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Strain control of the electronic structure in WS₂ homobilayers with 0° and 60° stacking angles

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Two-dimensional transition metal dichalcogenides combine attractive semiconductor properties with exceptionally strong light–matter interaction. Their mechanical robustness allows the modulation of their optical and electronic functionalities *via* strain. Bilayers introduce the stacking angle as an additional parameter, whose role in the strain response is still elusive. Here, we combine differential reflectance spectroscopy and density functional theory calculations to explore the strain response of WS₂ homobilayers with 0° and 60° stacking angles. The change of the excitonic resonance energies and linewidths depends on the stacking angle, highlighting the scope for the manipulation of the electronic structure of two-dimensional semiconductors *via* the synergistic harnessing of the strain and angle control parameters.

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Introduction

Two-dimensional transition metal dichalcogenides (TMDCs) combine attractive semiconductor properties and mechanical and chemical robustness with exceptionally strong light–matter interaction. As evidence of this, TMDC monolayers with sub-nanometer thickness have demonstrated a range of optical phenomena, including photodetection,¹ photovoltaics,² saturable absorption,³ optical gain,⁴ photocatalysis,⁵ electrooptical modulation,⁶ and optical parametric amplification.⁷

Strain can significantly modulate the band structure of TMDCs,^{8–19} resulting in a red-shift of the excitonic resonances by several tens of meV per % of uniaxial strain^{8–23} and, in some cases, inducing a crossover between direct and indirect semiconductor behavior.^{10,13,16} Moreover, strain also influences the strength of the electron–phonon coupling,^{24–28} resulting in a variation in the spectral linewidth of the exciton features and charge carrier mobility.^{29–32}

Experimental investigation of TMDCs' optical properties under strain has so far been largely limited to monolayer material. In bilayer TMDCs, the second atomic layer commonly

adopts specific stacking orientations, such as 0° rotation or 60° rotation, due to their enhanced thermodynamic stability compared to other possible configurations.³³ The few existing works on bilayer material have found direct-to-indirect bandgap transitions,^{13,14,16,25,34} a change in the exciton-phonon coupling³⁵ and a modulation of the Stokes shift.³⁶ None of the existing studies has yet assessed the role of the interlayer stacking angle in the strain response.

Here, we study the strain tunable optical properties of WS₂ homobilayers in 0° and 60° stacking configurations through combination of differential reflectance contrast (DR) and density functional theory (DFT) calculations. Experiments and calculations yield consistent linear strain gauge factors (GFs) that are slightly higher for the A exciton compared to the B exciton. Additionally, the measured strain GFs are about 25% higher for 60° stacking relative to 0° stacking. Our results are a first step toward a synergistic use of strain and stacking in the modulation of the electronic structures of two-dimensional semiconductors.

Methods

The WS₂ bilayer flakes were grown using a modified one-zone chemical vapor deposition process, as shown in our previous reports.^{33,37,38} First, the metal source WO₃ powder (Alfa Aesar, 99.8%) was loaded into the boat with the SiO₂/Si substrate facing the source materials. The source boat was placed at the center part of the growth furnace. Then, the sulfur powder was loaded onto the edge of the furnace with a movable inner tube and heated above 100 °C for more than 15 min to eliminate

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the water inside before growth. The furnace was then heated up to 750–850 °C with a heating rate of 25–30 °C min⁻¹ and kept at the growth temperature for 3–10 min. After growth, the furnace was cooled below 300 °C and then was opened for fast cooling to below 100 °C and the substrate was removed.

The flakes are transferred onto a flexible polycarbonate (PC) substrate with a thickness of 250 μm using a wet transfer method. A polydimethylsiloxane (PDMS) carrier substrate is first attached to the sample containing the WS₂ flakes. This assembly is then immersed in deionized water containing a small amount of ammonia, which facilitates the detachment of the PDMS layer along with the adhered flakes from the Si substrate. After detaching, the PDMS carrying the flakes is analyzed under the microscope to identify the flakes most suitable for transfer. The flakes are then mechanically transferred by gently pressing the PDMS against the PC substrate to ensure good contact, and by carefully peeling off the PDMS, leaving the WS₂ flakes securely attached to the PC substrate.³⁹

