Integrating Ohmic contacts into van der Waals (vdW) heterostructures is critical for realizing electronic and optoelectronic functionalities. However, to date no scalable methodology for gaining electrical access to buried monolayer two-dimensional (2D) semiconductors exists. Here we report viable edge contact formation to hexagonal boron nitride (hBN) encapsulated monolayer MoS\(_2\) for the first time. By combining reactive ion etching, \textit{in-situ} Ar\(^+\) sputtering and annealing, we achieve a relatively low edge contact resistance (46 ± 10 kΩ·μm), high mobility (up to \(\sim 30\, \text{cm}^2\, \text{V}^{-1}\, \text{s}^{-1}\)) and high on-current density (>50 μA/μm at \(V_{\text{gs}} = 3\, \text{V}\)), comparable to top contacts. Furthermore, the atomically smooth hBN environment also preserves the intrinsic MoS\(_2\) channel quality during fabrication, leading to a steep subthreshold swing (116 mV/dec) with a negligible hysteresis. Edge contacts exhibit a higher electron transmission probability than top contacts, as revealed by our quantum transport simulations, and can be arbitrarily narrow, which opens the door to further shrinkage of 2D device footprint.

We will now discuss the fabrication strategy that we developed. Detailed process parameters can be found in Supplementary Section.
**Figure 1. Fabrication of edge contacts.** (a-b) 3D illustration of the heterostructure assembly. 1L-MoS₂ is exfoliated on PDMS and transferred onto an hBN layer. Subsequently, the MoS₂ is fully encapsulated by stacking another hBN layer on top. UV-O₃ cleaning of the PDMS surface before exfoliating MoS₂ on it significantly reduces PDMS residues on MoS₂. (e) Differential interference contrast (DIC) optical image of a 1L-MoS₂ flake transferred on hBN (24 nm thick) and vacuum annealed. (d-g) 3D illustration of edge contact fabrication. (d) The hBN-MoS₂-hBN heterostructure is patterned by EBL and RIE to expose MoS₂ edges. (e) Before metalization, *in-situ* Ar⁺ sputtering is done at +15° and also -15°, inside a UHV chamber. This creates clean MoS₂ contact edges by removing MoOₓ and any adsorbed gas molecules. (f-g) Ti (5 + 5 nm) is then immediately deposited followed by Au (40 + 40 nm), both metals at +15° as well as -15°, to form 1D edge contacts. (h) Optical image of the MoS₂ sample shown in e, contacted via edge contacts after hBN encapsulation. In the devices outlined in red, the MoS₂ contact edges were not sputtered with Ar⁺, to act as a control. Ar⁺ treatment results in a lower contact resistance, as discussed later. The three sets of devices in h were aligned at 60° with respect to each other, in order to exclude any differences arising from the hexagonal crystal symmetry of hBN and allow for a more accurate comparison. For all devices, $L = 1 \mu m$ and the contact length $L_c = 0.5 \mu m$. Scale bars in e, h: 10 µm.

S1. Bottom hBN flakes were exfoliated directly on $p^+$/Si/SiO₂ (100 nm) substrates. 1L-MoS₂ and top hBN flakes were separately exfoliated on GelPak® PDMS (poly-dimethylsiloxane) stamps and transferred sequentially onto a suitable bottom hBN flake, as illustrated schematically in Figs. 1a, b. We found that PDMS can leave substantial residues behind after transfer which we minimized by pre-cleaning the PDMS surface in ultra-violet-ozone (UV-O₃) prior to exfoliation (see ref. 42 for details). After each transfer, the resulting stack was annealed at 200 °C in high-vacuum for 3 h to release trapped bubbles, wrinkles and strain (if any) induced by PDMS during transfer. Figure 1c shows the optical image of a 1L-MoS₂ flake transferred onto hBN from PDMS. To fully encapsulate the MoS₂, another hBN flake was subsequently transferred on top.

For device fabrication, bubble-free areas were chosen and patterned into rectangular sections by e-beam lithography (EBL) with PMMA (poly-methylmethacrylate) and reactive ion etching (RIE). Contact trenches were defined in a second EBL step and the exposed hBN-MoS₂-hBN was etched away by RIE to create MoS₂ edges for making contacts, as depicted in Fig. 1d (also see Supplementary Fig. S1). The samples were then loaded into an e-beam evaporator for metal deposition, which we found to be the most critical part of the whole fabrication process. An etched MoS₂ edge consists of dangling bonds as well as defects like Mo- and S-vacancies that are much more reactive than the basal plane of MoS₂. During the time elapsed between etching and metal deposition, O₂ and H₂O molecules can not only bind to such edge sites but also potentially convert unpassivated Mo into MoOₓ. However, MoOₓ, which is often used as a hole transport layer in solar cells, hinders electron injection into MoS₂ due to its high work-function. This scenario is in strong contrast to top contacts where MoOₓ formation is unlikely.

Hence, immediately before metal deposition, MoOₓ and any adsorbed O₂ or H₂O were removed by *in-situ* Ar⁺ sputtering at ±15° tilt angle to expose a fresh MoS₂ edge (Fig. 1e). Tilting the sample is necessary to access the etched hBN-MoS₂-hBN sidewalls shadowed by an overhanging PMMA bilayer with an inward slope and avoid re-deposition of sputtered PMMA over the MoS₂ edges. Ti-Au (5-40 nm) was then deposited at ±15° tilt under a base pressure of 1 × 10⁻⁵ mbar (Fig. 1f-g). After lift-off, the devices were annealed in Ar + H₂ at 300 °C for 3 hrs to improve the Ti-MoS₂ edge interface and reduce contact resistance (Supplementary Section S2). Note that the use of Ti is essential for providing good adhesion to hBN sidewalls. Without Ti, pure Au tends to reflow and lose contact during annealing at 300 °C (Supplementary Section S4). The final set of devices with edge contacts are shown in Fig. 1h.

