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A dielectric-defined lateral heterojunction in a monolayer semiconductor

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Abstract
Due to their low dimensionality, two-dimensional semiconductors, such as monolayer molybdenum disulfide, have a range of properties that make them valuable in the development of nanoelectronics. For example, the electronic bandgap of these semiconductors is not an intrinsic physical parameter and can be engineered through the dielectric environment around the monolayer. Here we show that this dielectric dependent electronic bandgap can be used to engineer a lateral heterojunction within a homogeneous MoS\textsubscript{2} monolayer. We visualize the heterostructure with Kelvin probe force microscopy and examine its influence on electrical transport experimentally and theoretically. We observe a lateral heterojunction with \textasciitilde90 meV band offset due to different bandgap renormalization of monolayer MoS\textsubscript{2} when it is on a substrate in which one segment is made from an amorphous fluoropolymer (Cytop) and another segment from hexagonal boron nitride. This heterostructure leads to a diode-like electrical transport with a strong asymmetric behaviour.
 Atomically thin semiconductors, such as monolayer transition metal dichalcogenides (TMDs)\(^1\)-\(^3\), provide a platform for investigating nanoscale quantum phenomena\(^4\)-\(^6\) and have a range of potential applications in nanoelectronics\(^7\)-\(^9\). A freestanding monolayer of a transition metal dichalcogenide experiences a reduced dielectric screening and an enhanced Coulomb interaction by virtue of its atomically thin structure. In contrast to bulk materials, electric field lines between charges inside a monolayer can extend substantially outside of the layer\(^10\)-\(^12\). This leads to an ineffective intrinsic screening that enhances electronic interaction and leads to large exciton binding energies between 0.2–0.7 eV in these materials\(^10\)-\(^18\). Furthermore, the electronic band structure of atomically thin 2D layers is not completely intrinsic to the material and can be strongly affected by the surrounding environment\(^13\)-\(^19\)-\(^23\). With both electron and hole experiencing the screening, the conduction and valence band edges shift in the opposite direction\(^13\)-\(^12\),\(^13\)-\(^21\),\(^23\). *Ab initio* calculations predict that there is a monotonic decrease of electronic bandgap energy with increasing dielectric screening, where the reduction of bandgap can reach the order of hundreds of meV relative to the bandgap of a freestanding monolayer\(^13\)-\(^20\),\(^22\),\(^24\)-\(^27\). Recent scanning tunneling spectroscopy\(^13\) and optical spectroscopy\(^20\),\(^22\) studies provided evidence that the bandgap renormalization phenomenon in atomically thin 2D semiconductors can indeed be significant. Such bandgap renormalization may have a profound effect on electrical transport in atomically thin 2D semiconductors; yet, the effect has not been investigated thoroughly and its implications in the development of applications based on 2D materials remains unclear.

In this Article, we design lateral heterojunctions within a homogeneous MoS\(_2\) monolayer exploiting the dielectric-dependent bandgap renormalization and explore its influence on electrical transport. We prepared a continuous monolayer MoS\(_2\), which has a segment on a high-\(\varepsilon\) substrate and an adjacent segment on a low-\(\varepsilon\) substrate (Fig. 1a). Due to the different degree of renormalization of the electronic bandgap introduced by the two substrates on each segment, the monolayer MoS\(_2\) forms an in-plane type-I heterojunction above the boundary of the two substrates (Fig. 1b,c). We used this sample configuration to perform Kelvin Probe Force Microscopy (KPFM) and electrical transport measurements across the heterojunction. KPFM\(^28\),\(^29\) examines the local variation of surface potential across the device channel\(^30\) and provides a direct determination of the band offset of the MoS\(_2\) heterojunction from the dielectric engineering. Electrical measurements show that the presence of the heterostructure has a significant effect on electrical transport through the device, leading to a strong asymmetric rectification behaviour. The experimentally observed transport phenomena can also be qualitatively reproduced in a numerical simulation of the device, which exhibits several unique aspects arising from the atomically thin layers. Such dielectric-defined heterostructure behaviour can be important for understanding electrical transport behaviour in atomically thin 2D layers and provide a new approach for engineering 2D nanoelectronic devices\(^4\),\(^31\).