To apply controlled uniaxial strain to the WS₂ flakes, a three-point bending setup adapted from ref. 40 and depicted in Fig. 1, right, was used. It consists of two identical manual linear micrometer Z stages, fixed onto a steel plate and supplemented with two homebuilt steel parts to attach the three cylinders that act as the pivots of the three-point-bending setup. The sample is placed in the central pivot, while the other pivots deflect the substrate from the sides, bending the sample and thus generating the uniaxial strain. This design ensures that the position of the sample remains nearly unchanged during the strain loading/unloading cycles. This eliminates the need for re-focusing and re-positioning the sample upon changing the strain in the optical measurements. We can achieve micrometric precision in controlling the deflection of the substrate, *i.e.* the displacement along the z-axis of the outer pivots. The applied strain ϵ is related to the distance D between the pivotal points, the deflection L , and the thickness t of the substrate by the following formula:

$$\epsilon = \frac{6Lt}{D^2} \quad (1)$$

This formula has been validated experimentally in ref. 40.

Calculations of the ground-state electronic properties were carried out by using the GPAW open-source code⁴¹ with a plane-wave cutoff energy of 600 eV. We use the van der Waals dispersion corrections vdW-DF⁴² and vdW-DF2⁴³ for the exchange–correlation functional. The momentum grid for ground-state self-consistent calculations was set to $k = 24 \times 24 \times 1$, and we used Fermi–Dirac smearing with 0.01 eV broadening. Original unstrained structures were relaxed both in lateral and perpendicular directions, while for the strained slabs we only perform the interlayer relaxation. With vdW-DF, this gives $a = 3.186$ Å for both 0° and 60° stacking angles, and W–W interlayer distances of $d = 6.655$ Å and $d = 6.662$ Å for 60° and 0° stackings, respectively. When the relaxation is done with vdW-DF2, we get the same unit cell parameter a , while W–W distances for 60° and 0° stackings are $d = 6.578$ Å and $d = 6.583$ Å. For both stackings we obtain an S–S distance within the layer of 3.19 Å (3.23 Å) with vdW-DF (vdW-DF2). For a more accurate description of the quasiparticle spectra, we use both the HSE⁴⁴ and many-body G₀W₀ corrections.⁴⁵ In the latter case we used $k = 24 \times 24 \times 1$ points and 80 bands in order to converge the screened Coulomb propagator, and we used 80 eV energy cutoff for the G vectors. The quasiparticle G₀W₀ correction was applied only to the relevant top-most two valence bands, and to the lowest two conduction bands.

The calculations of the electron–phonon interaction were performed by means of density functional perturbation theory⁴⁶ and the Wannier interpolation⁴⁷ scheme as implemented in QuantumEspresso⁴⁸ and EPW⁴⁹ codes. Here we tried to use the same parameters as in GPAW calculations in order to match the electronic properties as obtained with the two codes. For the pseudopotentials we used the norm-conserving PBE functional from the PseudoDojo library,⁵⁰ and we also use vdW-DF dispersion correction. The lattice parameters were the same as in GPAW inputs. For the phonon calculations we used $k = 12 \times 12 \times 1$ and $q = 6 \times 6 \times 1$ grids. In EPW calculations we use 22 maximally localized Wannier functions with the initial projections of d orbitals on the W sites and p orbitals on the S atom sites. Calculations of the Fan-Migdal electron self-energy that accounts for the electron–phonon coupling within the band structures⁵¹ are carried out on a $q = 120 \times 120 \times 1$ momentum grid.

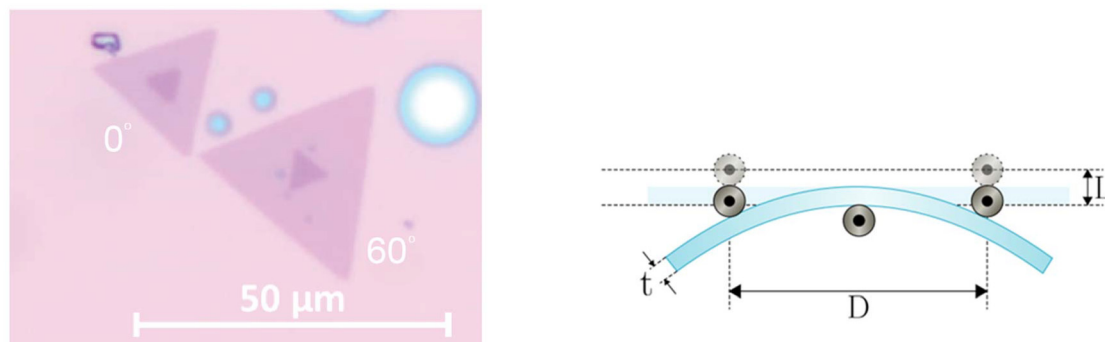


Fig. 1 Optical micrograph of as-grown bilayer flakes grown on SiO₂/Si before their transfer (left), and a scheme of the 3-point bending setup for strain investigation under an optical microscope (right).