**Electrical characterization**

Figure 2a shows the $I_D-V_{DS}$ output characteristics of an edge contacted 1L-MoS₂ transistor exhibiting n-type behavior. A slight non-linearity at low $V_{DS}$ indicates the presence of a small barrier at the contacts. The $I_D-V_{DS}$ transfer characteristics of the same device are plotted in Figs. 2b and 2c on linear and log scales, respectively. A high current density reaching 53.5 µA/µm at $V_{DS} = 3$ V with an on-off ratio >10⁷ can be observed. This clearly demonstrates that an efficient carrier injection is achievable via edge contacts, despite the lack of a 2D overlap between MoS₂ and Ti. In Fig. 2c, each curve is comprised of both forward and backward sweeps which display a very small hysteresis. A magnified plot of the subthreshold characteristics is shown in the inset of Fig. 2c and reveals a low subthreshold swing (SS) of 116 mV/dec maintained up to nearly 4 orders of magnitude. Realization of such a steep
that Ti can partially oxidize during evaporation, depending on the vacuum level inside the deposition chamber, and thereby result in TiO₂ formation at the contact interface. To inhibit the oxidation of Ti, we deposited Ti-Au on another set of devices (again without Ar⁺ sputtering) at a 10x lower base pressure of ~1 x 10⁻⁸ mbar, with negligible residual O₂ (Supplementary Section S5). However, a low $I_D$ is also observed in this case, revealing the existence of an $R_C$ dominated transport. This implies that a better vacuum does not lead to any appreciable change in the contact properties if Ar⁺ sputtering is not done. It must be emphasized that an optimum post-deposition annealing temperature is also crucial for improving the contact interface (Supplementary Section S2). Hence, our key finding here is that a clean MoS₂ edge (before metallization) and annealing (after metallization) are both essential for forming good edge contacts, like those demonstrated in Figs. 2b-d. This likely explains why such a high current density had not been observed previously.

Next, we want to characterize the intrinsic carrier mobility ($\mu_i$) and contact resistance ($R_C$) of our devices. For an ideal long-channel nMOSFET operating in the strong inversion regime, a linear dependence of $I_D$ on $V_{DS}$ is expected, given by

$$I_D = \mu_i C \frac{W}{L} \left[ V_{G,S} - V_T - V_{DS} / 2 \right] V_{DS}$$

where $V_T$ is the threshold voltage and the internal drain ($V_{DS,int}$) and gate ($V_{G,S}$) voltages are equal to the externally applied bias. Typically, $\mu_i$ is extracted from the slope of linear $I_D-V_{G,S}$ characteristics with the help of Eq. (2). However, Fig. 2b shows that $I_D$ grows sub-linearly with $V_{DS}$ for all $V_{G,S}$, which causes the mobility extracted in this manner to be underestimated. For a more accurate description of such $I_D-V_{G,S}$ behavior, the presence of finite contact resistances $R_C$ in series with the MoS₂ channel must be considered. In this scenario, the internal voltages seen by the channel get reduced to $V_{DS,int} = V_{DS} - 2 R_C R_D$ and $V_{G,S,int} = V_{G,S} - R_D R_C$. Note that $V_D$ also gets modified to $V_D + s R_D V_{DS}$, but the drain-induced barrier lowering (DBL) factor $s$ is small enough to be neglected in our long-channel devices. Equation (2) can then be re-written as

$$I_D = \mu_i C \frac{W}{L} \left[ (V_{G,S} - I_D R_C) - V_T - (V_{DS} - 2 I_D R_C) / 2 \right] V_{DS} - 2 I_D R_C$$

Rearranging Eq. (3) to solve for $I_D$, we obtain

$$\Rightarrow I_D = C \frac{W}{L} \left[ 1 - \theta (V_{DS} - V_T - V_{DS,2}) \right] \frac{W}{L} \left[ V_{DS} - V_T - V_{DS,2} / 2 \right] V_{DS}$$

where $\theta = 2 R_C \mu_i C \frac{W}{L}$

From Eq. (4), we can infer that when $R_C \neq 0$, $I_D$ increases sub-linearly with $V_{DS}$. To exclude the effect of $R_C$, one can first calculate $1/\sqrt{\theta}$, as shown by Ghibaudo et al. and Jain et al., where $\theta_m \equiv \partial I_D / \partial V_{G,S}$ is the transconductance of the device.

$$\frac{1}{\sqrt{\theta_m}} = \left( \frac{L}{\mu_i C \frac{W}{L}} \right)^{1/2} \left[ 1 + \theta (V_{DS} - V_T - V_{DS,2}) \right]$$

Upon multiplying Eqs. (4) and (5), $\theta$ can be eliminated and an expression commonly known as the $Y$-function is obtained, which depends linearly on $V_{G,S}$.

$$Y = \frac{I_D}{\sqrt{\theta_m}} = \left( \frac{\mu_i C \frac{W}{L}}{\theta_m} \right)^{1/2} \left[ V_{DS} - V_T - V_{DS,2} \right]$$

By plotting $Y$ vs. $V_{G,S}$ and using Eq. (6), the mobility ($\mu_i$) and threshold voltage ($V_T$) can be extracted from the slope ($S_y$) and x-intercept, respectively. Figure 3a is a plot of the $Y$-function for the data in Fig. 2b. It shows an approximately linear behaviour in the strong inversion regime from which a value of $\mu_i = 29.2 cm²/V·s$ can be derived. Lastly, we plot $1/\sqrt{\theta_m}$ vs. $V_{G,S}$ (Fig. 3b) and extract the slope ($S_y$) of the linear region.

