry, University of Arkansas, Fayetteville, Arkansas 72701, USA

<sup>4</sup>Institute for Solid State Physics, University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa, Chiba 277-8581, Japan

**Received:** 21 April 2026; **Revised:** 25 July 2026; **Accepted:** 24 August 2026

\*Address correspondence to Kai Chang, changkai@baqis.ac.cn; Salvador Barraza-Lopez, sbarraza@uark.edu

 **Cite this article:** *Nano Research*, 2026, 19, 94909142  
<https://doi.org/10.26599/NR.2026.94909142>

## Abstract

Monolayer lateral heterostructures (LHSs) composed of two-dimensional semiconducting ferroelectrics hold promise for non-volatile electronic and optoelectronic applications. Lattice misfit strain at these atomically sharp interfaces can significantly modulate in-plane polarization and related electronic properties, yet the direct characterization of the strain profile remains challenging. Here, we map the strain in SnTe-PbTe monolayer LHSs quantitatively *via* low-temperature scanning tunneling microscopy (STM). By combining moiré pattern simulation and geometric phase analysis, we achieve lattice parameter measurements with 0.02 Å precision—which substantially exceeds conventional STM resolution. Significant tensile strain is observed in SnTe regions, while PbTe sections exhibit much smaller strain. Density functional theory calculations attribute this asymmetric strain distribution to distinct atomic coordination in each monolayer semiconductor. These findings offer critical insights into strain engineering of ultrathin group-IV monochalcogenide heterostructures.

## Keywords

2D ferroelectrics, lateral heterostructures, strain distribution, scanning tunneling microscopy, density functional theory

## 1 Introduction

While layered materials are naturally suited for vertical heterojunctions with atomically sharp interfaces, devices based on two-dimensional (2D) materials and their lateral heterostructures may eventually evolve toward three-dimensional architectures containing both out-of-plane and in-plane heterostructures. Such an ambitious prospect may result in even more complex electronic and optoelectronic functionalities within limited spaces [1, 2]. Achieving this vision calls for the rational design and controlled creation of 2D LHSs having atomically sharp interfaces within a single monolayer [3, 4].

The earliest demonstration of 2D LHSs involved (identically coordinated) graphene and hexagonal boron nitride monolayers epitaxially grown [5-7]. Soon after, LHSs containing two different transition metal dichalcogenides (with identical coordination) were grown through chemical vapor deposition with techniques such as alternating-flux growth [3, 8, 9], one-pot synthesis [10, 11], or atomic substitution [12]. Atomically sharp one-dimensional (1D) interfaces with well-defined strain profiles in LHSs are now achievable [13]. Understanding strain distributions [14] and strain relaxation mechanisms at these interfaces is essential for optimizing interface quality and tuning material performance [15-17]. However, spatially resolved studies of strain are still limited due to the stringent precision requirements for its characterization, including the need for spatial resolution at the  $\sim 0.02$  Å scale for sub-percent strain (which often calls for interference-based techniques [18]), and highly surface-sensitive detection methods. Such studies are especially important in LHSs containing 2D ferroelectric semiconductors, whose polarization and electronic structures are highly sensitive to lattice strain. Here, we extract the strain distribution from high-resolution STM images of the LHSs between the monolayers of ferroelectric SnTe and paraelectric PbTe by moiré pattern simulation and geometric phase analysis (GPA) [13, 19].

## 2 Experimental

### 2.1 Sample growth

Experiments were carried out in a Unisoku USM1300 MBE-STM combined system. The base pressures were below  $2 \times 10^{-10}$  mbar in the MBE chamber and below  $1 \times 10^{-10}$  mbar in the STM chamber. Graphitized SiC(0001) substrates were prepared from phosphorus-doped, Si-terminated 4H-SiC single crystals in an UHV environment. After degassing, the substrates were annealed at 900 °C in a Si flux for 15 min to form atomically flat terraces and a Si-rich ( $3 \times 3$ ) reconstruction, followed by annealing at 1450 °C for 6 min (without Si flux) to obtain a surface predominantly covered by few-layer epitaxial graphene. High-purity PbTe and SnTe source materials (99.999%, Alfa Aesar) were evaporated from standard Knudsen cells; beam fluxes were controlled by mechanical shutters.

### 2.2 Scanning tunneling microscopy

STM measurements were performed in situ in UHV using the low-temperature STM

module at 4.7 K. Mechanically cut Pt–Ir tips were calibrated on Ag(111) prior to measurements.

### 2.3 Computational methods

Electric dipole [20] and band structure calculations were performed on single unit cells containing four atoms using density functional theory (DFT) in *VASP* [21]. It is known that theoretical and experimental structural parameters for SnTe differ. Therefore, the electric dipole and band structure calculations use the experimentally determined strain to change lattice parameters on a reference theoretical structure [22]. Additional structural calculations on structures containing 1272 atoms were performed with the SIESTA code [23], which employs localized numerical atomic orbitals [24] and is more efficient for this purpose. Energy and force convergence criteria were set to  $10^{-6}$  eV and  $10^{-3}$  eV/Å, respectively, in all DFT calculations.

### 3 Results and discussion

SnTe and PbTe belong to the group-IV monochalcogenide semiconductor family, and have applications in infrared detection [25, 26], photovoltaics [27, 28], thermoelectrics [29, 30], photostriction [31, 32], phase-change memories [33], valley-ferroelectric-coupled [34] non-volatile storage [13], among others. At room temperature, SnTe has a three-dimensional rock-salt structure that transitions into a layered structure when its thickness is reduced to less than eight atomic layers [35, 36] (a monolayer of those materials consists of two atomic layers). The ground state of SnTe monolayers [Figure 1(a)] displays an orthorhombic lattice (layer group  $Pmn2_1$ ) structurally analogous to black phosphorus with Sn and Te atoms occupying the two sublattices, leading to an in-plane polarization  $\mathbf{P}$  due to inversion symmetry breaking [37]. In contrast, pristine PbTe monolayers [Figure 1(b)] have a square lattice belonging to the centrosymmetric group  $Cmcm$  and are therefore paraelectric [38]. The cations (Sn or Pb) are slightly displaced out of the plane relative to the Te anions in these monolayers.

SnTe and PbTe monolayers form type-II band-aligned heterostructures and superlattices when grown by molecular beam epitaxy (MBE) on graphitic substrates [19]. By suppressing the surface diffusion in such LHSs [39], we have grown monolayer SnTe-PbTe LHSs with interdiffusion at the 1D interface limited to  $\sim 1$  nm, which permits the formation of tunnel junctions with barrier widths as small as 2 nm [13]. We achieved high-quality planar superlattices like the one displayed in Figure 1(c) after suppressing surface diffusion. Understanding the strain distribution and relaxation mechanisms across these 1D interfaces is an immediate next step toward designing the LHSs for practical non-volatile devices.

Due to their extreme sensitivity to local variations in the lattice constant [40], moiré patterns arising from the superposition of the lattices of a 2D material and the underlying substrate allow inferring strain distributions across monolayer heterojunctions and superlattices like those shown in Figures 1(c)-(e). Such strain has been used to engineer the out-of-plane rippling in  $\text{WSe}_2$  monolayers at the nanoscale [16]. Moirés were also crucial in determining the rhombohedral distortion angle (a

measure of ferroelectric strength) of SnTe monolayers [38, 41]. Next, we determine variations in the lattice constants across the LHS samples by analyzing their moiré patterns in Fourier space.

To ensure accurate measurements, structures with a minimum single-material width of at least 20 nm were analyzed. All STM data were acquired at 4.7 K to minimize thermal drift and scanning artifacts. We first determined the global lattice constants of pristine SnTe and PbTe monolayer nanoplates using their moiré patterns formed in conjunction with the graphitic substrate they are grown upon. Figure 2(a) shows a high-resolution image of a pristine PbTe monolayer nanoplate, and Figure 2(b) is its corresponding Fourier transform (FT) image. Three sets of spots can be identified in the FT image: (i) the orthorhombic Bragg spots of PbTe, indicated by the yellow circles; (ii) the hexagonal spots from a  $(6 \times 6)$  reconstruction of the SiC(0001) substrate beneath epitaxial graphene indicated by blue circles; (iii) monoclinic moiré spots from the overlaid PbTe and graphene, indicated by red circles. We reproduced the FT image by a numerical simulation (see the Supporting Information for details), in which the 2D lattice vectors  $\mathbf{a}_1$  and  $\mathbf{a}_2$  of the PbTe monolayer are the tunable parameters. The angle between these two vectors is fixed at  $90^\circ$ , hence there are three scalar variables in total (the magnitudes of  $\mathbf{a}_1$  and  $\mathbf{a}_2$ , and the rotation angle of  $\mathbf{a}_1$  from the zigzag direction of graphene). The spots from the  $(6 \times 6)$  reconstruction of SiC serve as a natural reference system that resists the parallelogram distortion induced by the drifting of the sample during scanning. We optimized these three parameters to best match the moiré pattern in Figure 2(b), and the corresponding  $\mathbf{a}_1$  and  $\mathbf{a}_2$  are the lattice vectors of the pristine PbTe monolayer. Since the moiré spots are extremely sensitive to the change of lattice vectors, the precision of this method is of the order of 0.02 Å, which is comparable with those reported in Reference [42] and corresponds to a strain sensitivity of  $\sim 0.1\%$ . This way, lattice parameters for the SnTe and PbTe monolayers are  $a_1 = 4.58 \pm 0.02$  Å,  $a_2 = 4.44 \pm 0.02$  Å [38] and  $a_1 = 4.62 \pm 0.02$  Å,  $a_2 = 4.58 \pm 0.02$  Å, respectively. A detailed description of the FT analysis is provided in the Supporting Materials. Note that the PbTe monolayer indeed exhibits a nearly square lattice within our experimental precision. Having these reference structural values, we measure strain on SnTe-PbTe monolayer LHSs next.

We fabricated two types of heterostructures to systematically investigate the strain distribution across SnTe-PbTe LHSs: “SnTe outside of PbTe” (SoP) LHSs, where a PbTe monolayer nanoplate serves as the core and a SnTe monolayer grows on its edges epitaxially, and “PbTe outside of SnTe” (PoS) LHSs, where the SnTe monolayer nanoplate forms the core and the PbTe monolayer is epitaxially grown outside SnTe afterwards. Figure 3(a) is an STM image of a SoP heterostructure. We performed high-resolution STM scans in the regions marked by the blue and red boxes, corresponding to the SnTe (blue box) and PbTe (red box) monolayer sections, respectively. Figures 3(b) and 3(c) display similar high-precision STM images within PoS heterostructures. FT analyses were then performed within the marked boxes to extract the lattice parameters of SnTe and PbTe monolayers within the SoP and PoS heterostructures [Figures 3(d)-(g)]; aided once more by simulated FT images—like

the ones initially showcased in Figure 2(c)—shown in Figures 3(h)-(k). By extracting the lattice parameters from the FT simulations, we find that the SnTe monolayer undergoes a noticeable lattice expansion when in a heterostructure: in the SoP heterostructure [Figures 3(a), (d), and (h)], the lattice parameters increase to  $a_1 = 4.64 \pm 0.01 \text{ \AA}$  and  $a_2 = 4.47 \pm 0.03 \text{ \AA}$ , respectively; in the PoS heterostructure they also expand to  $a_1 = 4.62 \pm 0.01 \text{ \AA}$  and  $a_2 = 4.49 \pm 0.01 \text{ \AA}$  [blue datapoints in Figure 3(l)]. The expansion leads to an increase in the electronic bandgaps for the SnTe monolayer, calculated to be 67 meV in the SoP structure, and 61 meV in the PoS case (Figure S5).