Theoretical calculations\(^21\)-\(^23\),\(^32\),\(^33\) show that the change in the bandgap of the 2D layer due to dielectric screening effect by the substrate(s) is most dramatic when the 2D layer has a low intrinsic dielectric constant (\(\varepsilon\)). In addition, a high contrast from the dielectric screening environment involving a low-\(\varepsilon\) substrate and a high-\(\varepsilon\) substrate is desirable to introduce a significant change in the bandgap of the 2D layer at the heterojunction. We choose the fluoropolymer Cytop (\(\varepsilon = 2.0–2.1\)) and hBN (\(\varepsilon(0) = 6.9, \varepsilon(\infty) = 5.0\) normal to \(c\)-axis\(^34\)) to serve as the \(\varepsilon_{\text{low}}\) and \(\varepsilon_{\text{high}}\) substrates respectively. The fluoropolymer Cytop substrate is one of the materials with the lowest dielectric constant that still allows ease of processing and device fabrication. Meanwhile, the straight edges of as-exfoliated thin hBN flake provide a boundary that is atomically sharp for a well-defined junction area. Moreover, both Cytop\(^35\) and hBN\(^36\) are known to be insulating layer with a low density of surface trap states.

**Heterojunction device design and electrical measurement**

We transferred a monolayer of MoS\(_2\) atop the boundary of an hBN flake on a Cytop film and then fabricated electrical contacts onto the monolayer to form a device channel that is perpendicular to the Cytop/hBN substrate boundary (Fig. 2a). The electrical measurements are then performed in 4-terminal configuration to minimize the influence of contacts. Fig. 2b shows the \(I-V\) measurement of the device for different back gate-source voltages (which we shall refer to as “gate voltage” for brevity) \(V_{gs} > 0\) V, which correspond to electron doping. With the MoS\(_2\) segment on Cytop grounded, the device exhibited a rectification behavior that is reminiscent of a diode. This rectification behaviour is consistent with the expected type-I heterojunction formation drawn in Fig. 1c, where the MoS\(_2\) segments above the \(\varepsilon_{\text{low}}\) and \(\varepsilon_{\text{high}}\) substrates have different electronic band gap due to dielectric screening. This behaviour is similar to an \(n-n\) heterojunction with MoS\(_2\) segment on Cytop (hBN) containing the depletion (accumulation) regime\(^37\).
In comparison, the reference MoS$_2$ monolayer device on a uniform Cytop film exhibits linear Ohmic-like behaviour (Fig. 2c), suggesting that the rectification arises from the presence of the heterojunction at the boundary between high-$\varepsilon$ and low-$\varepsilon$ substrates. Furthermore, we also conducted control experiments with MoS$_2$ monolayer on a step edge of an hBN flake that otherwise supports a uniform dielectric environment (Supplementary Fig. 7). Such control device shows symmetric output curves, which also substantiates that the rectification cannot be attributed only to the presence of step edge (e.g., strain-induced or otherwise) without introducing dielectric contrast.

A prominent feature of our MoS$_2$ heterojunction device behaviour is that the $I$-$V$ curve at forward bias that is higher than $V_{ch} \approx 0.1$ V is mostly linear. This behaviour is commonly found in a real diode, which can be described by a piecewise linear model with a "turn-on" voltage ($V_t$) before the device appears to be Ohmic-like$^{38}$. The turn-on voltage is often correlated to the potential landscape of the diode (e.g., built-in voltage in Si p-n diode), and it provides an estimate of conduction band offset across the heterojunction. Our low-temperature transport measurements yield a turn-on voltage $V_t \sim 90$ mV in the device (17 K, Fig. 2d).

**KPFM characterization**

Fig. 3a illustrates the KPFM measurement configuration, where lift mode with a constant tip height ($h = 30$ nm) is used and the DC component of bias voltage ($V_{bias}$) is applied to the sample. Fig. 3b displays the topography scan of atomic force microscope (AFM) from the MoS$_2$ heterojunction area at the Cytop/hBN substrate boundary. The averaged height profile (Fig. 3c) shows that the thickness of the hBN is around 10 nm. The exposed top surface in our devices allows for direct KPFM characterization.