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**Figure 2. I-V measurements of monolayer MoS₂ with edge contacts.**

(a) $V_{G,S}$ dependent two-probe $I_D-V_{G,S}$ characteristics of a 1L-MoS₂ transistor measured under ambient conditions. (b) $I_D$-$V_{G,S}$ characteristics of the same device demonstrating that edge contacts can support a high current density comparable to top contact devices with similar channel lengths but large metal-MoS₂ overlap areas. Inset: Optical image of the measured device (outlined). (c) The data from b with $I_D$ plotted on a log-scale showing both forward and backward sweeps to highlight the low hysteresis. Inset: Magnified plot of the subthreshold characteristics at $V_{G,S} = 2$ V, 3 V (only forward sweeps) exhibiting a steep slope and ~1 pA/µm off current. (d) $I_D$-$V_{G,S}$ characteristics of the next device (inset) showing current magnitudes comparable to top contact devices with similar channel lengths but large overlap areas. Inset: Optical image of the measured device (inset) showing current magnitudes comparable to top contact devices with similar channel lengths but large overlap areas.
we followed a slightly different approach and directly fitted Eq. (4) in the inversion regime for each $V_{GS}$ dataset. From these fits, an average $\mu_0 \approx 30 \text{cm}^2 \text{V}^{-1} \text{s}^{-1}$ was found, where the error margin represents one standard deviation. To study the influence of etched hBN sidewall profiles on edge contacts, we tested two different hBN etch recipes\textsuperscript{37,38}. Figures 3d-e are histograms of $R_C$ extracted from devices etched using the two recipes. For SF$_6$ + Ar etched devices, we estimate an average $R_C = (64.2 \pm 9.6) \text{k} \Omega \mu \text{m}$ at $V_{GS} = [1 \text{V}]$ (blue bars). Since our $I_{DS}-V_{GS}$ curves are slightly asymmetric in general (Fig. 2a), we extracted $R_C$ values from $I_{DS}-V_{GS}$ fits for both positive and negative $V_{GS}$. Some devices were also measured at $V_{GS} = [2 \text{V}]$ (orange bars) with an average $R_C-W = (46 \pm 10) \text{k} \Omega \mu \text{m}$. In contrast to SF$_6$ + Ar etched devices, those etched with CHF$_3$ + O$_2$ show a wider distribution (Fig. 3e) and a higher mean value of $R_C-W$ (75.3 $\pm$ 23.4 $\text{k} \Omega \mu \text{m}$. We attribute this increased variability to greater etching inhomogeneity resulting from CHF$_3$ + O$_2$ in comparison with SF$_6$ + Ar, which we discovered upon scanning electron microscopy of bare hBN sidewalls (Supplementary Fig. S1).

### Quantum transport simulations

In order to gain further insight into carrier transport through edge contacts and compare them with top contacts, we performed...
was also discovered in an earlier theoretical work. The effect of an applied gate bias was incorporated by shifting the MoS$_2$ conduction band minima to 1 eV below $E_F$. The Schottky barrier heights $\phi_{SB}$ for both cases are indicated by vertical arrows (e: edge, t: top). A higher $T(E)$ is clearly visible for edge contacts which have a more favorable orbital overlap between terminal Ti and Mo atoms. However, due to the nature of the band alignment simulated in b-c, a larger $\phi_{SB}^e = 0.72$ eV for edge contacts compared to $\phi_{SB}^t = 0.44$ eV for top contacts limits the overall current. Since experimentally measured $\phi_{SB}$ values are known to be significantly smaller than those indicated in b-c owing to Fermi level pinning and due to the inability of DFT to predict accurate band alignments, a more realistic scenario was evaluated by reducing both barrier heights by equal amounts. Calculated total current densities plotted as a function of $\phi_{SB}$. We find that for $\phi_{SB}^e < 0.48$ eV, $I^e$ exceeds $I^t$ due to the enhanced $T(E)$ allowed by edge contacts, implying that in real devices, the injected current density can be substantially increased by making use of edge contacts.

**Methods**

Spatially resolved density of states (DOS) distributions were computed for both structures and are displayed as color-coded band-diagrams in Figs. 4b-c. From these figures, the Ti-MoS$_2$ band alignments and the resulting Schottky barrier heights $\phi_{SB}$ can be discerned. A striking observation is that for the same metal-semiconductor combination, $\phi_{SB}$ varies substantially with the contact type, revealing an interface geometry dependent Fermi level pinning. Besides Ti, we found a similar trend for Au contacts (simulations not shown here), which was also discovered in an earlier theoretical work. The charge neutrality level (CNL) at the metal-MoS$_2$ interface is determined by the mid-point energy of the partial density of states distributions of the MoS$_2$ orbitals relevant for bonding in a given contact geometry, along x, y-directions for edge contacts and z-direction for top contacts. Specifically, the Mo $d_{xz}$ and $d_{yz}$ orbitals that are involved in edge contacts, only contribute to deep valence band states ($\sim 1$ eV below the true valence band maximum of MoS$_2$) and moves the CNL at the metal-MoS$_2$ edge interface away from the mid-gap and towards the MoS$_2$ valence band, thereby increasing the Schottky barrier height $\phi_{SB}^e$ for edge contacts. Note that although the DOS distributions of MoS$_2$ vary slightly between Figs. 4b and c due to the finite number of k-points used here to reduce the computational costs, this does not affect the respective Ti-MoS$_2$ band alignments.

To emulate the effect of an applied gate voltage, the MoS$_2$ conduction band minima in Figs. 4b-c were pushed to 1 eV below the Fermi level ($E_F$) by superimposing an exponentially decaying, electrostatic potential profile (see Methods). Under this scenario, energy dependent electron transmission probabilities, $T(E)$, were calculated in the limit of ballistic transport for both cases and are plotted in Figs. 4d-e. It is seen that edge contacts result in an increased electron transmission compared to top contacts, as anticipated by a previous computational study. This can be attributed to a shorter tunneling path (edge: 0.84 Å, top: 1.51 Å) and stronger orbital overlap between terminal Ti and Mo atoms when brought in contact laterally without an intermediate layer of S atoms. However, the presence of a finite $\phi_{SB}$ causes the onset of the enhanced $T(E)$ to lie above $E_F$ in Fig. 4d. But it must also be kept in mind that in real devices, the effective $\phi_{SB}$ is strongly dictated by Fermi level pinning and, which is mediated by defects and interface states. This leads to measured $\phi_{SB}$ values being significantly smaller than those predicted here by DFT.