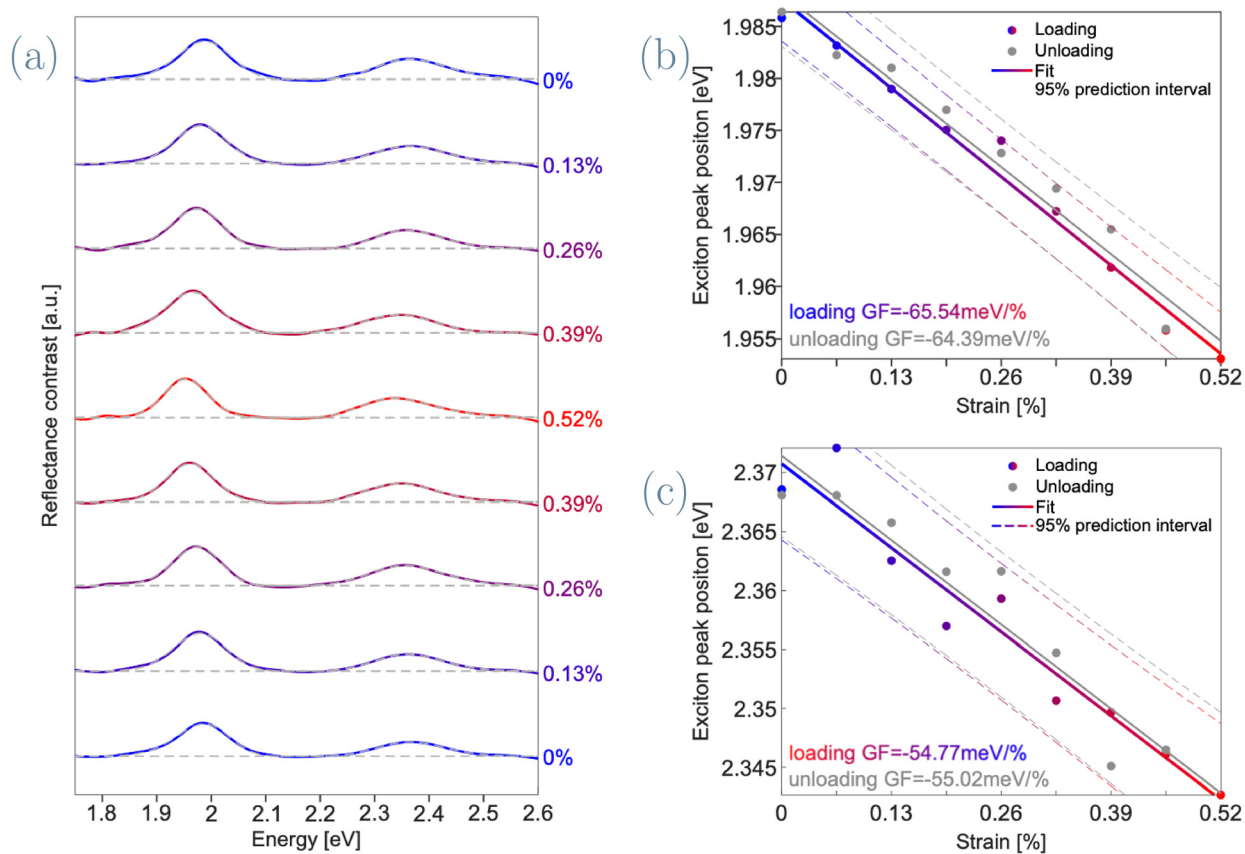


Fig. 2 (a) DR spectra of a 0° stacked WS₂ flake under strain from 0% to 0.52% and back to 0%. The curves are vertically shifted for clarity and drawn bottom to top in order of data acquisition. Determination of the strain GFs for the A exciton resonance (b) and the B exciton resonance (c).