In contrast, the PbTe monolayer experiences only minimal lattice changes when being a part of a LHS: within the SoP heterostructure, its lattice parameters are  $a_1 = 4.63 \pm 0.02 \text{ \AA}$  and  $a_2 = 4.59 \pm 0.02 \text{ \AA}$  [Figures 3(a), (e), and (i)]; in the PoS heterostructure they are  $a_1 = 4.60 \pm 0.02 \text{ \AA}$  and  $a_2 = 4.58 \pm 0.02 \text{ \AA}$  [red datapoints in Figure 3(l)].

These results indicate that the SnTe monolayer accommodates most of the lattice strain within LHSs. To emphasize this point, the blue datapoints in Figure 3(m) show that the unit cell of a SnTe monolayer experienced an area expansion of approximately 2% in both SoP and PoS LHSs, while the dots in red indicate that the area in the unit cell of PbTe monolayer is almost unchanged. The orthorhombic ratio  $a_1/a_2$  exhibits different trends in the two heterostructure types: it increases to 1.038 in SoP heterostructures (compared to 1.032 in a pristine SnTe monolayer) and it decreases to 1.029 in PoS heterostructures. This asymmetry in strain distribution suggests that the SnTe monolayer plays the dominant role in accommodating lattice mismatch within these lateral heterostructures, with minimal strain relaxation in PbTe monolayer sections. The intrinsic electric dipole  $P$  depends most strongly on changes in  $a_1$  and, according to our calculations, the (in-plane)  $P$  is predicted to increase by 20% with respect to its magnitude in the pristine structure in the PoS heterostructure (for which  $a_1$  increased by 0.9%), and by 25% in the SoP structure (in which  $a_1$  was bigger by 1.3%) [20, 21]. This is a very significant predicted enhancement of the electric dipole considering the amount of strain applied. The reliability of first-principles calculations for such relative, strain-induced polarization changes is well established: predictions that epitaxial strain enhances the spontaneous polarization [43] were confirmed experimentally in strained BaTiO<sub>3</sub> films [44]. (The strained PbTe monolayer remains centrosymmetric.)

Going beyond the estimation of average lattice parameters, we next map the spatial distribution of strain within SnTe and PbTe regions using GPA, a well-established technique that is often applied to transmission electron microscopy images for strain mapping [45]. The essence of GPA is to compare the phase of ideal crystal planes (defined by a  $g$ -vector) with the phase of planes measured from an image. By masking the FT at specific  $g$ -vectors, periodic components can be isolated and their phases extracted. The phase difference between the masked FT and the ideal lattice phase is used to refine the  $g$ -vector and analyze strain in homogeneous regions. From the phase information obtained for two non-collinear  $g$ -vectors, the displacement field is calculated, providing the basis for determining strain. Finally, strain, rotation,

and dilation of the sample are derived from the gradients of the displacement field, enabling a complete description of the material's deformation.

Due to the extreme sensitivity of GPA to small deformations, scanning artifacts such as piezo drift must be carefully addressed. To minimize these effects, we selected high-resolution STM images of PoS heterostructures and focused on the regions marked by the dashed boxes in Figures 4(a) and 4(b), ensuring that the analyzed regions are far away from the edges of the images, where the piezo drift is largest. Forward and backward scan images were separately processed and subsequently averaged to further suppress the nonlinear piezo distortions. No plane subtraction or detrending was applied to the displacement field; the only corrections were the forward/backward averaging, central cropping away from the image edges, and normalization of the strain zero of each map to its mean value (a scalar offset). Plane subtraction was deliberately avoided so as not to remove the physical strain gradient along the  $y$ -direction discussed below.

Strain maps along the  $x$ - and  $y$ -directions for the SnTe monolayer section [Figures 4(b) and (c)] and for the PbTe monolayer section [Figures 4(e) and (f)] reveal a continuous distribution of strain across the SnTe and PbTe monolayer regions. No point defects, dislocations, or abrupt lattice distortions were observed, indicating that the heterostructure maintains a continuous and defect-free crystal lattice within the field of view. Because these regions were deliberately chosen to be free of point defects and vacancies, the extracted strain reflects the intrinsic lattice deformation. A point defect would produce only a localized strain field decaying within a few nanometres, which cannot account for the systematic, region-wide  $\sim 2\%$  expansion confined to the SnTe sections; the asymmetry is further corroborated by its consistency across the two independent heterostructure geometries (SoP and PoS). We normalized the zero point of the strain percentage to the averaged strain value of each image, and the strain distribution is generally within  $\pm 0.5\%$  in SnTe and  $\pm 0.85\%$  in PbTe monolayer regions. Extracting the averaged strain distribution curves from the GPA images, we found that the strain distribution within the SnTe section shows a visible gradient along  $y$ , the direction perpendicular to the interface:  $\epsilon_{xx}$  is largest near the SnTe-PbTe junction, where the SnTe lattice is stretched toward registry with PbTe, and decays by  $\sim 0.5\%$  over  $\sim 35$  nm into the SnTe interior. This is the behavior expected for misfit-strain relaxation away from a coherent interface. An exponential fit yields characteristic relaxation lengths of 18 nm for  $\epsilon_{xx}$  and 24 nm for  $\epsilon_{yy}$  (Figure S2). In contrast, although the global analysis from FT does not reflect significant strain in PbTe sections, the fluctuation in strain distribution that is visible from GPA is stronger, and no clear strain gradient is observed. The junction itself is atomically coherent: single-frame atomic-resolution imaging across the SnTe-PbTe boundary of a lateral heterostructure island resolves both lattices simultaneously and reveals continuous atomic rows with no misfit dislocations over more than 100 nm (Figure S3). The two lattices are thus locked at the boundary, and the 2.2% mismatch must be accommodated by the long-range elastic strain quantified here, with the softer SnTe side carrying the relaxation. We note that, since the SnTe-PbTe heterostructures

studied here consist of only two atomic layers, the strain distribution may also reflect the inhomogeneity of the electronic states of the graphene/SiC substrate.

To further understand the microscopic mechanism of the asymmetric strain distribution between SnTe and PbTe, we created atomistic models of PoS and SoP LHSs having identical numbers of Sn and Pb atoms [Figures 5(a) and (b)] to determine strain unencumbered by artificially-induced anisotropies. Both structures contain 1272 atoms, with 9 nm diameters, and were optimized with the SIESTA density functional theory (DFT) code [23, 46]. The area expansion of individual unit cells within those LHSs is shown in Figures 5(c) and (d), respectively, and the strain profiles within the dashed rectangles on Figures 5(c) and 5(d) are displayed in Figure 5(e). Despite the smaller size of the simulated structures compared with the experimental structures shown above, we confirm that the PbTe monolayer experiences significantly smaller strain than that in the SnTe monolayer section in the same LHS. The unit cells of the SnTe monolayer in the core of a PoS LHS expand by 4%, while those of the PbTe monolayer in the core of a SoP LHS only shrink by 2%. This result is consistent with our experimental observation.

The different strain magnitudes in SnTe and PbTe monolayers can be understood from their distinct coordination environments. As displayed in Figure 1(a), because of the armchair-like structure, the atoms in SnTe monolayers are three-fold coordinated: each atom has two nearest neighbors within the same atomic layer and one in the other layer. However, the atoms in PbTe monolayers are five-fold coordinated, having four nearest neighbors within the same atomic layer and another with the opposite atomic layer, as Figure 1(b) shows. When experiencing tensile stress in a LHS, the three-fold coordination in SnTe allows variations in the bonding angle between Sn and Te atoms to induce lattice strain, which costs much less energy than varying the bonding length. While in PbTe, the five-fold coordination restricts the bonding angle, making its lattice stiffer under stress. For the same reason, it is also expected that the Young's modulus along the armchair direction of a SnTe monolayer is significantly smaller than that along the zigzag direction.

This coordination-number mechanism is not specific to SnTe/PbTe but is systematic across the group-IV monochalcogenide family. First-principles data [22] show that the relaxed lattices of all Pb-based monolayers (PbS, PbSe, PbTe) are square with five-fold-coordinated cations (a result robust across eleven exchange-correlation functionals), whereas the Sn-based monolayers (SnS, SnSe, SnTe) are orthorhombic with three-fold-coordinated cations (Table S1). Because the cation coordination determines whether strain is accommodated by bond-angle variations, which cost much less energy than changes of the bond length, we predict the same Sn-side strain localization in other Sn-/Pb-based monochalcogenide lateral heterostructures, such as SnSe/PbSe.

While it is known that the more compliant material takes up the larger share of misfit strain, this insight has not previously been directly imaged in the group-IV monochalcogenide family. The mechanism for strain release differs from that at play at graphene/hBN monolayer heterojunctions and those created by dissimilar

transition-metal dichalcogenide monolayers in two respects: whereas our junction is fully coherent (Figure S3), in the transition-metal dichalcogenide junctions the mismatch is largely relieved by misfit dislocations at the interface [40]; further, whereas the SnTe/PbTe asymmetry originates in the difference in cation coordination number itself, atoms across other heterojunctions share the same coordination.

The advances here are threefold: First, our self-calibrating moiré-Fourier method, referenced to the SiC(0001)-(6×6) superstructure, provides  $\sim 0.02$  Å ( $\sim 0.1\%$  strain) precision non-destructively and with surface sensitivity, whereas comparable precision previously required (scanning) transmission electron microscopy [18, 40]. Second, in contrast to TMD heterojunctions where strain chiefly tunes the electronic bands, here the asymmetric strain couples to a ferroelectric order parameter, with a predicted 20-25% enhancement of the in-plane polarization while the bands are only weakly affected. Third, we trace the asymmetry to a specific and transferable microscopic origin, the cation coordination number, which underlies the difference in stiffness between the two materials and provides a design rule that is expected to generalize across the group-IV monochalcogenide family.