Therefore, in order to evaluate a more realistic contact alignment, the Schottky barriers of both contacts were lowered by the same amount by artificially raising the metal Fermi levels in Figs. 4b-c. The total current was determined as a function of $\phi_{SB}$. We find that for $\phi_{SB} < 0.48$ eV, $I^e$ exceeds $I^t$ due to the enhanced $T(E)$ allowed by edge contacts, implying that in real devices, the injected current density can be substantially increased by making use of edge contacts.
contacts on heavily n-doped CVD grown 1L-MoS$_2$ on SiO$_2$.\textsuperscript{59} This was again suggested to be a consequence of MIGS, originating from metal wavefunctions that decay evanescently into the MoS$_2$. However, since these states have an imaginary \( k \)-vector which does not support electron propagation, their true nature and role in carrier injection needs to be resolved. Hence, the existence of a Schottky barrier as seen in our simulations is still relevant to consider.

**Discussion and conclusions**

Strictly speaking, the true bandstructure of a semiconductor is defined for a lattice with an infinitely repeating unit cell. At MoS$_2$ edges and grain boundaries, dangling bonds and Mo-, S-vacancies perturb the MoS$_2$ bandstructure and give birth to additional localized ‘edge states’ within the bandgap, as measured experimentally\textsuperscript{12,60}. Such states were also observed in air-exposed MoS$_2$\textsuperscript{12} and WSe$_2$\textsuperscript{61} devices, implying that adsorbed O$_2$ and H$_2$O do not fully passivate them. Elimination of edge states is essential for good edge contacts, which may be achieved by Ti-MoS$_2$ bonding. However, if a van der Waals gap or trapped air molecules are present between the MoS$_2$ edge and Ti, edge state passivation would be hindered, resulting in a high density of in-gap states at each electron injection site. By trapping incoming electrons, these states can cause a space charge region to build up which would repel further injected electrons. In this regard, \textit{in-situ} Ar$^+$ sputtering plays a key role in producing a clean MoS$_2$ edge immediately before Ti deposition. Subsequent annealing at 300 $^\circ$C promotes atomic rearrangement and Ti-MoS$_2$ bonding. The need for such extra measures does not arise in the case of edge contacts to graphene, where edge states (if any) are unable to trap carriers because of the absence of a bandgap. Even O$_2$ incorporation at the graphene edge was shown to have a negligible effect\textsuperscript{37}, thus greatly simplifying fabrication of edge contacts to graphene. This scenario is fundamentally different from top contacts where the injected electrons do not encounter any edge states since the translational symmetry of the underlying MoS$_2$ lattice is not broken (in the absence of interfacial reactions and defects) and on the contrary, a vdW gap is beneficial for avoiding Fermi level pinning\textsuperscript{62}.

Interactions between the contact metal and MoS$_2$ at the atomic scale and structural characteristics of the contact interface play a significant role in governing the performance of any contact. For edge contacts, where carrier transfer is restricted to a single atomic edge, an optimum metal-MoS$_2$ layer thickness is crucial. This makes them more challenging to fabricate compared to top contacts which impose fewer constraints and can tolerate local non-idealities to a greater extent due to the availability of a finite area. Our main achievement here lies in the development of an optimized process for realizing low resistance edge contacts with a very high density of current injection per atomic site. Further studies are needed nevertheless to unravel the rich physics and chemistry occurring at the edge contact interface. It is possible that unpassivated edge states at interface voids still undermine the performance of our devices and also cause undesired Fermi level pinning. Suitable chemical termination of dangling bonds could be a promising strategy to passivate edge states and de-pin the metal Fermi level. Apart from MoS$_2$, air sensitive TMDCs like HfS$_2$, ZrS$_2$, etc. where edge states are expected to lie at shallow levels close to the band extrema, which makes them more immune to defects, appear as attractive materials for edge contacts.\textsuperscript{63} Even though -\mu m long Ag-Au\textsuperscript{14} and Ti-Au\textsuperscript{49} top contacts on 1L-MoS$_2$ have resulted in a lower \( R_c \) than that obtained in this work, in order to be fair, a comparison should be made with top contacts scaled down to sub-nm overlap lengths. However, it is known that the \( R_c \) begins to increase considerably for contact lengths smaller than the current transfer length in both monolayers\textsuperscript{64} and multi-layer MoS$_2$.\textsuperscript{65} This implies that conventional contacts cannot be scaled down beyond a certain limit, thereby restricting the minimum achievable device footprint (gate length $+ 2 \times$ contact length). To ensure scaling of TMD based devices, scalable contact geometries that work efficiently irrespective of dimensions are necessary. Here we overcome this bottleneck via edge contacts, which do not require a 2D overlap with MoS$_2$ and thus, in principle, can be milled as narrow as possible. Another domain where edge contacts can outperform top contacts is multilayer TMDs, where carrier injection only via the topmost layer suffers from added interlayer hopping resistances that limit the current transport to top few layers,\textsuperscript{66} whereas with edge contacts every layer can be individually contacted for achieving higher current densities.

Lastly, the possibility to encapsulate 2D materials before processing with chemicals remains the biggest advantage of edge contacts for building clean devices. Fundamental studies rely on high interface quality and macroscopic homogeneity for uncovering new physical phenomena, which can benefit from edge contacts fabricated after encapsulation. Edge contacts are especially promising for 2D materials unstable in air for which fabrication of top contacts is challenging due to restrictions imposed by encapsulation inside an inert atmosphere before being exposed to air. Often such heterostructures are built in a top-down manner and the need to make contacts to buried layers demands pick-up of additional graphene sheets. In such scenarios, edge contacts provide a much higher flexibility in heterostructure assembly and can be scaled-up to integrated circuits employing multiple metal layers separated by insulating dielectric layers. To conclude, we envision that edge contacts will bring devices based on 2D materials one step closer to practical implementation and open up new pathways in 2D materials research.