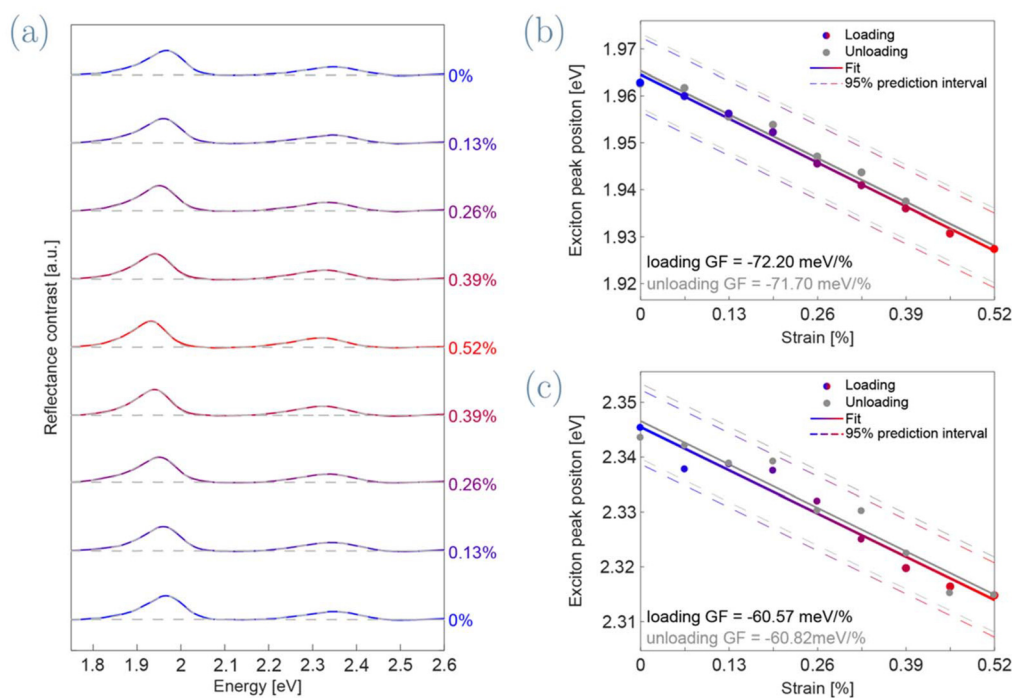


Fig. 3 (a) DR spectra of a 60° stacked WS₂ flake under strain from 0% to 0.52% and back to 0%. The curves are vertically shifted for clarity and drawn from bottom to top in order of data acquisition. Determination of the strain GFs for the A exciton resonance (b) and the B exciton resonance (c).



Results and discussion

Bilayer flakes with 0° and 60° stacking angles were synthesized using chemical vapor deposition.^{33,37,38} Representative optical micrographs of both stackings are shown in Fig. 1, left. The flakes are either hexagonal or triangular in shape, with the hexagonal ones typically having three long and three short edges, resembling triangles with truncated corners. Typical edge lengths of the (truncated) triangles are tens of μm . For 0° stacking, both top and bottom WS_2 layers appear as flakes with their (truncated) triangles oriented parallel to each other, while for 60° stacking they are rotated by 60° .^{52–57}

For strain dependent DR spectroscopy, a total of twelve flakes of 0° and thirteen flakes of 60° stacking angle were transferred onto flexible PC substrates. The DR is measured by illuminating the sample on a spot approximately $1.5 \mu\text{m}$ in diameter with white light from a halogen lamp and collecting

the reflected light. Strain is applied by bending the substrate in a loading (increasing strain) followed by an unloading sequence.⁵⁸ The DR spectra, shown in Fig. 2 and 3 for one example of each stacking angle, are dominated by the absorption of WS_2 , showing the characteristic A and B exciton resonances.^{59,60} To analyze the strain-dependent changes in the electronic structure, we fitted these spectra with a second-order polynomial to account for the scattering background and two skewed Gaussians to represent the main peaks broadened by electron–phonon coupling.^{61,62} For the unstrained samples, we obtained the A and B resonances at $1.979 \pm 0.002 \text{ eV}$ and $2.357 \pm 0.002 \text{ eV}$ for 0° stacking and $1.986 \pm 0.003 \text{ eV}$ and $2.371 \pm 0.006 \text{ eV}$ for 60° stacking. In both cases, the A and B resonances shift linearly to the red with increasing strain and reproducibly return almost to their original spectral positions upon strain release with only minor hysteresis. The slopes of the linear fits in Fig. 2b, c and 3b,c yield the experimental strain GFs.

