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Strain engineering in monolayer WS₂, MoS₂, and the WS₂/MoS₂ heterostructure

Xin He,^{1,a)} Hai Li,^{1,2,a)} Zhiyong Zhu,³ Zhenyu Dai,¹ Yang Yang,⁴ Peng Yang,^{1,2} Qiang Zhang,¹ Peng Li,¹ Udo Schwingenschlogl,¹ and Xixiang Zhang^{1,b)}

¹King Abdullah University of Science and Technology (KAUST), Physical Science and Engineering Division (PSE), Thuwal 23955-6900, Saudi Arabia

²Key Laboratory of Flexible Electronics (KLOFE) and Institute of Advanced Materials (IAM), Jiangsu National Synergetic Innovation Center for Advanced Materials (SICAM), Nanjing Tech University (NanjingTech), 30 South Puzhu Road, Nanjing 211816, China

³KAUST Supercomputing Laboratory, King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia

⁴Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

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Mechanically exfoliated monolayers of WS₂, MoS₂ and their van der Waals heterostructure were fabricated on flexible substrate so that uniaxial tensile strain can be applied to the two-dimensional samples. The modification of the band structure under strain was investigated by micro-photoluminescence spectroscopy at room temperature as well as by first-principles calculations. Exciton and trion emissions were observed in both WS₂ and the heterostructure at room temperature, and were redshifted by strain, indicating potential for applications in flexible electronics and optoelectronics. *Published by AIP Publishing.* [<http://dx.doi.org/10.1063/1.4966218>]

Graphene has attracted a huge amount of attention owing to its unique properties that are of fundamental interest and have potential applications in electronics,¹ optoelectronics,² spintronics,³ and other fields, such as sensor and energy storage.^{4,5} However, applications in both electronics and optoelectronics are largely limited by its zero bandgap. Tremendous efforts were made to open a bandgap in graphene, but the progress remains slow.^{6–10} Transition metal dichalcogenides (TMDs), being also layered materials with an S-M-S (M = Mo, W) sandwich structure bonded by van der Waals forces, recently were investigated extensively as a class of alternative two-dimensional materials.^{11,12} This is largely due to the fact that monolayer TMDs have direct bandgaps corresponding to the region of visible light, which indicates the potential for applications in optoelectronic devices.¹³ Moreover, monolayer TMDs are able to withstand large strain,¹⁴ and various research groups have predicted and confirmed that the band structure can be tuned effectively by strain.^{15–21}

van der Waals heterostructures consisting of different TMDs inherit superior electronic and optical properties from the individual TMD layers,^{13,22–26} and also often exhibit advanced features and functionalities not present in any component.^{27–31} Since many physical properties (e.g., electrical and optical) depend on the band structure, band structure tuning is of future importance. Even though for graphene and monolayer TMDs, such tuning through the application of strain was investigated extensively both theoretically and experimentally,^{14–21,32–37} there are only few theoretical studies on strain engineering in heterostructures,^{38–40} and experimental insight is still yet to be provided.

We therefore have studied the band structures of monolayers WS₂, MoS₂, and their heterostructure (WMoH) by

photoluminescence (PL) spectroscopy under uniaxial tensile strain from 0% to 0.64%. Only a neutral direct gap exciton peak was obtained for monolayer MoS₂, which showed a linear redshift under strain with a rate of 56 meV/%strain. Interestingly, both a neutral exciton peak (A) and a charged exciton (trion) peak (T) were observed in the PL spectra of the monolayer WS₂ and the heterostructure WMoH. Peaks A and T were redshifted under strain with rates of 46 meV/%strain and 43 meV/%strain in monolayer WS₂ and with rates of 53 meV/%strain and 62 meV/%strain in the WMoH. The shifts of the PL peaks reflect the changes of the optical bandgap as the exciton binding energy does not depend on strain.¹⁵ The bandgaps of monolayers WS₂, MoS₂ and the WMoH, thus, can be tuned by uniaxial strain.

Monolayer samples were obtained by mechanical exfoliation from bulk WS₂ and MoS₂ crystals that were purchased from the HQ Graphene Company. The thin samples were exfoliated onto different SiO₂/Si (90 nm, 500 μm) substrates, and the monolayer samples were identified by optical and atomic force microscopy, as shown in Figures 1(a) and 1(b) and their insets, respectively. Subsequently, the monolayer WS₂ was transferred onto the monolayer MoS₂ to form a double-layer heterostructure on the SiO₂/Si substrate with the help of PMMA and poly(dimethylsiloxane) (PDMS) (Figure 1(c)), using the method of Li *et al.*⁴¹ Since the two monolayers were partially stacked, it was possible to obtain their behaviors and that of the WMoH simultaneously as the applied strain was varied. To improve the interlayer coupling, the WMoH was annealed in a mild vacuum for 12 h (~60 mTorr, 120 °C)⁴² and then transferred onto a 300 μm thick polyethylene terephthalate (PET) film (Figure 1(d)). A PMMA film was employed to support the sample in the transfer process and to work as a clamp that prevents it from slipping during the straining process. Since PET is a flexible substrate, a reproducible uniaxial tensile strain can be applied

^{a)}X. He and H. Li contributed equally to this work.