**Methods**

**Electrical characterization.** I-V measurements were carried out using a Keithley 2602B source meter in two-probe configuration. All devices were measured at room temperature in air. For calculating \( g_m \), the \( I_C-V_G \) curves were smoothened by cubic spline interpolation in MATLAB to reduce the noise before differentiation.

**Computational details.** Transport through the Ti-MoS$_2$ interface was simulated using a quantum transport solver based on the non-equilibrium Green’s function (NEGF) formalism\textsuperscript{67}. The Hamiltonian of the system in equilibrium was determined \textit{ab initio} with the help of the DFT tool VASP\textsuperscript{68}. An approximately 20 nm long cell was constructed that contained large enough regions of both pure Ti and pure MoS$_2$ far from the interface where bulk-like behaviour could be expected. Ti was modeled with only 6 atomic layers in height, as adding more layers vertically did not significantly change the interface properties.\textsuperscript{41} Generalized gradient approximation (GGA) of Perdew, Burke, and Ernzerhof\textsuperscript{70} was applied. Van der Waals interactions between Ti and MoS$_2$ were included through the DFT-D2 method of Grimme\textsuperscript{70}. Ions close to the interface were relaxed by geometric optimization and the single-particle electron wavefunctions were determined. The results were then transformed into a set of maximally localized Wannier functions (MLWFs) with the Wannier90 code\textsuperscript{69}.

For calculating the transmission probabilities, the Hamiltonian of a system with a longer (50 nm) MoS$_2$ extension was created from the Hamiltonian matrix elements in the MLWF basis. This procedure is further detailed in Appendix B2 of ref.\textsuperscript{72}. Since the considered simulation domains are problematic for self-consistent NEGF simulations, a decaying exponential function ($\propto \exp[-x/\lambda]$ where the screening length $\lambda \approx 5$ nm) receding away from the metal contact was superimposed over the MoS$_2$ region to realistically model the electrostatic behavior. This is known to be a good approximation for the potential profile in the MoS$_2$ channel near the contacts under an applied gate voltage.\textsuperscript{73} The same potential profile was used for both contact geometries. Only ballistic transport was simulated (without including electron-phonon scattering).

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**Author Contributions**

ML, LN and AJ conceived the project. AJ developed the fabrication procedure, carried out the measurements and analyzed the experimental data. AS and ML performed the quantum transport simulations. MP built the electrical characterization setup, wrote the LabVIEW scripts for recording IV data and provided experimental support at various stages. TT and KW synthesized the hBN crystals used in this study. LN, ML and PB supervised the project. The manuscript was written by AJ with inputs from MP, AS, ML and LN.

**Competing Interests**

The authors declare no competing financial interests.

*Note added:* During the preparation of this manuscript, we became aware of another related work on edge contacts to MoS2.

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Supplementary Information

One-dimensional edge contacts to monolayer semiconductors

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List of Figures

S1 Etched hBN roughness ........................................................................... ii
S2 Edge contact metallization ......................................................................... iii
S3 Resistance reduction by annealing ............................................................ iv
S4 Hysteresis reduction by annealing .............................................................. iv
S5 SF6 + Ar etched devices ........................................................................ vi
S6 Pure Au edge contacts ............................................................................. vi
S7 Poor adhesion between Au and hBN ......................................................... vi
S8 Devices without Ar sputtering ................................................................... vii
S1. Fabrication details

**hBN-MoS$_2$-hBN heterostructure assembly**: Bottom hBN flakes were directly exfoliated on O$_2$ plasma cleaned p$^+$ Si/SiO$_2$ (100 nm) substrates using a blue tape (Nitto). Naturally occurring MoS$_2$ crystals (SPI Supplies) were exfoliated on viscoelastic PDMS stamps (Gel-Film® PF-40-X4 sold by Gel-Pak). We found that PDMS often has a significant amount of uncrosslinked (or ‘loosely bound’) dimethylsiloxane oligomers on its surface$^1$ which can contaminate 2D materials exfoliated on PDMS$^2$. In order to achieve high carrier mobilities and avoid unintentional doping, it is crucial to minimize PDMS residues and transfer MoS$_2$ in a pristine manner. Therefore, prior to MoS$_2$ exfoliation, all PDMS stamps were treated with UV-O$_3$ in a Bioforce Nanosciences UV-ozone ProCleaner for 30 min (manufacturer specified illumination intensity: 14.76 mW/cm$^2$), following the procedure outlined in ref. 2. UV-O$_3$ exposure breaks down unwanted surface oligomers and forms a residue free, few nm thin SiO$_2$ layer on the PDMS surface$^3$. After UV-O$_3$ treatment, PDMS stamps were left in ambient air for 2 h to deactivate the surface termination and cause a partial hydrophobic recovery of the PDMS surface. This wait interval prevents bonding between PDMS and the blue tape and helps to increase the yield during exfoliation.

Bulk MoS$_2$ crystals were then exfoliated on the clean PDMS stamps after 2 h and monolayer flakes were identified in an optical microscope. For transfer, PDMS stamps with MoS$_2$ were placed on a transparent quartz plate and aligned on top of suitable bottom hBN flakes on SiO$_2$ using a SUSS MicroTec MJB4 mask aligner. All transfers were carried out in air. Upon coming in contact, the hBN-MoS$_2$ stacks were heated to ~65 °C for 2 min with a Peltier module kept underneath the Si/SiO$_2$ substrates. After allowing for a few minutes to cool down, the PDMS stamps were then slowly detached. The transferred MoS$_2$ flakes on hBN were annealed at 200 °C for 3 h in high vacuum (2 × 10$^{-6}$ mbar) to remove any remaining PDMS residues and release transfer induced compressive strain as well as accumulated bubbles/wrinkles in MoS$_2$$^2$. The same procedure was followed to transfer the top hBN flakes onto the MoS$_2$ - (bottom) hBN stacks and the resulting heterostructures were again vacuum annealed at 200 °C for 3 h to reduce the density of bubbles.