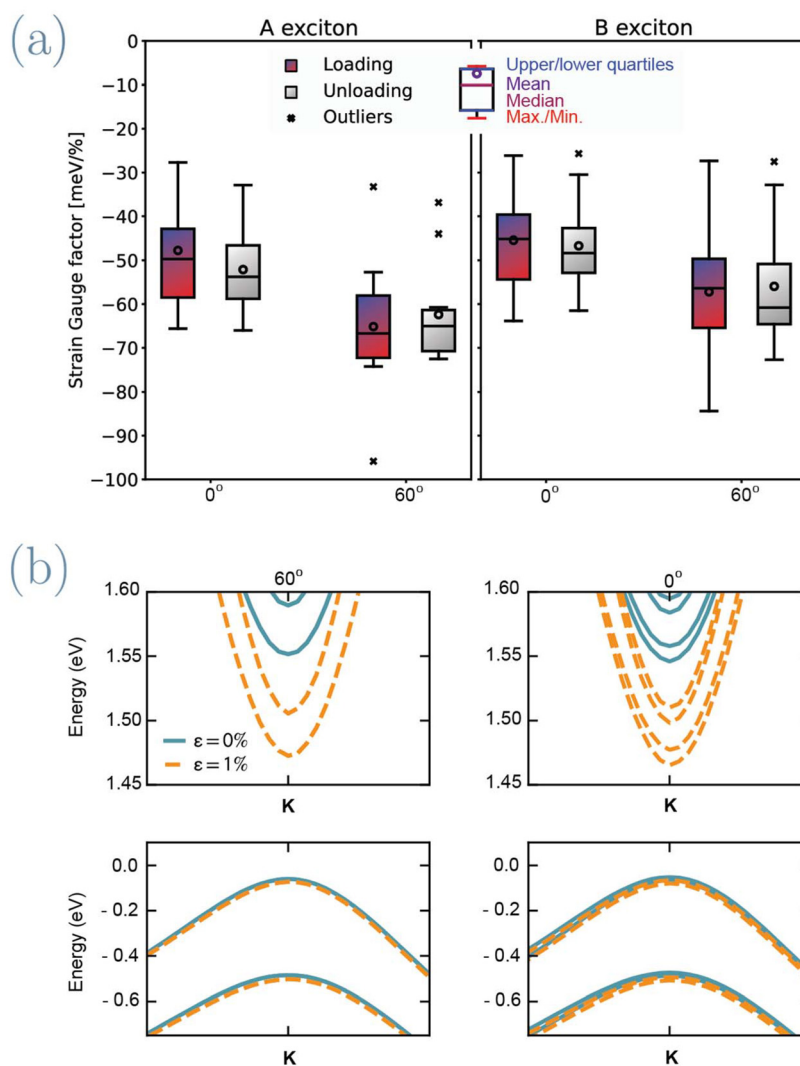


Fig. 4 (a) Statistical analysis of the strain GFs for excitons A and B in 0° and 60° stacking bilayers of WS_2 on various flakes. (b) The energy bands of bilayer WS_2 for 0° and 60° stacking angles calculated using density functional theory.



The statistical analysis of the 12 0°-stacked and the 13 60°-stacked flakes shown in Fig. 4a and Table 1 yields strain GFs whose absolute values are about 10% higher for the A than the B resonance, and 25% higher for 60° than for 0° stacking. The calculated band structures in Fig. 4b show that at the *K* point, where the electronic transitions associated with the A and B resonances take place, the conduction bands shift to lower energy upon strain application, while the valence bands remain almost unaffected, resulting in red-shifted optical transitions with GFs in good agreement with the experimental values (see Table 1). According to our theoretical analysis, a small difference between the strain GFs of the A and B excitons could arise from the modification of spin-orbit coupling with strain. For instance, in the case of 0° stacking the spin-orbit-coupling splitting between the valence bands is 422 meV, which is then modified to 428 meV upon 1% strain. A similar effect is observed for 60° stacking, where the splitting increases from 425 meV to 430 meV with 1% strain. The increase of the spin-orbit splitting counteracts the strain-

induced decrease of the band gap and therefore results in a lower absolute strain GF for the B exciton compared to the A exciton.