The local electronic structure of these lateral heterostructures has been characterized by scanning tunneling spectroscopy previously: the type-II band alignment was measured directly by  $dI/dV$ , with the conduction and valence band edges of SnTe monolayers 0.42 eV and 0.37 eV above those of PbTe, and spatially resolved spectra across SnTe-PbTe-SnTe junctions yielded the local density of states and the tunnel-barrier profiles [13, 19]. To probe the strain response of the band structure directly, we performed spatially resolved  $dI/dV$  spectroscopy along a line crossing a SnTe-PbTe junction (Figure S4). The band edges are spatially uniform in the interior of the SnTe monolayer: far from the junction the gap is constant at  $1490 \pm 3$  meV, in quantitative agreement with Ref. [13], over distances across which the misfit strain relaxes; the electrostatic band bending of the junction is screened by the graphene substrate to within a few nanometers, and the occupied-state map resolves the standing waves produced by in-plane scattering at ferroelectric domain walls [13]. In a small ferroelectric domain closer to the junction the apparent gap is larger by only  $15 \pm 4$  meV; because the lowest domain-wall standing wave is offset from the true band edge by a finite-size confinement energy comparable to this difference, we do not assign it to strain. These measurements bound any strain-induced band-edge shift to a few tens of meV, consistent with the calculated bandgap increase of 61-67 meV at the strain levels measured here, and far smaller than the 0.3-0.4 eV type-II band offsets [13]. This weak band response, contrasted with the strong predicted polarization response, is itself a consequence of the bond-angle-mediated strain accommodation in three-fold-coordinated SnTe.

#### 4 Conclusions

In conclusion, we investigated the strain distribution within monolayer SnTe-PbTe lateral heterostructures using high-resolution STM, moiré pattern simulation, GPA, and DFT calculations. By applying a self-calibrating method to

analyze moiré patterns, we achieved a precision of 0.02 Å in local lattice parameter measurements. Through a comparative study of SoP and PoS LHSs, we identified a coherent epitaxial interface with a highly asymmetric strain distribution, where strain is predominantly localized in the SnTe regions, while the PbTe regions remain relatively unstrained. Furthermore, spatial strain analysis indicates a continuous, defect-free lattice throughout the heterostructure, and single-frame cross-junction imaging establishes an atomically coherent boundary free of misfit dislocations. First-principles calculations further elucidate the origin of this asymmetric strain distribution as arising from the different coordination environments of the cations: SnTe, with three-fold coordination, accommodates lattice deformations more readily than PbTe, which has a more rigid five-fold coordination. Supported by first-principles data across the group-IV monochalcogenide family, this cation-coordination mechanism is expected to govern strain partitioning generically in Sn/Pb-based monochalcogenide monolayer lateral heterostructures. These findings provide key insights into strain in group-IV monochalcogenide semiconductor LHSs, and underscore the importance of atomic-scale strain engineering in these 2D materials.

#### **Data availability**

All data needed to support the conclusions in the paper are presented in the manuscript and the Electronic Supplementary Material. Additional data related to this paper may be requested from the corresponding authors upon request.

#### **Acknowledgments**

Z.G., C.L., W.W., C.Y. and K.C. are supported by Quantum Science and Technology-National Science and Technology Major Project (2023ZD0300500), National Natural Science Foundation of China (12304189, 12304206), and Beijing Municipal Science & Technology Commission (Grant No. Z221100002722013). J.-R.J. and S.S.P.P. acknowledge funding from the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – Project number 314790414. S.P.P., J.D.M. and S.B.-L. acknowledge financial support from MonArk NSF Quantum Foundry from the U.S. National Science Foundation under Award No. DMR-1906383. Calculations were carried out at the Pinnacle Supercomputer, funded by the NSF under award OAC-2346752.

#### **Declaration of competing interest**

All the contributing authors report no conflict of interests in this work.

#### **Author contribution statement**

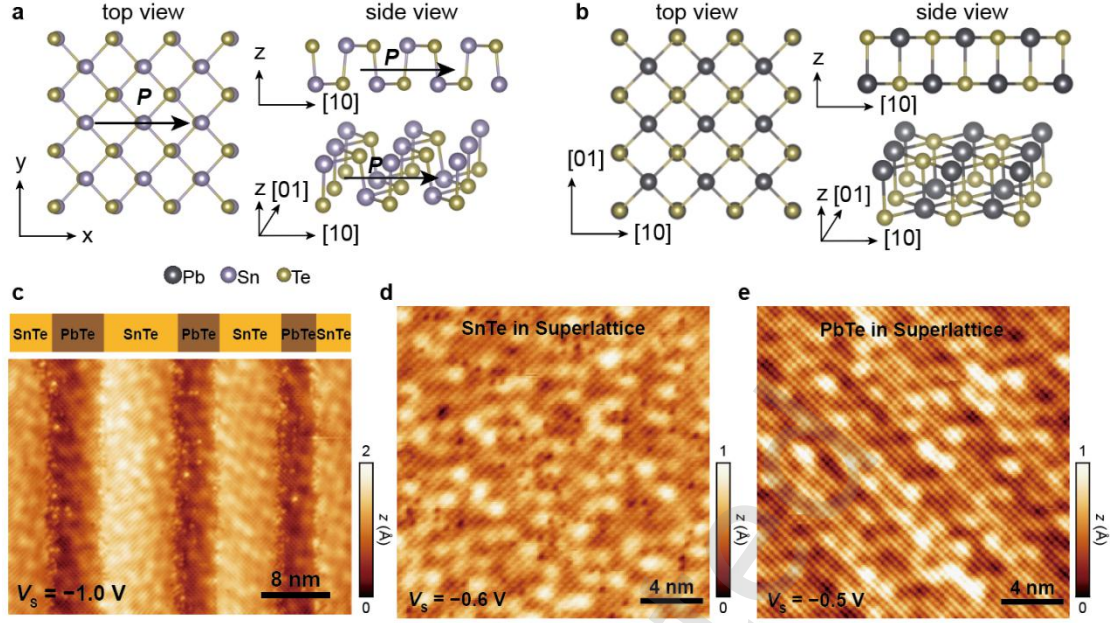
K.C. conceived the project and directed the experimental work. Z.G. conducted the MBE growth and STM experiments, performed the moiré-based strain analysis and geometric phase analysis. J.-R.J. (directed by S.S.P.P.), W.W., and C.Y. contributed to MBE/STM measurements. C.L. developed the code for the moiré-spot Fourier

analysis. S.P.P. and J.D.M. performed DFT calculations and analyzed strain distributions on atomistic structures created by S.B.-L. K.C. and S.B.-L. wrote the manuscript with input from all the authors.

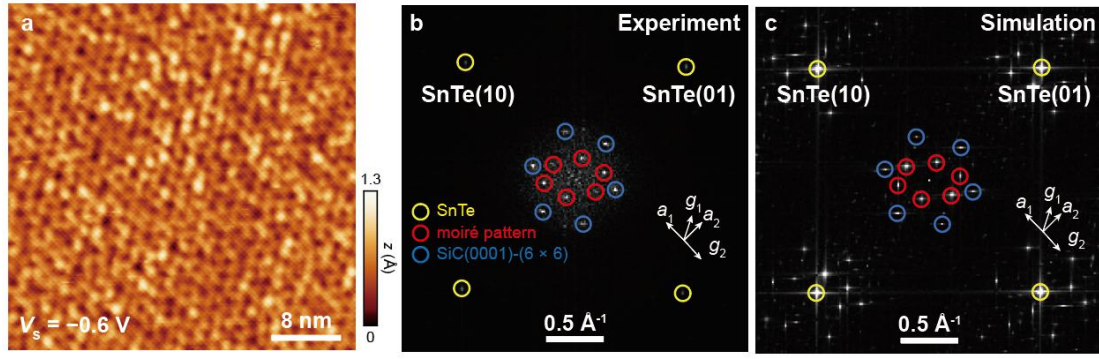
#### **Use of AI statement**

During the revision of this work the authors used artificial-intelligence tools for language editing and for assistance with data-analysis code. The authors reviewed and edited the content as needed and take full responsibility for the content of the published article.

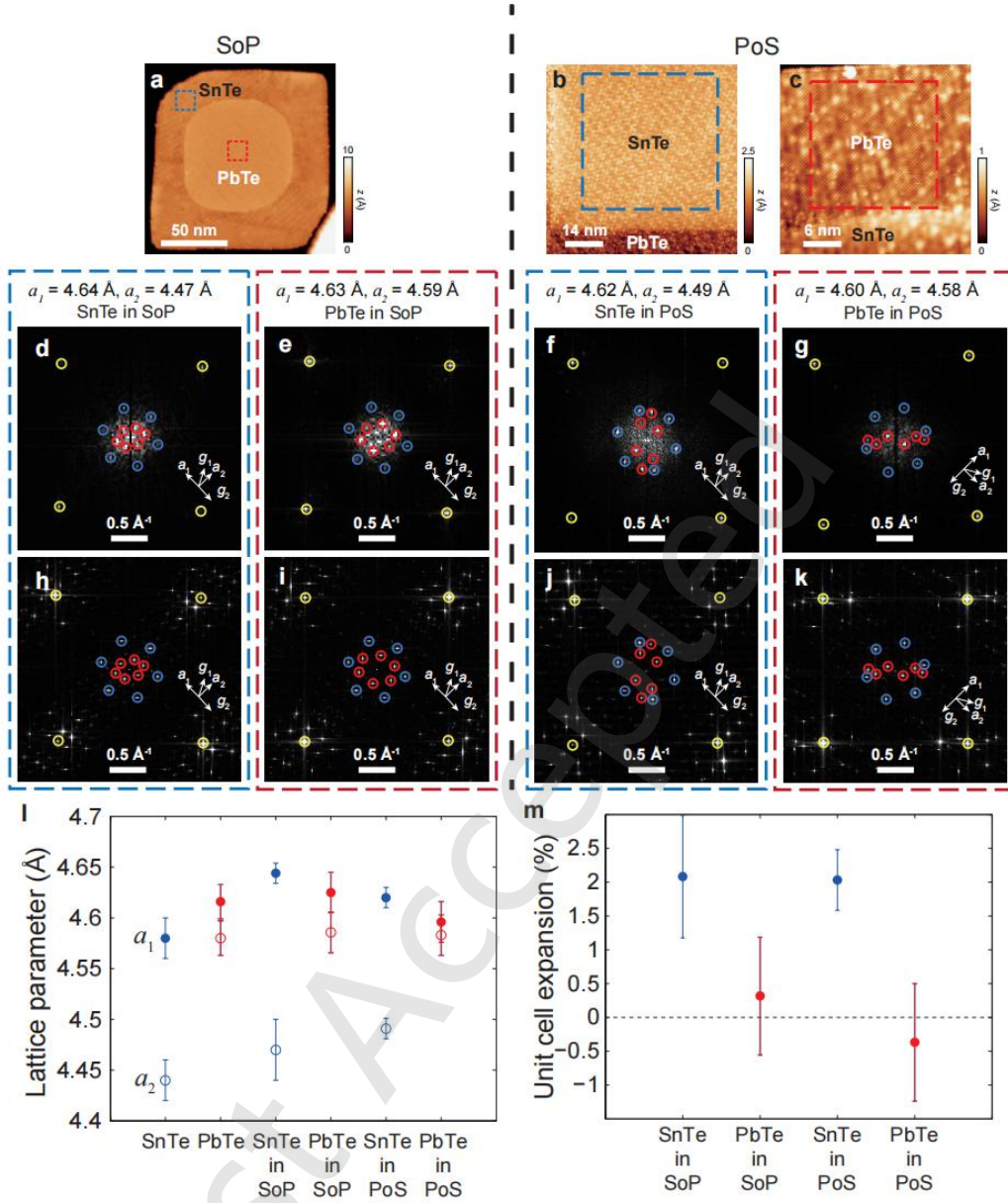
Just Accepted



**Figure 1.** Schematics of (a) SnTe and (b) PbTe monolayers. (c) Diagram (top) and low-temperature STM image (bottom,  $V_s = -1.0$  V,  $I = 10$  pA) of a SnTe-PbTe monolayer LHS. The difference in the apparent height of SnTe and PbTe monolayer sections comes from their type-II band alignment. (d) Atomically resolved image of a SnTe monolayer section within a superlattice ( $V_s = -0.6$  V,  $I = 10$  pA). (e) Atomically resolved image of a PbTe monolayer section in a superlattice ( $V_s = -0.5$  V,  $I = 50$  pA).