**Electron beam lithography (EBL) and etching**: Clean, bubble-free areas in the hBN-MoS$_2$-hBN heterostructures were chosen and patterned into well-defined rectangular channels by EBL (RAITH150 Two) with a bilayer of PMMA 50k (4% in chlorobenzene) and 950k (4.5% in anisole). Each layer was spin-coated at 5000 rpm for 45 s and baked at 180 °C for 4 min. After EBL (electron dose: 400 µC/cm$^2$ at 30 kV), PMMA was developed in MIBK:IPA (1:3) for 60 s and exposed areas were etched away by reactive ion etching (RIE) in an Oxford Plasmalab 80 Plus system. For making edge contacts into the rectangular channels, EBL and RIE were repeated again. RIE was performed with either (a) CHF$_3$ + O$_2$ plasma (40 + 4 sccm, 50 W power and 37.5 mTorr pressure, etch rate: ∼36 nm/min)$^4$ or (b) SF$_6$ + Ar plasma (20 + 20 sccm, 50 W power and 100 mTorr pressure, etch rate: >90 nm/min)$^5$. Scanning electron microscope (SEM) images of the hBN surfaces resulting from the two etching recipes are shown in Fig. S1 for comparison and reveal some striking differences. Reactive ion etching of hBN with CHF$_3$ + O$_2$ proceeds primarily via chemical interactions that strongly favor etching along certain in-plane crystal directions. It can be noticed in Fig. S1a that this highly anisotropic etch rate leaves behind a high density of hBN pyramids in the etched regions and forms sidewalls with very narrow triangular crevices (red dotted lines). It is reasonable to assume that during metal deposition over such hBN sidewalls, Ti grains might not fill these fine crevices entirely, resulting in a loss of contact with the MoS$_2$ edge at certain spots.

![Figure S1. Etched hBN roughness. (a) Tilted view SEM images of contact trenches in a test hBN flake, etched half-way through with CHF$_3$ + O$_2$ for 210 s. The etched regions display a very rough bottom surface, with partially etched hBN pyramids, and sidewalls featuring narrow, vertical crevices with triangular facets, arising from the crystallographic planes of hBN. Two such crevices have been indicated by red dotted lines. (b) SEM images of a curved trench etched in another (thinner) hBN flake with SF$_6$ + Ar for 20 s. It exhibits a smooth bottom SiO$_2$ surface with a significantly reduced density of unetched hBN pyramids. No triangular crevices like those indicated in a could be resolved in this flake, although considerable sidewall roughness is still present. All images were taken immediately after etching, without removing PMMA, in order to avoid deposition of any organic residues that might smear out the sharp hBN features and reduce image contrast. Upon interaction with the electron beam (5 keV), the PMMA layer retracted away from the sides, allowing hBN to be imaged. Scale bars: 200 nm in all images.](image-url)
Moreover, within a single device, source and drain contacts formed along parallel etched trenches would have different faceting due to the 60° rotational symmetry of hBN (and not 90°), giving rise to asymmetric $I_{ds}$-$V_{gs}$ characteristics. In case of SF$_6$ + Ar (1:1), the introduction of Ar adds a physical sputtering contribution to the etch process. This leads to more isotropic in-plane etching, resulting in sidewalls devoid of triangular facets, as shown in Fig. S1b and lower contact variability (see Fig. S5).

**Metal deposition and annealing:** This is the most critical part of our fabrication process. As discussed in the main text, etched MoS$_2$ edges have a large number of dangling bonds which host in-gap edge states and act as adsorption sites for air molecules (O$_2$, H$_2$O). These adsorbed species could likely hinder covalent bonding between the contact metal (Ti) and MoS$_2$, leaving edge states unpassivated, which subsequently act as traps for injected carriers. Moreover, Mo atoms located at the edge can oxidize to form MoO$_x$ which, owing to its high work-function, would pose a further barrier for electron injection. Therefore, in order to limit MoS$_2$ oxidation after RIE, the samples were immediately loaded into an electron beam evaporator (Plasys MEB550S) for metal deposition, with only a few minutes of air exposure in between. While loading, the etched contact trenches were aligned parallel to the axis of the tilting motor and thereafter, the samples were not rotated in-plane at any point during sputtering and evaporation. To remove any MoO$_x$ and form a clean MoS$_2$ edge just before metal deposition, the contact edges were sputtered *in-situ* with an Ar$^+$ ion beam at +15° and -15° tilt (Fig. S2b) for 15 s each (250 V beam voltage, 50 V acceleration voltage, 10 mA beam current).

Ti (5 nm) was then deposited at 0.2 nm/s rate under a base pressure of $1 \times 10^{-7}$ mbar, first at +15° tilt and then 5 nm again at -15° tilt, as depicted in Fig. S2c. Tilting was necessary to avoid shadowing of the MoS$_2$ edge by the overhanging bilayer PMMA sidewalls. In this manner, a nearly conformal Ti layer could be deposited over the hBN sidewalls despite the rough topography, as visible in Fig. S1d. Au (40 + 40 nm) was then deposited the same way. Note that the choice of deposition angle was constrained by the PMMA undercut angle in our case. Deposition at 20° caused the PMMA sidewalls to be also partially coated with Ti-Au, leaving behind vertical ears upon lift-off, while 30° resulted in no lift-off. After lift-off in hot acetone, the samples were annealed at 300 °C in Ar + H$_2$ (380 + 20 sccm) for 3 h inside a quartz tube furnace to improve the contacts. Finally, for electrical characterization, wire-bonds were made manually with a 25 μm diameter tungsten wire and silver epoxy (CircuitWorks® CW2400). The epoxy was cured at 80 °C for 30 min in a vacuum oven. Unlike conventional ultrasonic wire-bonding, Ag epoxy helped to prevent shorting with the Si back-gate through the 100 nm SiO$_2$ layer.