The theoretical results presented in Table 1 are obtained with G_0W_0 as well as with the inclusion of electron-phonon renormalization to the electron energies, when the structure is relaxed with vdW-DF2 functional. In that case, the GF of A exciton for 60° is around 4% higher than for 0° stacking. With only G_0W_0 one obtains GFs of -80 meV per % and -81.3 meV per % for 0° and 60° stackings, respectively. Very similar results are obtained with HSE functional [GF(0°) = -81.3 meV per % and GF(60°) = -82.7 meV per %], as well as with the HSE functional when the structure is relaxed with vdW-DF2 [GF(0°) = -79.5 meV per % and GF(60°) = -80.4 meV per %]. Besides that we note that the results obtained without HSE or G_0W_0 provide the trend that opposes the experimentally observed GFs. Namely, in that case we obtain GF(0°) = -76.8 meV per % and GF(60°) = -67 meV per % for structures relaxed with both vdW-DF and vdW-DF2. With this one concludes that theory provides very similar results for GFs, but with slightly higher value for the 60° stacking, in agreement with the experimental observation, especially when both the non-local electron-electron (beyond semi-local PBE and vdW corrections) and electron-phonon corrections are included. This highlights the need to include non-local electron-electron and electron-phonon interaction to accurately model the stacking dependence of the strain GFs.

Table 1 Experimental and calculated strain GFs for A and B excitons in WS₂ for 0° and 60° stacking angle

	A ₀	A ₆₀	B ₀	B ₆₀
Exp. mean (meV per %)	-50 ± 2	-64 ± 3	-46 ± 2	-57 ± 4
Exp. median (meV per %)	-51	-66	-47	-59
Calculated (meV per %)	-73	-76	-61	-66