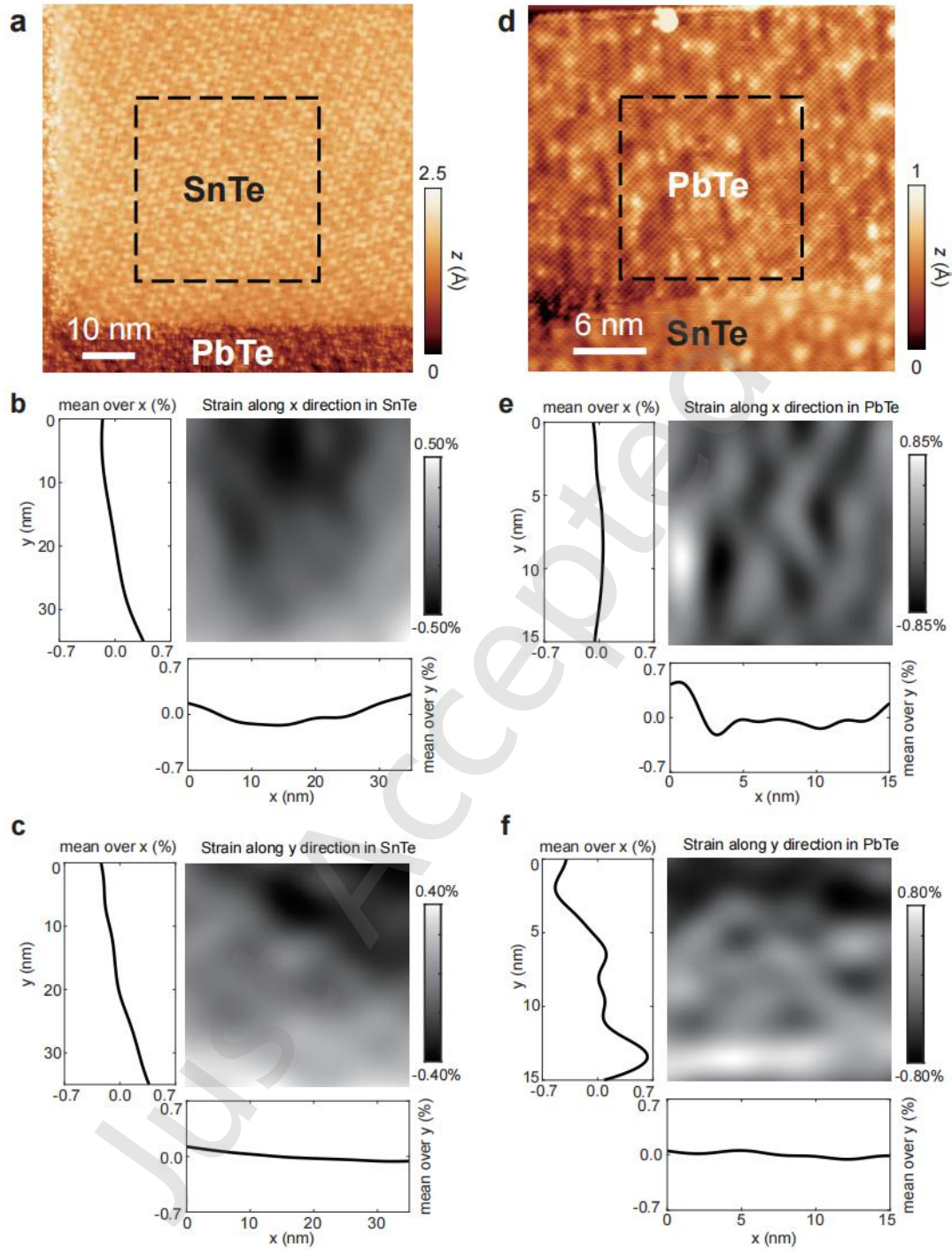


**Figure 2.** (a) High-resolution STM image of a pristine PbTe monolayer ( $V_s = -0.6$  V,  $I = 50$  pA). (b) Fourier-transform of the STM image and (c) simulated FT of a pristine PbTe monolayer on epitaxial graphene. The optimal lattice parameters for the pristine PbTe monolayer found with this procedure are  $a_1 = 4.62 \pm 0.02$  Å and  $a_2 = 4.58 \pm 0.02$  Å.



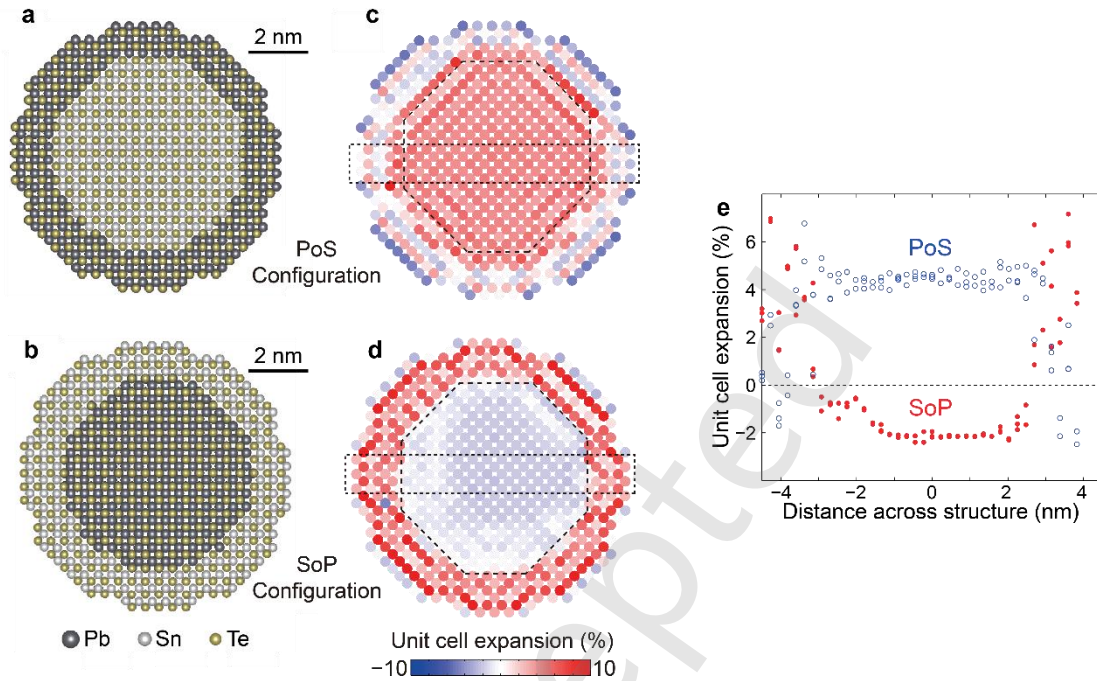
**Figure 3.** (a) STM image of a SoP LHS ( $V_s = 1.6$  V,  $I = 30$  pA). (b,c) STM images within PoS LHSs acquired at  $V_s = -0.6$  V,  $I = 10$  pA and  $V_s = -0.9$  V,  $I = 50$  pA, respectively. The difference in the apparent height of SnTe and PbTe monolayers comes from their type-II band alignment. (d-g) Fourier transforms of the STM images within red and blue squares in subplots (a) and (b). (h-k) Optimal simulated Fourier transforms, with lattice parameters of SnTe or PbTe monolayers best matching the experimental data in subplots (d-g). There are three sets of spots: (1) orthorhombic ones from SnTe or PbTe monolayers marked in yellow, (2) hexagonal ones from the SiC(0001)-(6×6) superstructure drawn in blue, and (3) another set of irregular spots resulting from the moiré pattern between the hexagonal graphene lattice and the orthorhombic SnTe or PbTe monolayer lattices (red circles). (l) Summary of lattice parameters  $a_1$  and  $a_2$  extracted from freestanding SnTe and PbTe monolayer nanoplates, and from SoP and PoS heterostructures by the moiré pattern simulation method. Error bars reflect the uncertainty arising from the resolution of the Fourier transformed images. (m) Average expansion of the area of a single unit cell in the heterostructures, in comparison with those in freestanding SnTe and PbTe monolayer

nanoplates, calculated from the data in (l).



**Figure 4.** (a) Same high-resolution STM image of the SnTe region in a PoS LHS as shown in Figure 3(b). (b),(c) Spatial distribution of the strain in SnTe along the  $x$ - and  $y$ -directions within the black dashed box in (a), extracted by GPA method. The zero point of the strain percentage is normalized to the averaged value of the whole image. No detrending or plane subtraction was applied. The SnTe-PbTe interface runs along  $x$ ;  $y$  is the direction perpendicular to the interface. The curves are the averaged strain distribution along the  $x$ - and  $y$ -directions. (d) Same high-resolution STM image of the PbTe region in a PoS LHS as shown in Figure 3(c). (e),(f) Spatial distribution of the

strain in PbTe along the  $x$ - and  $y$ -directions within the black dashed box in (d), with similar averaged curves of strain distribution as those in (b) and (c).



**Figure 5.** Atomistic structures of (a) PoS and (b) SoP monolayer nanoplates from first-principles calculations. Each model contains 318 Pb atoms, 318 Sn atoms, and 636 Te atoms. (c) and (d): Maps of the local unit cell area expansion in the atomistic PoS and SoP nanoplates from first-principles calculations. (e) Unit cell expansion extracted along the dashed rectangles in subplots (c) and (d): SnTe monolayer sections undergo the largest strain consistently.