As KPFM typically requires the sample to be sufficiently conducting, we performed KPFM on the MoS$_2$ when it is electrostatically gated to its on-state (electron accumulation) at high gate voltage. Fig. 3d shows the map of $V_{bias}$ that was applied to the sample to cancel the electrostatic force between the tip and the sample, which is imaged at $V_{gs} = 50$ V. Meanwhile, Fig. 3e shows the corresponding averaged $V_{bias}$ profile. The $V_{bias}$ magnitude is related to the work function of the sample and that of the tip by $\phi = V_{bias} + W_{f,tip}$ (see Supplementary Fig. 8). Therefore, the difference in local work function between two segments of the sample that are imaged by the same tip is given by:

$$\Delta W_{f,\text{sample}} = e \Delta V_{bias}$$  \hspace{1cm} (1)

Two distinct areal regions of $V_{bias}$ are seen in Fig. 3d that correlates well with the two segments of MoS$_2$ on Cytop and hBN from the topographic image (Fig. 3b). By using the averaged line profile in Fig. 3e, we therefore conclude that the work function difference ($\Delta W_f = W_{f,\text{low}} - W_{f,\text{high}}$) of MoS$_2$ on the Cytop and hBN substrate is -90 ± 20 meV at $V_{gs} = 50$ V. Here, the negative sign means that the vacuum level of MoS$_2$ on Cytop is lower than that on hBN.

The conduction band offset can be obtained from the work function difference by

$$\Delta E_c = -\Delta W_f - kT \ln \left[ \frac{\exp \left( \frac{m^* n_{\text{low}}}{m^* kT} \right)}{\exp \left( \frac{m^* n_{\text{high}}}{m^* kT} \right)} \right]$$  \hspace{1cm} (2)

with the carrier density $n = C_g (V_{gs} - V_{ch})/e$, where $V_{ch}$ is the gate threshold voltage, and $m^*$ is the effective mass of electrons. Because the serial gate capacitance ($C_g$) at $\varepsilon_{\text{high}}$ and $\varepsilon_{\text{low}}$ side of the device does not differ significantly (the geometric capacitance of the 285 nm SiO$_2$ substrate dominates the serial capacitance), the ratio $n_{\text{low}}/n_{\text{high}}$ becomes closer to unity at high gate voltage. Applying these considerations to equation (2) in combination with (1) suggests that performing the measurement at the high gate voltage provides two major benefits: first, it counters the doping contribution from the environment to allow the relative carrier density on both sides of the junction to be more balanced since the charge density is dominated by that induced by the gate. Secondly, as the consequence of $n_{\text{low}}/n_{\text{high}} \approx 1$, KPFM measurements at high gate
voltage allow direct interpretation of the conduction band offset from the $V_{\text{bias}}$ contrast. Fig. 3e therefore implies that $\Delta E_c \approx -e\Delta V_{\text{bias}} \sim 90$ meV for our experimental condition, i.e., $E_c$ for MoS$_2$ on Cytop is positioned higher than that on hBN.

The heterojunction measured by KPFM is consistent with the electrical transport data. It suggests that dielectric engineered bandgap difference is around $\Delta E_g \approx 2\Delta E_C = -180 \pm 40$ meV (illustrated in Fig. 1c), assuming electron-hole symmetry. We compare this experimental result with the theoretical calculation of the electronic bandgap of MoS$_2$ within the $ab$ initio $GW_0$ approach as implemented in the BerkeleyGW package and account for the dielectric screening effect from the substrates using the in-plane substrate averaging approach (details regarding the $GW_0$ calculation is in Supplementary Note 4). The $GW_0$ calculation shows that the bandgap of MoS$_2$ on a similar dielectric fluoropolymer as Cytop, after accounting of surface roughness (Supplementary Fig. 3), is larger than that of MoS$_2$ on hBN by $120 \pm 40$ meV, of which the CBM offset is $\sim 70 \pm 20$ meV (Fig. 3f). Our calculations reveal that the roughness of the Cytop surface decreases the effective dielectric screening experienced by MoS$_2$; the same calculation performed on a perfectly smooth Cytop-like substrate results in a CBM offset of $\sim 40$ meV. The calculated bandgap and CBM offset agree well with the experimental results, with overlapping error bars. The CBM and VBM offsets are also approximately symmetric.