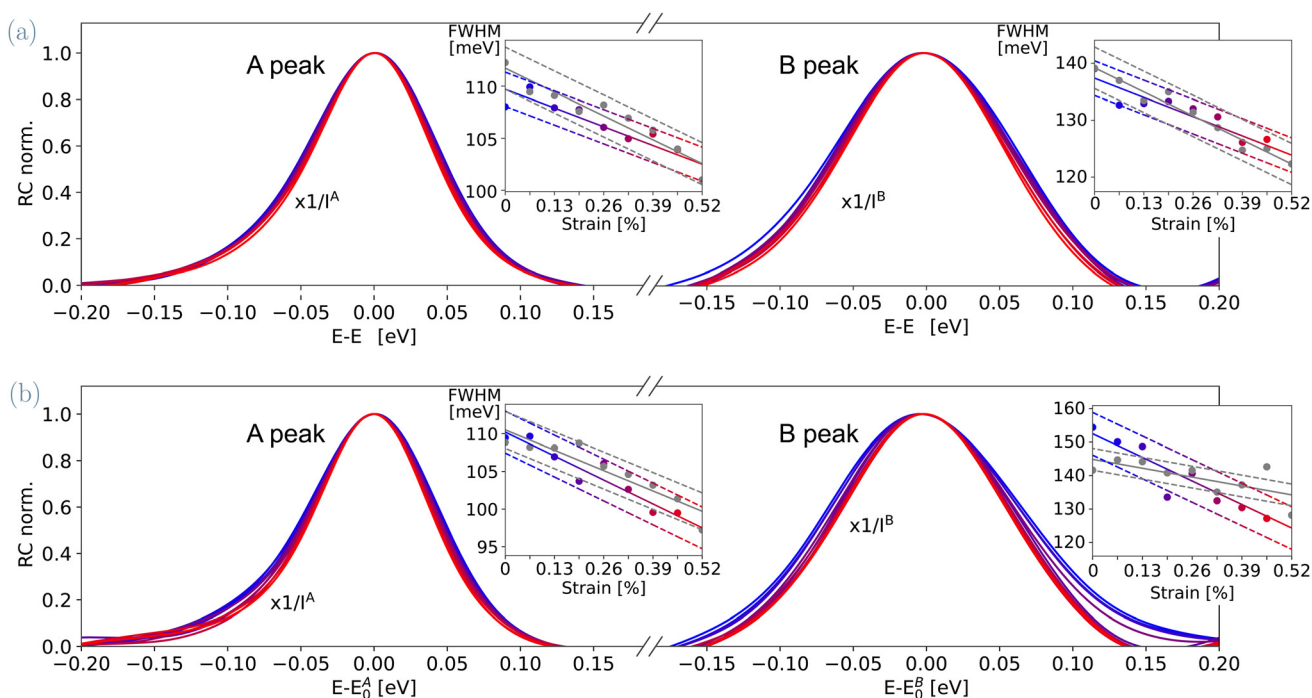


Fig. 5 FWHM variation in the reflectance contrast spectra of 2L-WS₂ at different applied strains for one flake each in 0° (a) and 60° (b) stacking angle. On the left side, the spectra of the A peak, normalized with respect to its intensity and centered at the A peak center are presented, highlighting the variation in FWHM as a function of strain. On the right side, the spectra of the B exciton peak, normalized and centered, are shown. Inset graphs show the strain-dependent FWHMs as a function of the applied strain.



We additionally note that the Q valley (shown later) is only slightly affected by the strain, so that the energy difference between the valence K valley and conduction Q valley is almost unchanged.

We will now examine how strain affects the A and B peak widths, which are determined by the electron–phonon coupling. Examples for the strain-dependent full width at half maximum (FWHM) values are given in Fig. 5 for the A and B peaks in both stacking angles. For the unstrained samples, the FWHMs statistically averaged over all flakes are 106 ± 1 meV and 144 ± 1 meV for A and B in 0° stacking and 122 ± 4 meV and 146 ± 3 meV for 60° stacking. Upon strain application, the A and B peaks in both stackings become progressively higher and narrower, without a significant change of their area. Hence, strain reduces the widths of the excitonic resonances without appreciably changing their oscillator strength. Again, the effect is stronger for 60° stacking, though to a lesser extent than for the resonance energies.

In Fig. 6 we show the results for the calculations of the electron–phonon scattering and its impact on the electron and

hole state broadening when uniaxial strain is applied on 2L WS_2 with 60° stacking angle. Panel (a) shows the modification of the electron–phonon-induced scattering rate of valence and conduction band states when the system is strained by 1%. The biggest change in broadening occurs for the conduction band valley around the K point, where the scattering rate is reduced by ~ 20 meV. The broadening of the valence band states at the K point is increased by less than that; hence the net effect is that the broadening of the electron–hole excitations is decreased for the excitation energies close to the band gap. In the simplest approach, the combined broadening of electron and hole pairs is a solid approximation for the scattering rate of electron–hole bound states, *i.e.*, excitons,⁶³ so the presented results serve as a qualitative explanation for the behavior of the exciton FWHM as a function of strain as obtained in Fig. 5. In fact, we show that the strain-induced decrease of the FWHM of A and B excitons in 2L WS_2 could be explained through the reduced electron–phonon scattering rate of conduction electrons in the K valley, which in turn comes from the strain-induced modified scattering phase space between Q