![Figure S2. Edge contact metallization.](image)

(a) Sketch showing possible existence of MoO$_x$ at the Ti-MoS$_2$ interface (top) whereas a MoO$_x$-free interface is desired (bottom). (b) Schematic illustration of a hBN-MoS$_2$-hBN heterostructure mounted upside-down inside an e-beam evaporator chamber, undergoing *in-situ* Ar$^+$ sputtering at +15° and -15° tilt to remove MoO$_x$ (if any) and absorbed O$_2$, H$_2$O molecules from both MoS$_2$ contact edges before metal deposition. (c) Schematic illustration of Ti deposition at +15° and -15° tilt, immediately after Ar$^+$ sputtering. (d) SEM image of a test hBN flake featuring a conformal deposition of Ti over the hBN sidewall, despite its roughness. Scale bar: 100 nm.
S2. Significance of annealing

Post metal-deposition annealing is commonly employed to lower the contact resistance \( R_c \) in 2D material devices. We tested several temperatures for this purpose and found that for edge contacts annealed in Ar + H\(_2\) (380 + 20 sccm), \( R_c \) reduced with increasing temperatures up to 400 \(^\circ\)C, as shown in Fig. S3a. At the same time, the high interface quality of our devices remained preserved due to hBN encapsulation, as evidenced by the unchanged steep subthreshold slope and negligible hysteresis in all \( I_D-V_{GS} \) plots in Fig. S3b. However, we observed that high temperatures can affect the long-term ambient stability of our devices to a certain extent. Besides this, we also varied the annealing time at a fixed temperature but did not notice a substantial change in \( I_D \) after a total duration >1.5 h (Fig. S3c). Considering both these facts, a temperature of 300 \(^\circ\)C and time 2-3 h were therefore chosen as optimum for our fabrication recipe. Lastly, un-annealed devices measured directly after metal deposition and lift-off, can sometimes exhibit a large hysteresis in the transfer characteristics, as seen in Fig. S4a. Annealing can help to get rid of such hysteresis (Fig. S4b).

Thus, we can conclude that annealing is indispensable for edge contacts. Several processes can occur simultaneously during annealing: metal-MoS\(_2\) covalent bonding, reduction of interfacial oxides and sulfur atoms by H\(_2\) molecules, inter-diffusion of edge atoms (metal into MoS\(_2\) or vice-versa), defect migration and edge reconstruction. Presently, it is unclear which process dominates in case of edge contacts and is responsible for the reduction of \( R_c \) upon annealing, although Fig. S3c points towards a weaker contribution of diffusion, which is a slow, time-dependent process. Understanding the various mechanisms at play and developing more effective annealing procedures is an interesting subject for future studies.

Figure S3. Contact resistance reduction by annealing. (a) \( I_D-V_{GS} \) characteristics of the 1L-MoS\(_2\) device, presented in Figs. 2a-c of the main text, measured after annealing in Ar + H\(_2\) at three different temperatures. It can be seen that the current density increases monotonically with the annealing temperature, implying a reduction in \( R_c \) upon annealing. This enhancement can possibly be attributed to improvement of the edge contact interface, leading to reduced scattering/trapping of electrons and thus, more efficient current injection. (b) \( I_D-V_{GS} \) data shown in a, plotted on a log-scale, exhibiting a consistently steep subthreshold slope after each annealing cycle. Moreover, all plots comprise of both forward and backward sweeps that display very small hysteresis (sweep directions marked by arrows). This indicates that in our devices, the MoS\(_2\) crystal quality and the low interface trap density (\( \sim 10^{11} \) eV\(^{-1}\) cm\(^{-2}\)), remain preserved by hBN encapsulation and do not deteriorate, at least up to 400 \(^\circ\)C. (c) \( I_D-V_{GS} \) Characteristics of the same device after annealing at 300 \(^\circ\)C for 30 min, 1 h and 3 h, incrementally. These results reveal that prolonged annealing (>1.5 h), at a fixed temperature, does not cause any significant change in the contact properties. All measurements were done in air at room temperature after each annealing.

Figure S4. Hysteresis reduction by annealing. \( I_D-V_{GS} \) transfer characteristics of 1L-MoS\(_2\) devices with Ti-Au (10-60 nm) edge contacts, (a) as-fabricated and (b) after annealing in Ar + H\(_2\) at 200 \(^\circ\)C for 3 h. The as-fabricated devices exhibit a large hysteresis between the forward and reverse sweeps, which nearly vanishes upon annealing, accompanied by a shift in the threshold voltages to lower values. The gate voltage sweep directions have been indicated by arrows. Inset: Optical image of the measured devices. In this sample, the SiO\(_2\) thickness was 285 nm and no in-situ Ar\(^+\) sputtering was performed (which explains the lower \( I_D \) compared to Fig. S3). Scale bar: 4 \( \mu \)m.
S3. Data from additional devices

Here we show I-V data from devices in which edge contacts were etched with SF$_6$ + Ar. The MoS$_2$ flake shown in Fig. S5a was exfoliated on PDMS and transferred to hBN (Fig. S5b-c). After encapsulating the MoS$_2$ with another hBN and patterning the resulting stack into two rectangular segments, edge contacts were fabricated on each (Fig. S5d). The $I_D$-$V_{DS}$ characteristics of one such device are plotted in Fig. S5e and display a nearly linear behavior without any sign of saturation, at least until 3 V. In Fig. S5f, the $I_D$-$V_{GS}$ curves of two representative devices are shown and exhibit similar characteristics, indicating a low-variability in contacts etched with SF$_6$ + Ar, as discussed in Section S1 above. All curves in Fig. S5f have been fitted with the model used in the main text. The excellent quality of the fits further corroborates the validity of the model. Log-scale $I_D$-$V_{GS}$ plots are shown in Fig. S5d, revealing a steep subthreshold slope and high on/off ratio, similar to Fig. 2c of the main text. These measurements, together with those in the main text, demonstrate that with our fabrication procedure, edge contacts can be made reproducibly.