Energy band modelling

We model the electrical potential and charge transport through the junction numerically to understand the unusual electrical transport from an atomically thin 2D heterojunction. While the rectification behaviour of the heterojunction is consistent with the predicted band alignment in Fig. 1c, the transport data cannot be aptly modelled with a thermionic emission theory commonly used to describe a Schottky diode, in which the current level predicted from a thermionic emission mechanism is several orders of magnitude larger than that measured herein (Supplementary Note 1 and Supplementary Fig. 1-2). The thermionic emission model fails in atomically thin 2D layers because these 2D materials tend to have rather low mobility, and the drift-diffusion behaviour of charge carriers plays a dominant role in the transport across the heterojunction. To accurately model the device behaviour, we introduce a carrier density dependent electron mobility in MoS$_2$ by $\mu(n) = \mu_0/[1 + \exp(\alpha n)]$. Here, the mobility has a constant value of $\mu_0$ at high doping but drops significantly at low doping. This functional form is reminiscent to an activated behaviour with a certain density of trap states, and the relevant parameters are obtained through gate-dependent transport data from a homogeneous MoS$_2$ monolayer (Supplementary Fig. 5f-g). The density-dependent mobility is especially relevant at the depletion region, which would experience increased local electrical resistance due to lowered carrier density (Fig. 4d).

Fig. 4 shows the calculated band diagram and the associated band bending of MoS$_2$ around the Cytop and hBN substrates for the conduction band edges at zero, forward, and reverse applied bias (see method in Supplementary Note 2). The electron density $n_0$ at $x < 0$ (at Cytop) is assumed to be $\sim 2 \times 10^{13}$ cm$^{-2}$. The zero bias calculation result (Fig. 4a) captures the built-in potential on each side of the junction ($\psi_1$ and $\psi_2$ for MoS$_2$ on hBN and Cytop, respectively) because of the work function differences between the two segments of MoS$_2$. In the case of a biased channel, the current flow is a response of a voltage drop over the whole channel: $V_{ch} = E_F(z = -L) - E_F(z = L)$ that shifts the Fermi level out of equilibrium. However, we see from both Fig. 4b and 4c that the voltage drop primarily transpires at the heterojunction, ensuring that the heterojunction property to define the $I-V$ behaviour of the device.

In the forward bias (Fig. 4b), the voltage drop across the heterojunction reduces the net built-in potential into $\psi_1 - V_1$ and $\psi_2 - V_2$, respectively. A net current will flow with the electrons moving from the segment on Cytop to that on hBN. At a finite temperature, electrons moving in this direction will see an energy barrier for transport across the heterojunction. However, this energy barrier becomes negligible at a sufficiently large applied bias $V_{ch} > V_1$, as illustrated in Fig. 4b. In other words, $\psi_2 - V_2 \approx 0$ and the transport across the junction should be mostly dominated by the sheet resistance of MoS$_2$ away from the junction and appears Ohmic-like. As an approximation, the $\psi_2 - V_2 \approx 0$ condition is achieved when the total built-in voltage across the junction: $\psi_1 = \psi_1 + \psi_2 \approx V_1$. We believe that this picture might explain the $I-V$ behaviour for the heterojunction as discussed in Fig. 2. An equivalent diode circuit for the junction is shown in the inset of Fig. 4b: the heterojunction is comprised of an internal built-in potential $V_i$ that needs to be compensated by applying an external potential, following which the current-voltage behaviour is dictated by a resistance $R_s$.
in series due to the MoS$_2$ segment away from the junction. Our simulated $I$-$V$ plot (Fig. 4e) reproduces the threshold-like behavior of the device.

Conclusions

We have reported an operational device application of bandgap renormalization in 2D materials via dielectric screening, and shown that a dielectric-engineered lateral heterojunction can strongly modify electrical transport in monolayer MoS$_2$. Since heterostructures are fundamental building blocks in electronics, such dielectric engineering can provide a powerful new route for realizing more complex device architecture. Our findings also have implications for the efforts to incorporate 2D materials in optoelectronics, in order to improve functionality (for example, spin-valley current for information encoding$^{42}$) and drive miniaturization$^{43,44}$.