## References

- [1] Novoselov, K. S.; Mishchenko, A.; Carvalho, A.; Castro Neto, A. H. 2D materials and van der Waals heterostructures. *Science* **2016**, *353*, aac9439.
- [2] Liu, Y.; Huang, Y.; Duan, X. Van der Waals integration before and beyond two-dimensional materials. *Nature* **2019**, *567*, 323-333.
- [3] Zhang, Z.; Chen, P.; Duan, X.; Zang, K.; Luo, J.; Duan, X. Robust epitaxial growth of two-dimensional heterostructures, multiheterostructures, and superlattices. *Science* **2017**, *357*, 788-792.
- [4] Dean, C. R.; Young, A. F.; Meric, I.; Lee, C.; Wang, L.; Sorgenfrei, S.; Watanabe, K.; Taniguchi, T.; Kim, P.; Shepard, K. L. et al. Boron nitride substrates for high-quality graphene electronics. *Nat. Nanotechnol.* **2010**, *5*, 722-726.
- [5] Ci, L.; Song, L.; Jin, C.; Jariwala, D.; Wu, D.; Li, Y.; Srivastava, A.; Wang, Z. F.; Storr, K.; Balicas, L. et al. Atomic layers of hybridized boron nitride and graphene domains. *Nat. Mater.* **2010**, *9*, 430-435.
- [6] Liu, Z.; Ma, L.; Shi, G.; Zhou, W.; Gong, Y.; Lei, S.; Yang, X.; Zhang, J.; Yu, J.; Hackenberg, K. P. et al. In-plane heterostructures of graphene and hexagonal boron nitride with controlled

- domain sizes. *Nat. Nanotechnol.* **2013**, *8*, 119-124.
- [7] Levendorf, M. P.; Kim, C.-J.; Brown, L.; Huang, P. Y.; Havener, R. W.; Muller, D. A.; Park, J. Graphene and boron nitride lateral heterostructures for atomically thin circuitry. *Nature* **2012**, *488*, 627-632.
- [8] Gong, Y.; Lin, J.; Wang, X.; Shi, G.; Lei, S.; Lin, Z.; Zou, X.; Ye, G.; Vajtai, R.; Yakobson, B. I. et al. Vertical and in-plane heterostructures from WS<sub>2</sub>/MoS<sub>2</sub> monolayers. *Nat. Mater.* **2014**, *13*, 1135-1142.
- [9] Duan, X.; Wang, C.; Shaw, J. C.; Cheng, R.; Chen, Y.; Li, H.; Wu, X.; Tang, Y.; Zhang, Q.; Pan, A. et al. Lateral epitaxial growth of two-dimensional layered semiconductor heterojunctions. *Nat. Nanotechnol.* **2014**, *9*, 1024-1030.
- [10] Sahoo, P. K.; Memaran, S.; Xin, Y.; Balicas, L.; Gutiérrez, H. R. One-pot growth of two-dimensional lateral heterostructures via sequential edge-epitaxy. *Nature* **2018**, *553*, 63-67.
- [11] Chen, K.; Wan, X.; Xie, W.; Wen, J.; Kang, Z.; Zeng, X.; Chen, H.; Xu, J. Lateral Built-In Potential of Monolayer MoS<sub>2</sub>-WS<sub>2</sub> In-Plane Heterostructures by a Shortcut Growth Strategy. *Adv. Mater.* **2015**, *27*, 6431-6437.
- [12] Zhang, S.; Liu, H.; Zhang, F.; Zheng, X.; Zhang, X.; Zhang, B.; Zhang, T.; Ao, Z.; Zhang, X.; Lan, X. et al. Controllable Synthesis of WSe<sub>2</sub>-WS<sub>2</sub> Lateral Heterostructures via Atomic Substitution. *ACS Nano* **2024**, *18*, 30321-30331.
- [13] Chang, K.; Ji, J.-R.; Gao, Z. A.; Huamán, A.; Cao, R.-Q.; Wang, W.-L.; Yue, C.; Liu, C.; Barraza-Lopez, S.; Parkin, S. S. P. Ferroelectrically switched valley-dependent transmission in SnTe-PbTe-SnTe monolayer lateral heterostructures. *Nat. Commun.* **2025**, *16*, 11063.
- [14] Naumis, G. G.; Herrera, S. A.; Poudel, S. P.; Nakamura, H.; Barraza-Lopez, S. Mechanical, electronic, optical, piezoelectric and ferroic properties of strained graphene and other strained monolayers and multilayers: an update. *Rep. Prog. Phys.* **2024**, *87*, 016502.
- [15] Li, M.-Y.; Shi, Y.; Cheng, C.-C.; Lu, L.-S.; Lin, Y.-C.; Tang, H.-L.; Tsai, M.-L.; Chu, C.-W.; Wei, K.-H.; He, J.-H. et al. Epitaxial growth of a monolayer WSe<sub>2</sub>/MoS<sub>2</sub> lateral p-n junction with an atomically sharp interface. *Science* **2015**, *349*, 524-528.
- [16] Xie, S.; Tu, L.; Han, Y.; Huang, L.; Kang, K.; Lao, K. U.; Poddar, P.; Park, C.; Muller, D. A.; DiStasio, R. A. et al. Coherent, atomically thin transition-metal dichalcogenide superlattices with engineered strain. *Science* **2018**, *359*, 1131-1136.
- [17] Yang, S.; Chen, Y.; Jiang, C. Strain engineering of two-dimensional materials: Methods, properties, and applications. *InfoMat* **2021**, *3*, 397-420.
- [18] Nguyen, K. X.; Jiang, Y.; Lee, C.-H.; Kharel, P.; Zhang, Y.; van der Zande, A. M.; Huang, P. Y. Achieving sub-0.5-angstrom-resolution ptychography in an uncorrected electron microscope. *Science* **2024**, *383*, 865-870.
- [19] Chang, K.; Villanova, J. W. D.; Ji, J.-R.; Das, S.; Küster, F.; Barraza-Lopez, S.; Sessi, P.; Parkin, S. S. P. Vortex-Oriented Ferroelectric Domains in SnTe/PbTe Monolayer Lateral Heterostructures. *Adv. Mater.* **2021**, *33*, 2102267.
- [20] Resta, R. Macroscopic polarization in crystalline dielectrics: the geometric phase approach. *Rev. Mod. Phys.* **1994**, *66*, 899-915.
- [21] Kresse, G.; Hafner, J. Ab initio molecular dynamics for liquid metals. *Phys. Rev. B* **1993**, *47*, 558-561.
- [22] Poudel, S. P.; Villanova, J. W.; Barraza-Lopez, S. Group-IV monochalcogenide monolayers: Two-dimensional ferroelectrics with weak intralayer bonds and a phosphorenelike monolayer

- dissociation energy. *Phys. Rev. Mater.* **2019**, *3*, 124004.
- [23] Soler, J. M.; Artacho, E.; Gale, J. D.; García, A.; Junquera, J.; Ordejón, P.; Sánchez-Portal, D. The SIESTA method for ab initio order- N materials simulation. *J. Phys.: Condens. Matter* **2002**, *14*, 2745.
- [24] Junquera, J.; Paz, Ó.; Sánchez-Portal, D.; Artacho, E. Numerical atomic orbitals for linear-scaling calculations. *Phys. Rev. B* **2001**, *64*, 235111.
- [25] Xie, Y.; He, Q.; Guo, J.; Li, X.; Wei, J.; Zhang, Y.; Gu, C.; Lu, P.; Shen, X. Dual-Polarity Response in Self-Powered Infrared SnTe Photodetector with Double Symmetric Schottky Junctions. *Adv. Opt. Mater.* **2024**, *12*, 2400632.
- [26] Song, L.; Tang, L.; Hao, Q.; Yang, C.; Teng, K. S.; Wang, H.; Yue, B.; Li, J.; Wei, H. Large-area SnTe nanofilm: preparation and its broadband photodetector with ultra-low dark current. *Opt. Express* **2022**, *30*, 14828-14838.
- [27] Panday, S. R.; Barraza-Lopez, S.; Rangel, T.; Fregoso, B. M. Injection current in ferroelectric group-IV monochalcogenide monolayers. *Phys. Rev. B* **2019**, *100*, 195305.
- [28] Wang, Z.; Wang, F.; Xu, G.; Cao, X.; Xi, Y.; Huang, Y.; Xu, X. Dispersion of Ultrafast Nonlinear Shift Current in SnTe Revealed by Photon-Energy-Dependent Terahertz Emission Spectroscopy. *Adv. Opt. Mater.* **2025**, *13*, 2403030.
- [29] Wang, L.; Moshwan, R.; Yuan, N.; Chen, Z.-G.; Shi, X.-L. Advances and Challenges in SnTe-Based Thermoelectrics. *Adv. Mater.* **2025**, *37*, 2418280.
- [30] Villanova, J. W.; Barraza-Lopez, S. Anomalous thermoelectricity at the two-dimensional structural transition of SnSe monolayers. *Phys. Rev. B* **2021**, *103*, 035421.
- [31] Haleoot, R.; Paillard, C.; Kaloni, T. P.; Mehboudi, M.; Xu, B.; Bellaiche, L.; Barraza-Lopez, S. Photostrictive Two-Dimensional Materials in the Monochalcogenide Family. *Phys. Rev. Lett.* **2017**, *118*, 227401.
- [32] Luo, D.; Zhang, B.; Sie, E. J.; Nyby, C. M.; Fan, Q.; Shen, X.; Reid, A. H.; Hoffmann, M. C.; Weathersby, S.; Wen, J. et al. Ultrafast Optomechanical Strain in Layered GeS. *Nano Lett.* **2023**, *23*, 2287-2294.
- [33] Schenk, F. M.; Zellweger, T.; Kumaar, D.; Bošković, D.; Wintersteller, S.; Solokha, P.; De Negri, S.; Emboras, A.; Wood, V.; Yarema, M. Phase-Change Memory from Molecular Tellurides. *ACS Nano* **2024**, *18*, 1063-1072.
- [34] Chang, K.; Miller, B. J.; Yang, H.; Lin, H.; Parkin, S. S. P.; Barraza-Lopez, S.; Xue, Q.-K.; Chen, X.; Ji, S.-H. Standing Waves Induced by Valley-Mismatched Domains in Ferroelectric SnTe Monolayers. *Phys. Rev. Lett.* **2019**, *122*, 206402.
- [35] Chang, K.; Kaloni, T. P.; Lin, H.; Bedoya-Pinto, A.; Pandeya, A. K.; Kostanovskiy, I.; Zhao, K.; Zhong, Y.; Hu, X.; Xue, Q.-K. et al. Enhanced Spontaneous Polarization in Ultrathin SnTe Films with Layered Antipolar Structure. *Adv. Mater.* **2019**, *31*, 1804428.
- [36] Kaloni, T. P.; Chang, K.; Miller, B. J.; Xue, Q.-K.; Chen, X.; Ji, S.-H.; Parkin, S. S. P.; Barraza-Lopez, S. From an atomic layer to the bulk: Low-temperature atomistic structure and ferroelectric and electronic properties of SnTe films. *Phys. Rev. B* **2019**, *99*, 134108.
- [37] Barraza-Lopez, S.; Fregoso, B. M.; Villanova, J. W.; Parkin, S. S. P.; Chang, K. Colloquium: Physical properties of group-IV monochalcogenide monolayers. *Rev. Mod. Phys.* **2021**, *93*, 011001.
- [38] Chang, K.; Liu, J.; Lin, H.; Wang, N.; Zhao, K.; Zhang, A.; Jin, F.; Zhong, Y.; Hu, X.; Duan, W. et al. Discovery of robust in-plane ferroelectricity in atomic-thick SnTe. *Science* **2016**, *353*,

274-278.