^{b)}Xixiang.Zhang@kaust.edu.sa

FIG. 1. (a) and (b) The AFM topographic images of monolayers WS₂ and MoS₂ on the SiO₂/Si substrate obtained using the tapping mode; the optical images of the corresponding samples are shown in the insets. (c) and (d) The optical images of the WS₂/MoS₂ heterostructure on, respectively, the SiO₂/Si and PET substrates. (e) Schematic drawing of the two-point bending apparatus. The length of the PET substrate is 34.8 mm.

to the samples using the two-point bending apparatus shown in Figure 1(e). The applied strain is given by $\varepsilon = \tau/2R$, where τ is the thickness and R is the radius of curvature of the PET film.¹⁵ A laser ($\lambda = 532$ nm) with $\sim 1 \mu\text{m}^2$ focused spot was used for excitation. All the PL spectra were collected on a Jobin-Yvon HR 800 Raman system at room temperature. The power of the laser was kept at $\sim 5.5 \mu\text{W}$ to avoid heating of the samples.

To understand how the applied strain affects the band structure, three materials are addressed: an isolated monolayer WS₂, an isolated monolayer MoS₂, and the WMoH. Considering the much smaller sizes of the samples (and their relative locations) in comparison with the size of the two-point bending apparatus (Figure 1(e)), it is safe to ignore the difference in the strain applied to them. To ensure reproducibility, each measurement was repeated three times by changing the applied strain. The dependence of the peak positions on the strain was found to be reproducible, which confirmed that there was no slip between the samples and substrate, and thus that the employed technique is reliable.

Although PL spectra of the strained monolayer MoS₂ were studied by other groups,^{15,17,19} they were collected also in this study for comparison, see Figure S1 (supplementary material). The results are in good agreement with the previous

data,^{15,17,19} which confirm that the technique used in this study is correct, and that there was no slip during the straining process.

Without strain, two peaks appeared in the PL spectra of WS₂, see Figure 2(a). Peak A at higher energy of 2.036 eV is due to the neutral exciton emission (E_X) and peak T at 1.995 eV is due to the trion emission (E_T). Since the trion emission is closely related to the carrier density, it is sensitive to the laser power, as reported by Currie *et al.*⁴³ The observation of trion emission under $5.5 \mu\text{W}$ laser light indicated that the trion binding energy was significantly larger than the thermal energy at room temperature. The obtained binding energy of 41 meV is calculated by subtracting E_T from E_X . Under strain, both peaks redshifted, similar to the monolayer MoS₂, implying a reduction in the bandgap. The positions of the exciton and trion peaks in the PL spectra are shown in Figure 2(b) as a function of the applied strain. Both peaks redshifted linearly, but with slightly different rates: 46 meV/%strain for peak A and 43 meV/%strain for peak T. This result indicates clearly that the band structure can be effectively tuned by strain.^{15–17,19,34}

FIG. 2. (a) The PL spectra of the monolayer WS₂ under strain from 0% to 0.64%. Peak T (red) corresponds to the WS₂ trion and peak A (green) to the WS₂ exciton. The dashed lines are guides to the eye highlighting the redshift of the peaks. (b) The strain dependence of the peak T and peak A energies extracted from (a).

The PL spectra of a typical WS₂/MoS₂ heterostructure on SiO₂/Si, before and after annealing, are shown in Figure S2 (supplementary material) indicating that the coupling is improved by annealing.⁴² The PL spectra obtained for the annealed WMoH under strain in Figure 3(a) show only the WS₂ peaks. This can be explained by the fact that the annealing creates regions of strong coupling between MoS₂ and WS₂. In these regions, the bandgap is indirect so that the PL signal is small. In addition, their presence has effects on MoS₂ in weakly coupled regions, which become depleted of holes due to the availability of the energetically higher valence band in strongly coupled regions,⁴² as shown in Figure 4, which suppresses the MoS₂ peak. On the other hand, the WS₂ peaks are not suppressed since the energy level of the conduction band minimum is not modified by the coupling.⁴² Analysis of the two WS₂ peaks by Lorentz fitting shows that both are redshifted with increasing strain (Figure 3(b)), indicating that the energy band structure of the WMoH can be tuned by strain as well. The redshift rate was obtained as 53 meV/%strain for the exciton peak and 62 meV/%strain for the trion peak after linear fitting. Due to the different redshift rates, the two peaks

FIG. 3. (a) The PL spectra of the WS₂/MoS₂ heterostructure under strain from 0% to 0.64%. Peak T (red) corresponds to the WS₂ trion, and peak A (green) corresponds to the WS₂ exciton. The dashed lines are guides to the eye highlighting the redshift of the peaks. (b) The strain dependence of the peak T and peak A energies extracted from (a).