In practical applications, all aspects of manufacturing must be considered. For instance, the monolithic integration of 2D materials in circuitry requires interfacing with other components, such as substrate, electrodes, and interconnections. Each component may screen the 2D materials, resulting in different degree of bandgap renormalization across the channel. Notably, the bandgap of MX$_2$ should decrease significantly upon interfacing with electrodes due to the high permittivity of metals and thus a heterojunction is expected to form at each border between the MX$_2$ segments with and without metal contact. Although the behaviour of metal-MX$_2$ junction is dominated by other mechanisms such as Fermi-level pinning$^{45,46}$, recent work suggests the possibility to prevent pinning by minimizing disorders and interface states at the metal-MX$_2$ junction$^{47,48}$. At such limit, accounting for bandgap renormalization is essential to fully understand the physics of electrical contact to MX$_2$ monolayers.

Although we have used Cytop and hBN substrates in order to simplify fabrication, the bandgap renormalization is a general phenomenon in 2D semiconductors and the heterojunction should form with other combinations of dielectrics. The constraint for low $\varepsilon_{\text{low}}$ substrate may be satisfied by other established materials in industry, such as electronic-grade plastic substrates$^{49,50}$ with well-developed scalability and processability. Additionally, an advantage of such polymeric surfaces is the absence of dangling bonds, leading to a low density of surface trap sites. If conventional high-$\varepsilon$ dielectrics are used, an abrupt heterojunction is affordable by patterning with state-of-the-art microfabrication technology. Another scalable approach also includes using CVD-grown 2D lateral heterojunction as the substrate if the material combination has a significant dielectric contrast$^{51,52}$. We also believe that the influence from interface trapping and substrate doping for non-optimized surface can be minimized if the heterojunction is operated at high carrier density as defined by the electrostatic gating, where the difference in the work functions between low- and high-$\varepsilon$ channel segments are primarily due to the bandgap renormalization.

Methods

Device fabrication. Cytop (CYTOP CTL-809M, Asahi Glass Co.) is mixed into CTL180 (Asahi Glass Co.) in 2:7 v/v and spincoated at 1000 rpm for 1 min to a uniform thickness of ~70 nm on highly doped Si substrates with 285 nm SiO$_2$. The Cytop-coated substrate is then heated at a hotplate for 5 min at 100°C and then 5 min at 150°C. Crystal of hBN is then exfoliated on the Cytop surface. The hBN flakes with thickness of 5-15 nm that have a flat side edge are identified from optical microscopy and confirmed with AFM imaging. Monolayers of MoS$_2$ are exfoliated onto a PDMS stamp and dry-transferred$^{53,54}$ to the flat edge of such hBN flake (Supplementary Fig. 4a,b). For all devices, 100 nm Au film is deposited for the electrode of MoS$_2$ using a standard electron beam lithography (EBL) process with two layers of EBL resist (495PMMA A4 and 950PMMA A4, MicroChem). We found that exposing the Cytop film to a short, low power N$_2$ plasma (10 sccm, 5 W for 1 s) before the hBN exfoliation can help to produce better spincoating of the resists on Cytop.
**Data availability**

The data that support the plots within this paper and other findings of this study are available from the corresponding author upon reasonable request.

**References**

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**Author contribution**


**Financial and non-financial competing interests**

The authors declare no competing interests.

**Additional information**

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Figure 1 | Engineering 2D heterojunction through dielectric-dependent bandgap renormalization. a, Schematic illustration of the heterostructure. Two substrates with different dielectric constant ($\varepsilon_{\text{low}} < \varepsilon_{\text{high}}$) are used to locally vary the MoS$_2$ electronic bandgap. b, The expected band alignment of isolated monolayer MoS$_2$ situated on $\varepsilon_{\text{low}}$ substrate (Cytop) and on $\varepsilon_{\text{high}}$ substrate (hBN), respectively. The segment of MoS$_2$ monolayer on Cytop and that on hBN are assumed to have the same electron doping density from the electrostatic gating. c, The band alignment from (b) if the MoS$_2$ segments at the two substrates are in contact and reach equilibrium following Anderson’s rule. A type-I lateral heterojunction forms with an energy barrier for electron transport in the conduction band.