- [39] Ji, J.-R.; Gao, Z. A.; Poudel, S. P.; Cao, R.-Q.; Chen, T.; Li, L.; Liu, C.; Barraza-Lopez, S.; Parkin, S. S. P.; Chang, K. Surface Diffusion in SnTe-PbTe Monolayer Lateral Heterostructures. *Adv. Funct. Mater.* **2026**, e24380.
- [40] Zhang, C.; Li, M.-Y.; Tersoff, J.; Han, Y.; Su, Y.; Li, L.-J.; Muller, D. A.; Shih, C.-K. Strain distributions and their influence on electronic structures of WSe<sub>2</sub>-MoS<sub>2</sub> laterally strained heterojunctions. *Nat. Nanotechnol.* **2018**, *13*, 152-158.
- [41] Barraza-Lopez, S.; Kaloni, T. P.; Poudel, S. P.; Kumar, P. Tuning the ferroelectric-to-paraelectric transition temperature and dipole orientation of group-IV monochalcogenide monolayers. *Phys. Rev. B* **2018**, *97*, 024110.
- [42] Zhang, Y.; Baek, J.-H.; Lee, C.-H.; Jung, Y.; Hong, S. C.; Nolan, G.; Watanabe, K.; Taniguchi, T.; Lee, G.-H.; Huang, P. Y. Atom-by-atom imaging of moiré transformations in 2D transition metal dichalcogenides. *Sci. Adv.* **2024**, *10*, eadk1874.
- [43] Ederer, C.; Spaldin, N. A. Effect of Epitaxial Strain on the Spontaneous Polarization of Thin Film Ferroelectrics. *Physical Review Letters* **2005**, *95*, 257601.
- [44] Choi, K. J.; Biegalski, M.; Li, Y. L.; Sharan, A.; Schubert, J.; Uecker, R.; Reiche, P.; Chen, Y. B.; Pan, X. Q.; Gopalan, V. et al. Enhancement of Ferroelectricity in Strained BaTiO<sub>3</sub> Thin Films. *Science* **2004**, *306*, 1005-1009.
- [45] Hÿtch, M. J.; Snoeck, E.; Kilaas, R. Quantitative measurement of displacement and strain fields from HREM micrographs. *Ultramicroscopy* **1998**, *74*, 131-146.
- [46] Rivero, P.; Garcia-Suarez, V. M.; Pereniguez, D.; Utt, K.; Yang, Y.; Bellaiche, L.; Park, K.; Ferrer, J.; Barraza-Lopez, S. Systematic pseudopotentials from reference eigenvalue sets for DFT calculations. *Comput. Mater. Sci.* **2015**, *98*, 372-389.

## Electronic Supplementary Material

### Asymmetric strain distribution in ferroelectric/paraelectric SnTe-PbTe monolayer lateral heterostructures

Zi'Ang Gao<sup>1</sup>, Jing-Rong Ji<sup>2</sup>, Shiva Prasad Poudel<sup>3</sup>, Jose D. Mella<sup>3</sup>, Wen-Lin Wang<sup>1</sup>,  
Chengguang Yue<sup>1</sup>, Chong Liu<sup>1</sup>, Stuart S. P. Parkin<sup>2</sup>, Salvador Barraza-Lopez<sup>3,4,\*</sup> and  
Kai Chang<sup>1,\*</sup>

<sup>1</sup>*Beijing Key Laboratory of Fault-Tolerant Quantum Computing, Beijing Academy of Quantum Information Sciences, Beijing 100193, China*

<sup>2</sup>*Max Planck Institute for Microstructure Physics, Weinberg 2, Halle 06120, Germany*

<sup>3</sup>*Department of Physics, University of Arkansas, Fayetteville, Arkansas 72701, USA  
and MonArk NSF Quantum Foundry, University of Arkansas, Fayetteville, Arkansas  
72701, USA*

<sup>4</sup>*Institute for Solid State Physics, University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa,  
Chiba 277-8581, Japan*

\*Address correspondence to Kai Chang, changkai@baqis.ac.cn; Salvador Barraza-Lopez, sbarraza@uark.edu

Supporting information to <https://doi.org/10.26599/NR.2026.94909142>

## 1. Determination of Lattice Constants from Moiré-Spot Fourier Analysis

Figure S1 shows the Fourier-transform (FT) analysis used to quantify lattice and rotational variations. In the experimental FT (Fig. S1a), the moiré spots are highlighted by red circles. Only three moiré spots ( $M_1$ ,  $M_2$ , and  $M_3$ ) are labeled explicitly; the other three moiré spots are related to these by inversion symmetry about the FT origin. The SnTe monolayer Bragg spots are highlighted by yellow circles. Two of the four Bragg spots ( $A_1$  and  $A_2$ ) are labeled (the remaining two, appearing at the bottom of the image, are their inversion-symmetric counterparts).

To track the reciprocal-space displacement of these peaks, we connect selected spots to the FT origin  $O$  and define the vectors  $OM_1$ ,  $OM_2$ ,  $OA_1$ , and  $OA_2$ . These vectors are shown in the simulated FT (Fig. S1b) for clarity ( $OM_1$  and  $OM_2$  are shown in red;  $OA_1$ , and  $OA_2$  in yellow). The simulated FT reproduces the experimental FT closely, confirming the quality of the fit.  $\theta$  is defined as the angle between the basis vector of graphene and the  $OA_1$  direction of the SnTe monolayer. When  $a_2$  and  $\theta$  are held fixed and  $a_1$  is varied, the moiré vector  $OM_1$  and the Bragg vector  $OA_1$  shift approximately along the same direction (Fig. S1c). Likewise, when  $a_1$  and  $\theta$  are held fixed and  $a_2$  is varied,  $OM_2$  and  $OA_2$  move approximately along the same direction (Fig. S1d). In addition, changing the relative rotation angle  $\theta$  between the SnTe/PbTe monolayers and graphene leads to a systematic displacement (rotation) of the moiré spots (Fig. S1e).

The moiré spots are more sensitive to changes in lattice parameters than the Bragg spots (i.e., the former move over a larger range). Therefore, we selected the moiré spots with the largest displacement to determine the lattice parameters.

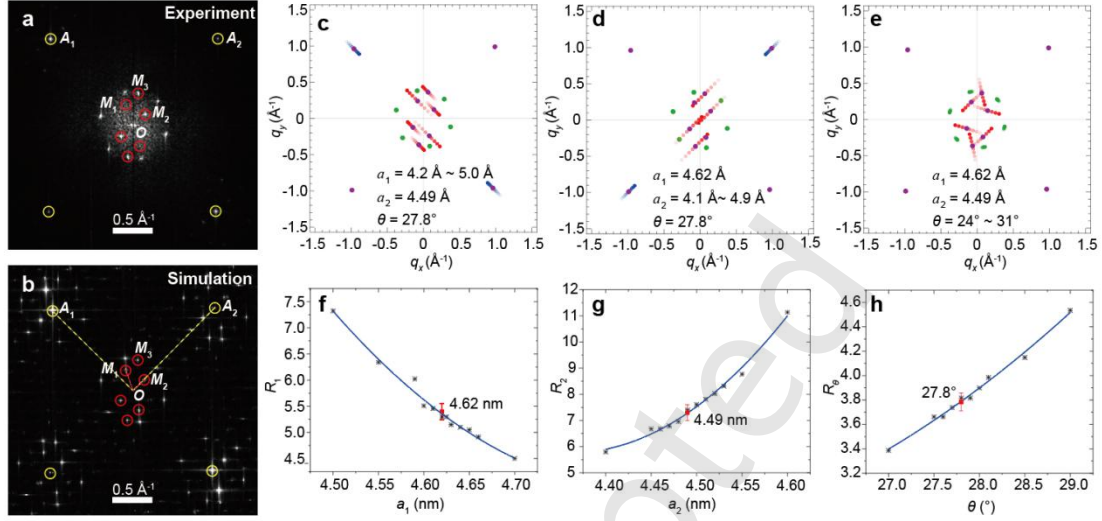
We first roughly measure  $a_1$ ,  $a_2$ , and  $\theta$  directly from the FT images, the measurement provides a basic range for optimizing the moiré pattern simulation. We then simulated multiple moiré pattern FT images by varying  $a_1$ ,  $a_2$ , and  $\theta$  independently, and calculated the ratios

$$R_1 = \frac{|OA_1|}{|OM_1|}, R_2 = \frac{|OA_2|}{|OM_2|}, R_\theta = \frac{|OA_3|}{|OM_2|},$$

where  $|OM_i|$  and  $|OA_i|$  are the distances from the FT origin  $O$  to the selected moiré spot  $M_i$  and Bragg spot  $A_i$ , respectively. Within a small parameter range ( $\pm 0.1$  Å for  $a_1$  and  $a_2$ , and  $\pm 1^\circ$  for  $\theta$ ),  $R_1$ ,  $R_2$ , and  $R_\theta$  are monotonic functions of  $a_1$ ,  $a_2$  and  $\theta$  respectively. Since there are three parameters to optimize, the simulation was performed in an iterative way: we first fix  $a_2$ ,  $\theta$  and vary  $a_1$ ; then vary  $a_2$  with the other two parameters fixed; and finally vary  $\theta$ . This optimization loop was carried out several times until the obtained lattice parameters are stable within the ranges of  $\pm 0.02$  Å and  $\pm 0.1^\circ$ .

Notably, the ratios  $R_i$  act as a self-calibrating factor that can minimize systematic errors such as the nonlinear response of the piezo actuators in the STM scanner, calibration errors, and thermal drift of the sample. When those systematic errors are stable within a single image, they can be largely eliminated by this self-calibrating method because they apply the same distortion to  $OM_i$  and  $OA_i$  and therefore do not

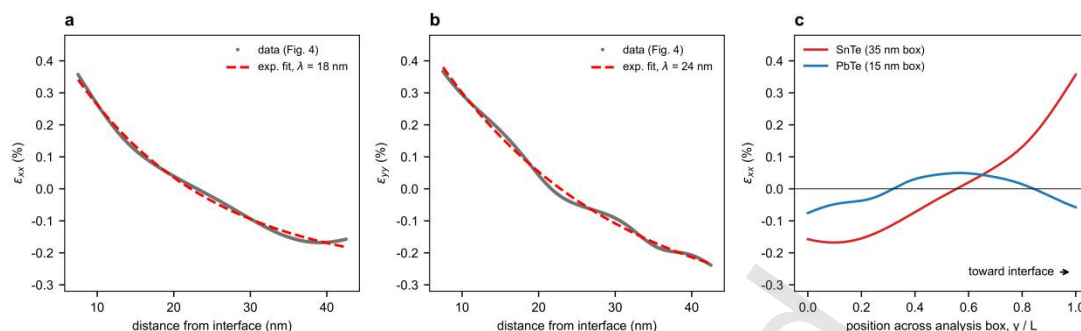
significantly affect  $R_i$ . This method reduces the uncertainty in  $a_1$  and  $a_2$  to  $\sim 0.01$ - $0.02$  Å, and the uncertainty in  $\theta$  to  $\sim 0.1^\circ$ . The analysis above suggests that SnTe monolayer sections experience a larger lattice strain than PbTe monolayer sections.