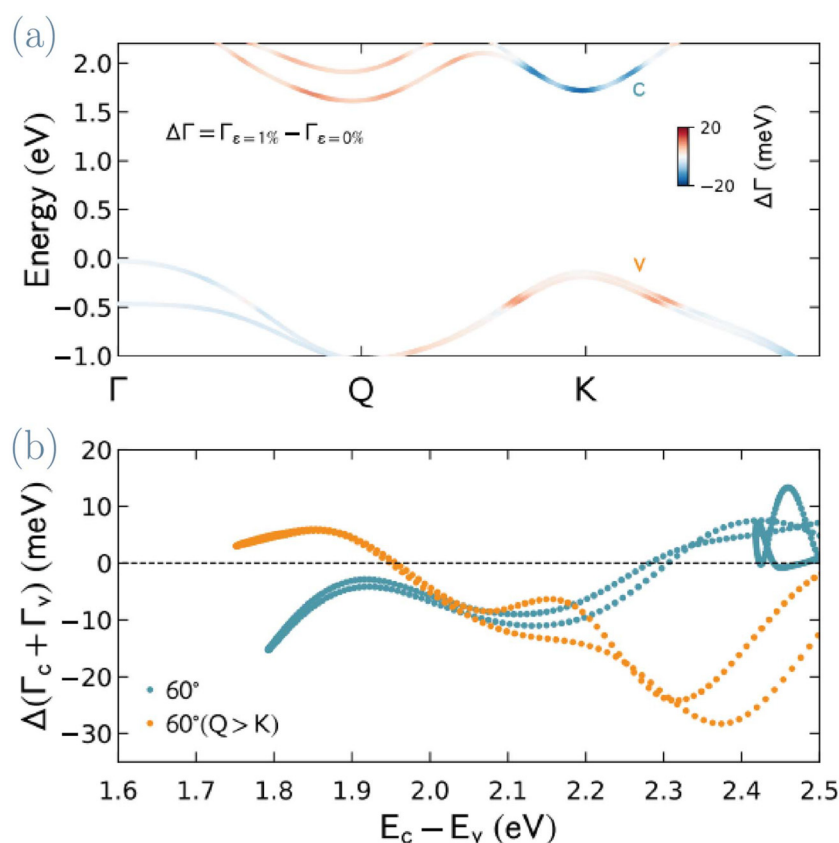


Fig. 6 The impact of strain on electron–phonon-related broadening of electron–hole excitations in 2L WS_2 with 60° stacking angle. (a) Band structure of valence and conduction states where the color depicts the change of the electron state broadening due to applied uniaxial strain of 1%. The conduction (valence) states around the K valley show decrease (increase) of the electron–phonon-related broadening. (b) The total change of the electron–hole scattering rate due to strain as a function of electron–hole excitation energy. The blue dots show the results for the 60° stacking angle, while the orange dots are for the same stacking configuration but when the S–S distance is altered so that the energy of the Q valley is lifted above the K valley. The results show that the broadening of the electron–hole excitations (such as excitons) would decrease with applied strain if the energy of the K valley were above the Q valley.



and K valleys. In particular, the applied strain shifts the Q valley to higher energies,⁶⁴ which reduces the scattering phase space for the K valley. This effect is reversed when the original unstrained structure of 2L WS₂ is adjusted in such a way that the energy of the Q valley is above the K valley (orange dots). Therefore, the negative trend of FWHMs in 2L WS₂ indicates that these materials are indirect gap semiconductors, or at the very edge of direct-to-indirect band-gap transition.^{34,35}

Both the 0° and 60° stacking angles have rather similar small interlayer distances (0.662 and 0.655 nm, respectively), and consequently similar strong interlayer coupling. For stacking angles between 0 and 60°, larger interlayer distances and consequently weaker coupling is found.⁶⁵ An increase in interlayer spacing raises the energy of indirect ($\Lambda \rightarrow \Gamma$ and $K \rightarrow \Gamma$) electronic transitions, while the direct $K \rightarrow K$ transition energy remains nearly unchanged.⁶⁶ This trend leads to an indirect-to-direct gap crossover at large interlayer spacing. For 0° and 60° stacking, the bilayers have an indirect band gap, as seen in Fig. 6a. Despite the calculated high sensitivity of the valence band maximum at the Γ point, for the applied strain values up to 0.52%, no direct-to-indirect band gap crossover is expected. Such crossovers usually appear as kinks in either the strain-dependent peak positions or widths.^{13,25} The absence of such kinks in our experimental data confirms that the band gap remains indirect over the observed strain range.

Conclusion

Our joint experimental and computational investigation highlights the stacking dependent linear strain GFs of the excitonic resonance energies and the electron–phonon coupling strength of bilayer WS₂. Both examined stacking angles have low interlayer distance and strong interlayer coupling. Even stronger effects can be expected if intermediate stacking angles are included, where a much larger variation of the interlayer coupling leads to a quasi-direct bandgap behavior and the appearance of an interlayer exciton. Our work is a first step towards synergistic harnessing of both strain and twist angles as control parameters for the functionality of two-dimensional semiconductors. For example, the twist angle could be used to calibrate the sensitivity of a strain sensor or to adjust the signal weight in neuromorphic straintronic devices.⁶⁷

Author contributions

I. L.-G., V. J. and B. R. carried out the strain-dependent optical experiments.

Q. L. fabricated the samples.

D. N. performed the calculations.

I. L.-G. and V. J. analyzed and visualized the data.

N. V., A. C.-G., C. G. and X. Y. provided funding and supervised the work.

C. G., D. N., I. L.-G. and V. J. wrote the paper with input from all authors.

Conflicts of interest

There are no conflicts to declare.

Abbreviations

TMDC	Transition metal dichalcogenide
DR	Differential reflectance
GF	Gauge factor
PC	Polycarbonate
PDMS	Polydimethylsiloxane
FWHM	Full width at half maximum

Data availability

Raw data is available on https://drive.google.com/drive/folders/1vEs91D4aqiCYMXz03WhyRq2MQGDPxY-o?usp=share_link.

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