Figure 2 | Current-voltage characteristics of MoS$_2$ heterojunction device. a, Optical micrograph of an MoS$_2$ monolayer that is partially situated on Cytop and on hBN substrates. The white dashed line denotes the location of the monolayer that acts as the device channel. The MoS$_2$ segment on hBN received the high bias potential (drain). Scale bar: 2 µm. b, The output characteristics of the device with various back gating at the temperature of 200 K. c, The output characteristics of a reference MoS$_2$ monolayer device on a uniform Cytop substrate measured at 200 K. Inset: The micrograph of the reference device. Scale bar: 2 µm. d, The output characteristics of the heterojunction device at 17 K in log-log scale. The forward bias current is fitted with a straight line that extrapolates to a turn-on voltage of 90 mV. Inset: the same data in linear scale.

Figure 3 | KPFM characterization of the MoS$_2$ heterojunction formation from differences in the degree of local dielectric screening. a, Schematic of the KPFM setup with $V_{\text{bias}}$ applied to the sample. For the measurements herein, the device is back gated to $V_{\text{gs}} = 50$ V and the lift height of the tip is set to $h = 30$ nm. b, The topography image recorded in tapping mode AFM. c, The height profile, averaged from the area inside the white-dashed rectangle in (b). d, The spatially mapped $V_{\text{bias}}$ from the same area as in (b). e, The $V_{\text{bias}}$ profile from (d), also averaged similarly from the same area as in (e). Given that $\Delta E_c = -e\Delta V_{\text{bias}}$ in the measurement configuration, the KPFM result demonstrates that the conduction band edge of MoS$_2$ on Cytop substrate is higher by 90 meV than that of MoS$_2$ on hBN. f, Results from GW calculations of the bandgap and band alignment of monolayer MoS$_2$ that is freestanding without substrate screening effect (left), that is placed on a surface of a fluoropolymer (middle), and that is placed on a hBN substrate (Scale bars in (b) and (d) corresponds to 500 nm).

Figure 4 | Simulation results of the energy band bending at the 2D heterojunction. a,b,c The conduction band edges and Fermi levels are calculated at (a) zero bias, (b) forward biased (current: 80 nA/µm), and (c) reverse biased condition (current: -6 nA/µm). In the three cases, the MoS$_2$ segment on Cytop is assigned to be electrically grounded. Under small forward bias ($V_{\text{gh}} = V_{\text{t}} + V_{\text{f}}$), an electron traversing the heterojunction from the segment on Cytop to that on hBN experiences an energy barrier due to the built-in voltage. However, for large enough bias beyond the turn-on voltage ($V_{\text{gh}} > V_{\text{f}}$), electrons traversing the heterojunction (blue circle) do not experience significant energy barrier and the current-voltage characteristic is determined by the resistance of the channel instead of the junction. Inset in (b): a schematic of the diode modelling according to piecewise linear model. d, Carrier density distribution across the junction under different bias condition. e, Simulated current-voltage characteristics with a carrier density-dependent mobility. All calculations are performed using carrier density of $2.0 \times 10^{12}$ cm$^{-2}$ at 140 K.
(a) Schematic diagram of the device with $V_{ds}$ as the drain-source voltage.

(b) Graph showing the drain current density $J_{ds}$ as a function of channel voltage $V_{ch}$ at 200 K, with different gate voltages $V_{gs}$:
- $V_{gs} = 55$ V: red line
- $V_{gs} = 45$ V: orange line
- $V_{gs} = 35$ V: green line
- $V_{gs} = 25$ V: blue line

(c) Graph showing the drain current density $J_{ds}$ as a function of channel voltage $V_{ch}$ with a control experiment at 200 K:
- $V_{gs}$ values: 50 V, 40 V, 30 V, 20 V, 10 V

(d) Graph for a different temperature, 17 K, showing $V_{gs} = 55$ V:
- $V_{f} \sim 90$ mV