**Figure S1.** Self-calibrating method for determining the lattice parameters utilizing the moiré patterns formed by the overlapping graphene and SnTe/PbTe monolayer lattices. **a**, Fourier transformed image of the data in Figure 3b, which corresponds to the SnTe monolayer part of a PoS LHS. **b**, The Fourier transformed image of a simulated pattern with the superposition of a SnTe monolayer, graphene, and SiC(0001)-(6×6) lattices. The optimal lattice parameters of the SnTe monolayer are  $a_1 = 4.62 \pm 0.01$  Å and  $a_2 = 4.49 \pm 0.01$  Å. **c-e**, Movement of moiré spots in response to the variation of  $a_1$ ,  $a_2$  and  $\theta$ . Here  $\theta$  is defined as the angle between the basis vector of graphene and the  $OA_1$  direction of the SnTe monolayer. The lighter to darker red spots in **c** indicate the trace of the movement of moiré spots in response to the change of  $a_1$  from 4.2 Å to 5.0 Å, while  $a_2$  and  $\theta$  are fixed. Similar demonstrations of changing  $a_2$  and  $\theta$  are displayed in **d** and **e**. **f-h**, Method to determine lattice parameters from the moiré pattern. We define three ratios between the magnitudes of reciprocal vectors:  $R_1 = OA_1/OM_1$ ,  $R_2 = OA_2/OM_2$ , and  $R_\theta = OA_2/OM_3$ . These ratios change monotonically with  $a_1$ ,  $a_2$  and  $\theta$ , thus the lattice parameters can be extracted by finding the experimental values from the curves. The error bars correspond to the uncertainty of measuring the ratios from the experimental data.

## 2. Strain Relaxation Length in the SnTe Monolayer Section

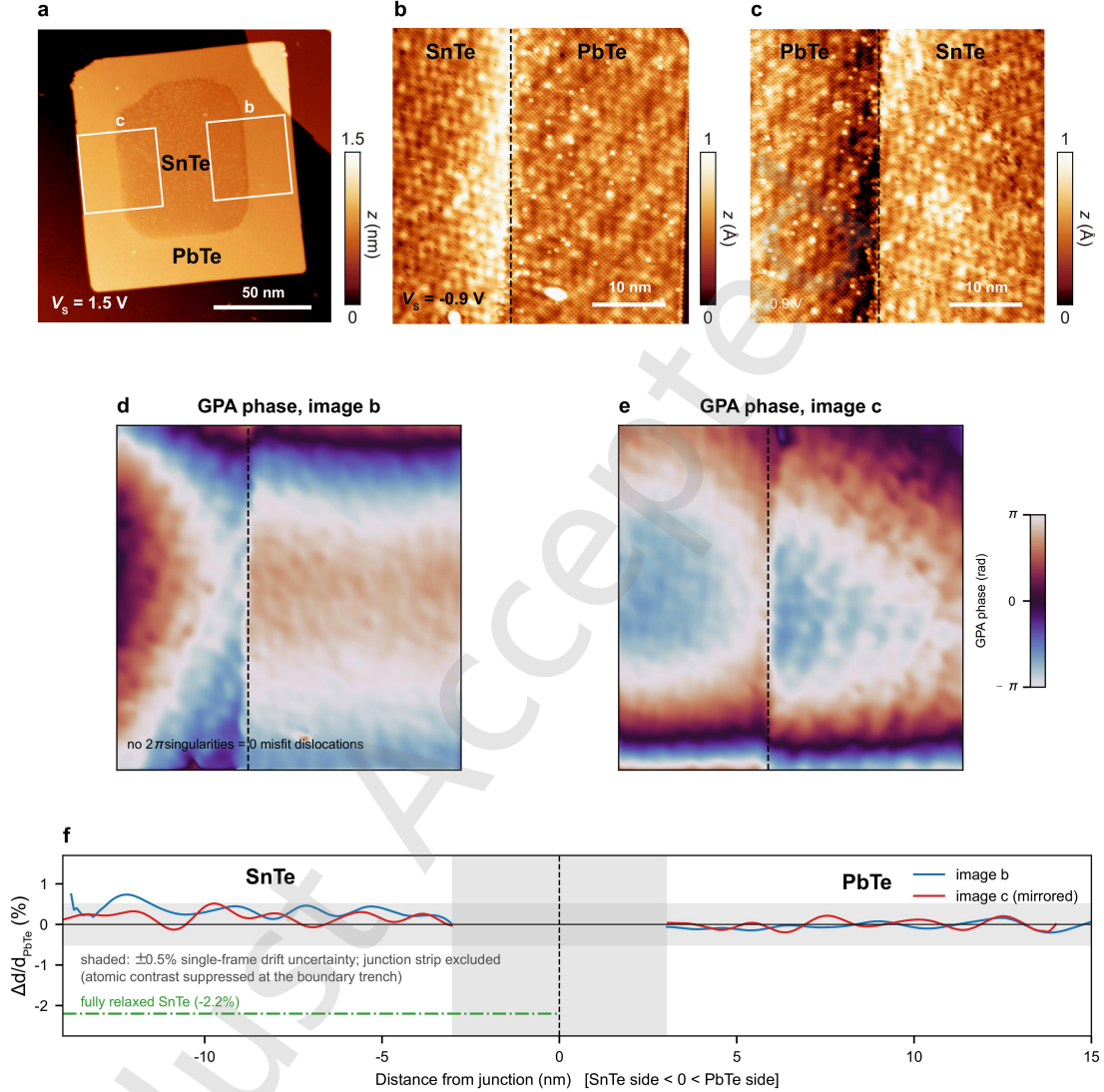
Figure S2 quantifies the strain relaxation length in the SnTe monolayer section from the GPA data of Figure 4.



**Figure S2.** Strain relaxation length in the SnTe monolayer section. **a**, Laterally averaged  $\epsilon_{xx}$  extracted from the GPA map in Figure 4b, plotted against the distance from the SnTe-PbTe interface. The red dashed line is a fit to an exponential decay, which describes the profile well and gives a relaxation length  $\lambda = 18$  nm. **b**, The same analysis for  $\epsilon_{yy}$  from the GPA map in Figure 4c, giving  $\lambda = 24$  nm. The fitted  $\lambda$  is insensitive to the exact position assumed for the interface. **c**, Laterally averaged  $\epsilon_{xx}$  of the SnTe and PbTe analysis regions in Figure 4, plotted against the normalized position across each analysis box ( $y/L$ , with  $L = 35$  nm for SnTe and 15 nm for PbTe). A monotonic trend toward the interface is present only in the SnTe section; the net  $\epsilon_{xx}$  variation across the PbTe box is  $\sim 0.05\%$ .

### 3. Atomic-Resolution Imaging Across the SnTe-PbTe Junction

Figure S3 shows single-frame atomic-resolution STM imaging across the SnTe-PbTe monolayer junction of a lateral heterostructure island. The island consists of a SnTe monolayer core laterally enclosed by a PbTe monolayer section, and it was grown by the same lateral epitaxy procedure as the other heterostructures in this work.



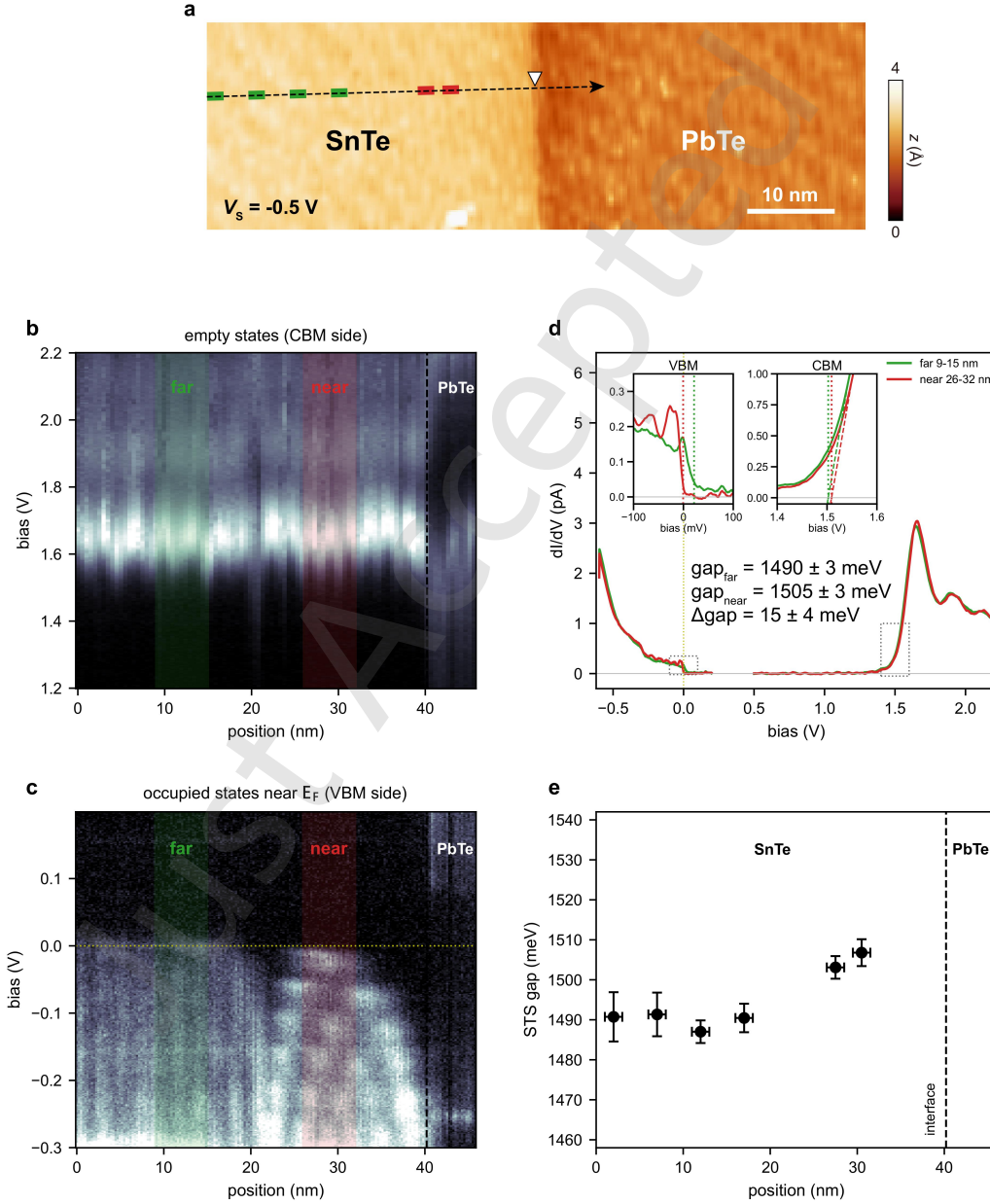
**Figure S3.** Atomically coherent SnTe-PbTe lateral junction imaged within single STM frames. **a**, Overview image ( $V_s = +1.5$  V,  $I = 10$  pA,  $150 \times 150$  nm<sup>2</sup>,  $T = 4.7$  K) of a lateral heterostructure island consisting of a SnTe core laterally enclosed by PbTe grown from its edges. White boxes mark the locations of panels b and c. **b**, **c**, Atomic-resolution images ( $V_s = -0.9$  V,  $I = 50$  pA,  $40 \times 40$  nm<sup>2</sup>) across two opposite segments of the junction, forming a mirror pair: SnTe left / PbTe right in b, reversed in c. At this bias the SnTe surface appears brighter; the dashed line marks the junction. The topographs are shown with line-wise background subtraction for display only; all quantitative analysis was performed on the raw data. **d**, **e**, GPA phase maps of the atomic rows in b and c, respectively (phase referenced to the PbTe-side mean of each frame; regions with negligible atomic contrast are left blank). The phase varies smoothly across the junction, with no  $2\pi$  fork singularities, the signature of a misfit

dislocation, in either image or scan direction: zero misfit dislocations are detected along the >100 nm of junction sampled in these and two additional frames (not shown), whereas relaxation of the 2.2% mismatch at the boundary would require one edge dislocation every ~20 nm. The slow smooth phase variations lie at the sub-percent level of the single-frame systematics and are not interpreted; only the topology of the phase enters the analysis. **f**, Row-spacing profiles perpendicular to the junction for the mirror pair: local spacing of the Bragg-filtered row family (one projection of the in-plane lattice), averaged along the junction (forward/backward scans averaged; no detrending), referenced to the PbTe-side mean of each frame; the  $\pm 3$  nm junction strip is excluded because the atomic contrast is suppressed in the boundary trench, and image c is mirrored so that the SnTe side lies at negative distances.