Figure S5. SF$_6$ + Ar etched devices. (a) Optical image of a 1L-MoS$_2$ flake exfoliated on UV-O$_3$-cleaned PDMS. (b) Differential interference contrast (DIC) image of the same flake after having been transferred to hBN (25 nm thick) and vacuum annealed. (c) AFM topography map of the 10µm × 10µm region outlined in b, displaying a pristine MoS$_2$ surface with few interfacial bubbles (bright spots). Inset: Cross-section profile along the green dashed line, revealing a thickness close to monolayer. (d) Optical image of six devices built using the MoS$_2$ flake in b after hBN encapsulation. In all devices, $L = 1$ µm, $W = 3$ µm and the contact length $L_c = 0.5$ µm. The edge contacts outlined in blue were etched by RIE with SF$_6$ + Ar while those in red with CHF$_3$ + O$_2$. (e) $I_D$-$V_{GS}$ characteristics of the device labeled as 1 in d, exhibiting almost symmetric and linear (for $V_{DS} > 0.5$ V) transport behavior up to 3 V. (f) $I_D$-$V_{GS}$ characteristics of identical devices 1 and 2 showing very similar current densities. The dashed curves are fits obtained using the model in Eq. 4 (main text). The respective threshold voltages $V_T$, extracted from the fits, were subtracted from $V_{GS}$ in all plots, for a better comparison. (g) $I_D$-$V_{GS}$ characteristics of device 2 (same as in f) plotted on a log-scale, displaying an on/off current ratio $>10^7$ and a steep subthreshold slope (inset), maintained up to three orders of magnitude.
S4. MoS$_2$ FETs with pure Au edge contacts

In addition to Ti-Au, we also fabricated edge contacts with pure Au (i.e. without any Ti adhesion layer), since Au has been reported to result in low resistance contacts to MoS$_2$. Figure S6 shows the optical images of an hBN encapsulated 1L-MoS$_2$ sample with Au edge contacts, together with the I-V characteristics of one device. However, this sample was among the very few that were successfully fabricated since, in general, Au was found to often result in devices that did not conduct at all. Upon closer inspection of failed samples in an SEM, we noticed gaps between Au and hBN in several contacts, as shown in Fig. S7. By comparing the morphology of Au before and after annealing, we observed that during annealing at 300 °C, Au tends to reflow and lose contact with hBN due to poor adhesion. This occurred despite Au deposition at an angle so as to completely cover the hBN sidewalls. Therefore, we infer that pure Au is not suitable for edge contacts, in combination with high-temperature annealing.

Figure S6. Pure Au edge contacts. (a) Optical image of a 1L-MoS$_2$-hBN heterostructure on a Si/SiO$_2$ (285 nm) substrate. (b) Final stack after top hBN transfer and Au (60 nm) edge contacts fabrication. The encapsulated MoS$_2$ flake has been demarcated by white dashed lines. No Ar$^+$ sputtering was performed for this sample. (c-d) $I_D$-V$_{DS}$ and $I_D$-V$_{GS}$ characteristics of the device outlined by the black dashed rectangle in (b).

Figure S7. Poor adhesion between Au and hBN. (a) Schematic illustration of Au losing contact with MoS$_2$ encapsulated between two hBN layers. (b-d) SEM images of actual devices revealing gaps between hBN sidewalls and Au after annealing at 300 °C. Such gaps often cause devices to not conduct, making Au without an adhesion layer, highly unreliable for use in edge contacts.
S5. Edge contacts without Ar⁺ sputtering

In the most general case, Ti-MoS₂ edge contacts can be considered to be composed of Ti-TiOₓ-(air molecules)-MoOₓ-MoS₂ junctions. For improving the contact performance, it is important to determine the role of each interfacial species. As discussed in the main text, we fabricated several devices without sputtering the MoS₂ contact edges with Ar⁺, in order to leave air molecules and MoOₓ (if any) intact. The transfer characteristics of three such devices, shown in Fig. S8a, exhibit a substantially lower \( I_D \) compared to Ar⁺ sputtered devices fabricated on the same hBN-MoS₂-hBN stack (see Fig. 1h of the main text). Furthermore, it has been found previously by X-ray photoelectron spectroscopy (XPS)⁹ that Ti can oxidize to form TiOₓ when deposited under moderately high vacuum conditions (\(~1 \times 10^{-6} \) mbar). To inhibit TiOₓ formation and study its effect, Ti-Au was deposited at \( \sim 1 \times 10^{-8} \) mbar on another sample (Fig. S8b), again without Ar⁺ sputtering. Before metal deposition on the contacts, Ti (80 nm) was evaporated into the chamber while keeping the sample surface covered by a shutter, to capture residual O at the contact edges with Ar⁺ sputtering. The current density in these devices is 5-8x lower compared to those on the same sample that were Ar⁺ sputtered. Ti-Au deposition was done at \( \sim 1 \times 10^{-7} \) mbar. Inset scale bar: 3 \( \mu \)m. (b) Optical image of another set of control devices in which, Ar⁺ sputtering was again not performed and additionally, Ti-Au was deposited at a base pressure of \( \sim 1 \times 10^{-8} \) mbar to prevent TiOₓ deposition. The channel lengths \( L \) range from 0.25-3 \( \mu \)m. (c) \( I_D-V_{GS} \) characteristics of the devices shown in b. Despite the higher vacuum, \( I_D \) in this case too is similar to a and much lower than that obtained after Ar⁺ sputtering. Moreover, no correlation with \( L \) is discernible, indicating a high \( R_C \) in every device. All \( I_D-V_{GS} \) plots shown in a and c were recorded after annealing in Ar + H₂ at 200 °C for 3 h. The characteristics of un-sputtered devices did not improve considerably upon further annealing at higher temperatures.

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