FIG. 4. The band alignment and charge transfer between the strongly and weakly coupled regions of the WS₂/MoS₂ heterostructure.

overlapped less and less, as shown in Figure 3(a). Compared with Figure 2(a), the trion peaks are much weaker, which can be attributed to a reduced hole density in WS₂ due to the presence of the strongly coupled regions as seen above.

To examine whether the strain distribution is uniform in the sample, the PL measurements were performed at three positions randomly chosen within the layers of WS₂, MoS₂, and WMoH on the PET substrate. It is found that the peak positions of the PL spectra obtained from those three positions within each layer are the same (see Figure S3) (supplementary material), indicating a uniform distribution of the applied strain. This observation is in good agreement with a previous report.⁴⁴

To gain more quantitative understanding of the strain effects on the bandgap evolution, we have performed the first-principles calculations using the full-potential linearized augmented plane-wave code WIEN2k.⁴⁵ The lattice constants from Ref. 46 were adopted for the monolayer WS₂ ($a = 3.197$ Å) and monolayer MoS₂ ($a = 3.193$ Å), whereas for the WMoH ($a = 3.195$ Å), the average of the lattice constants of the two individual materials was used.⁴⁶ Two-dimensional structures were generated by adding a vacuum layer of 20 Å thickness. Uniaxial strain along the zigzag or armchair direction was simulated by stretching in this direction only, in accordance with the experimental setup, as lateral movement of the sample was prohibited by the strong adhesion with the substrate. For the muffin-tin radius, values of 2.0 bohr for S and 2.2 bohr for Mo/W were used. High accuracy is achieved by employing a $10 \times 10 \times 1$ k-mesh and setting $R_{\text{mt}}K_{\text{max}} = 8.0$. The atomic positions were fully relaxed with a force tolerance of 0.1 mRy/bohr for all structures. The generalized gradient approximation to the exchange-correlation functional⁴⁷ was employed for both the lattice optimization and electronic structure calculations. Spin-orbit coupling was simulated using the second variation approach.

The electronic band structures of monolayers WS₂, MoS₂, and the WMoH are addressed in Figure 5 for strain along the armchair direction and in Figure S4 for strain along the zigzag direction (supplementary material). Without strain, both the valence band maximum and conduction band minimum are located at the K point for MoS₂ and WS₂, giving rise to a direct bandgap. The size of the bandgap as a function of the applied strain is shown in Figure 6. For unstrained monolayers WS₂ and MoS₂, the bandgaps are 1.51 eV and

FIG. 5. The Electronic band structures of the monolayer MoS₂ (a), monolayer WS₂ (b), and the WS₂/MoS₂ heterostructure (c) without strain. The changes of the valence band maximum and conduction band minimum are shown in (d)–(f) under strain along the armchair direction.

1.57 eV, respectively, which are smaller than the experimental values of 2.03 eV and 1.87 eV, since density functional theory underestimates bandgaps. While for WMoH without strain, the valence band maximum and conduction band minimum are located at the Γ and K point, respectively, resulting in an indirect bandgap. Under strain, the bandgap is modified in a linear manner, see Figure 6, similar along the zigzag and armchair directions. For 1% strain, the predicted bandgap reductions are 64 meV for WS₂, 55 meV for MoS₂, and 65 meV for the WMoH, which are consistent with our experiments.

We have investigated the bandgap modulation of monolayers WS₂, MoS₂, and the WMoH under strain, using both experimental and theoretical methods. Neutral excitons with large binding energies were observed in both the unstrained and strained samples in each case, whereas charged excitons (trions) were only observed in monolayer WS₂ and the WMoH. Both the neutral exciton (56 meV/%strain, 46 meV/%strain, and 53 meV/%strain for monolayers MoS₂, WS₂, and the WMoH, respectively) and trion (43 meV/%strain and 62 meV/%strain for monolayer WS₂ and the WMoH, respectively) peaks showed redshifts under strain, indicating decreasing bandgaps. The tunability of the band structures by strain implies potential applications in flexible electronics and optoelectronics.

FIG. 6. Theoretical evolution of the bandgap of monolayers WS₂, MoS₂, and the WS₂/MoS₂ heterostructure under strain from 0% to 0.9% along the zigzag and armchair directions.

See [supplementary material](#) for the PL spectra of the monolayer MoS₂ under strain, PL spectra of a typical WS₂/MoS₂ heterostructure before and after annealing, PL spectra uniformity in WS₂, MoS₂, and WS₂/MoS₂ regions before and after straining and electronic band structures of monolayers WS₂, MoS₂, and the WMoH under strain along the zigzag direction.

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