No lattice discontinuity is resolved at the junction: the profiles stay within the  $\pm 0.5\%$  single-frame drift uncertainty (gray band in Figure S3f), far from the  $-2.2\%$  step expected for an incoherent boundary (green dash-dotted line in Figure S3f). The sub-percent strain relaxation itself cannot be separated from the single-frame systematics here: the expected relaxation profile (dark-green dashed curve;  $\lambda \approx 20$  nm with the amplitude measured in Figure 4b) lies entirely within the gray band, and the relaxation is quantified instead by the large-area GPA of Figure 4 and Figure S2. Together, the data establish an atomically coherent junction whose lattice mismatch is accommodated by the long-range elastic strain quantified in Figure 4.

#### 4. Scanning Tunneling Spectroscopy Across a SnTe-PbTe Monolayer Junction

Figure S4 presents spatially resolved  $dI/dV$  spectroscopy acquired along a line crossing the SnTe-PbTe monolayer junction of a lateral heterostructure grown by the lateral epitaxy procedure of Refs. 13 and 39 of the main text; the  $\sim 45$ -nm segment spanning the SnTe interior and the junction is shown. Empty-state and occupied-state line maps were recorded along the identical path, so that the conduction- and valence-band edges, and hence the local gap, can be followed as a function of distance from the junction.



**Figure S4.** Spatially resolved  $dI/dV$  across a SnTe-PbTe monolayer lateral junction. **a**, STM topography of the junction region ( $V_s = -0.5$  V,  $I = 10$  pA;  $80 \times 25$  nm<sup>2</sup>). The dashed arrow marks the  $dI/dV$  line-spectroscopy path and the triangle marks the junction, located at position 40 nm along the line; green and red blocks mark the far (9-15 nm) and near (26-32 nm) analysis windows. **b**, Empty-state  $dI/dV$  line map (2.5

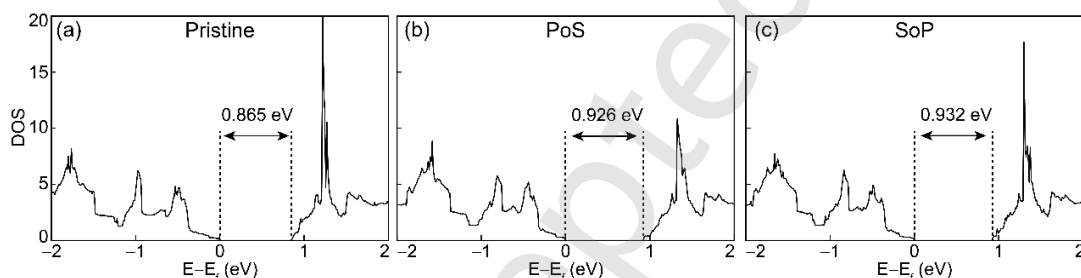
to 0.5 V, lock-in modulation 20 mV) covering the SnTe conduction-band edge. **c**, Occupied-state dI/dV line map near  $E_F$  (−0.6 to 0.2 V, modulation 6 mV) covering the SnTe valence-band edge; the arc-like features within ~20 nm of the junction arise from in-plane scattering at ferroelectric domain walls (Ref. 13 of the main text) and preclude a meV-level valence-edge reading there. **d**, Window-averaged spectra from the two equal-width windows; the insets zoom on the valence- and conduction-band edges. The conduction-band edge is read by linear extrapolation of the rising edge to the in-gap baseline (dashed lines); the valence-band edge is read directly, as the first rise above the in-gap noise floor (dotted lines). The quoted gap values are means of the individual 2-nm-window readings of panel e. **e**, STS gap versus position along the line (2-nm windows on a regular grid; error bars give the systematic spread of the reading criteria; positions 18-26 nm are omitted because of the domain-wall scattering visible in c). See text for the interpretation of the small gap difference between the two windows.

Two observations follow: First, the band edges are spatially uniform in the SnTe monolayer interior: in the wall-free region far from the junction the gap is constant at  $1490 \pm 3$  meV, with a spread of only a few meV over distances across which the misfit strain relaxes (Figure S2), and the absolute gap agrees with the published spectroscopy of this system (Ref. 13 of the main text). The electrostatic band bending of the junction itself is confined to within a few nanometers by the metallic screening of the graphene substrate, and the occupied-state map resolves the standing waves produced by in-plane scattering at ferroelectric domain walls (Ref. 13 of the main text). Second, the apparent gap in the near window is larger by only  $15 \pm 4$  meV, a magnitude consistent with our calculations once the partial relaxation of the misfit strain between the two windows is accounted for. Since scattering at the domain walls that bound this small domain can shift the apparent band edges by a comparable amount, we regard this agreement as a consistency check rather than an isolated measurement of the strain effect.

## 5. Electronic Band Gap of Strained SnTe Monolayers

We applied the experimentally determined strain to the lattice parameters of the reference theoretical structure (Ref. 22 of the main text). The resulting strains are  $\sim 0.87\%$  along  $a_1$  and  $\sim 1.13\%$  along  $a_2$  for PoS, and  $\sim 1.31\%$  along  $a_1$  and  $\sim 0.68\%$  along  $a_2$  for SoP. The lattice parameters using the optPBE-vdW functional are  $a_1 = 4.642$  Å,  $a_2 = 4.577$  Å for pristine SnTe,  $a_1 = 4.683$  Å,  $a_2 = 4.628$  Å for PoS, and  $a_1 = 4.703$  Å,  $a_2 = 4.608$  Å for SoP.

The density of states of pristine and strained SnTe was calculated with VASP, using a Monkhorst-Pack k-point mesh and 2000 energy grid points, to study the effect of strain on the electronic band gap. Figure S5 presents the density of states and the corresponding energy gaps. The electronic band gap increases by comparable amounts under the two strain conditions: 61 meV for PoS and 67 meV for SoP.



**Figure S5.** Density of states for **a**, pristine SnTe, **b**, PoS, and **c**, SoP.  $E_f$  is the Fermi energy, aligned with the VBM. The left and right dotted vertical lines correspond to the VBM and CBM, respectively. The numerical value indicates the electronic band gap.

## 6. Relaxed Lattice Parameters of Group-IV Monochalcogenide Monolayers

Table S1 lists the relaxed in-plane lattice parameters of group-IV monochalcogenide monolayers computed with eleven exchange-correlation functionals, taken from the Supplemental Material of Ref. 22 of the main text.

**Table S1.** Relaxed in-plane lattice parameters (Å) of group-IV monochalcogenide monolayers across eleven exchange-correlation functionals, reproduced from the Supplemental Material of Ref. 22 of the main text (Poudel *et al.*, Phys. Rev. Mater. **3**, 124004 (2019)). All Pb-based monolayers (PbS, PbSe, PbTe) relax to a square lattice ( $a_1 = a_2$ ) with five-fold-coordinated cations for every functional listed. SnSe relaxes to an orthorhombic lattice ( $a_1 > a_2$ ) with three-fold-coordinated cations for all functionals except LDA and vdW-DF-CX, which are known to overbind and yield square lattices. The same orthorhombic, three-fold-coordinated ground state holds for SnS and SnTe monolayers (Refs. 22, 36, and 38 of the main text), consistent with the experimentally measured orthorhombic lattice of SnTe in this work. This cation-controlled contrast in coordination underlies the difference in stiffness discussed in the main text.

| Functional         | SnSe $a_1/a_2$  | PbS $a_1/a_2$   | PbSe $a_1/a_2$  | PbTe $a_1/a_2$  |
|--------------------|-----------------|-----------------|-----------------|-----------------|
| LDA                | 4.1924 / 4.1924 | 4.1187 / 4.1187 | 4.2771 / 4.2771 | 4.5092 / 4.5092 |
| PBE                | 4.3818 / 4.2936 | 4.2369 / 4.2369 | 4.4007 / 4.4007 | 4.6383 / 4.6383 |
| PBE LASPH          | 4.3850 / 4.2927 | 4.2371 / 4.2371 | 4.4010 / 4.4010 | 4.6388 / 4.6388 |
| optPBE-vdW         | 4.4697 / 4.2948 | 4.2514 / 4.2514 | 4.4216 / 4.4216 | 4.6604 / 4.6604 |
| optPBE-vdW LASPH   | 4.4718 / 4.2938 | 4.2515 / 4.2515 | 4.4217 / 4.4217 | 4.6607 / 4.6607 |
| optB86-vdW LASPH   | 4.3019 / 4.2699 | 4.1966 / 4.1966 | 4.3634 / 4.3634 | 4.5948 / 4.5948 |
| vdW-DF2            | 4.7903 / 4.3636 | 4.3556 / 4.3556 | 4.5412 / 4.5412 | 4.8029 / 4.8029 |
| vdW-DF2 LASPH      | 4.7857 / 4.3653 | 4.3556 / 4.3556 | 4.5408 / 4.5408 | 4.8026 / 4.8026 |
| vdW-DF2-B86R LASPH | 4.3280 / 4.2736 | 4.2043 / 4.2043 | 4.3718 / 4.3718 | 4.6061 / 4.6061 |
| vdW-DF-CX LASPH    | 4.2534 / 4.2534 | 4.1759 / 4.1759 | 4.3405 / 4.3405 | 4.5685 / 4.5685 |
| SCAN+rVV10 LASPH   | 4.4586 / 4.2041 | 4.1962 / 4.1962 | 4.3590 / 4.3590 | 4.5881 / 4.5881 |