

Correlating Carrier Localization to Optoelectronic Behavior of Monolayer MoS₂

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Abstract

In nanoscale semiconductor devices, electrical conductivity is significantly influenced by inherent disorder. This study examines the electrical transport properties of a single-layer MoS₂ field-effect transistor on a few-layered hBN substrate. Temperature-dependent transport measurements reveal that electrical conductivity is predominantly governed by a combination of simple activated and variable-range hopping mechanisms. The calculations on the experimental data yield a localization length around 5 nm for a typical defect density near the Fermi energy as $10^{14} \text{ eV}^{-1} \text{ cm}^{-2}$. Additionally, optoelectronic transport measurements exhibit temperature-dependent persistent photoconductivity, attributed to electron localization within defect states. Calculations based on the temperature-dependent photoconductivity relaxation indicate a localization length of 7 nm, suggesting a direct correlation between the two phenomena.

Keywords

Two-dimensional semiconductor, Transition metal dichalcogenide, Electrical Transport, Variable range hopping, Carrier localization, Optoelectronic Transport, localization length

Introduction

Structural defects¹ happen to be one of the ingredients to modify the electronic properties of any material.² Vacancy³ in the atomic structure of any semiconductor creates low energy states in the band structure, which could host charge carriers.⁴ The influence of structural defects¹ and the resulting carrier localization^{5–8} are of particular interest, as they can give rise to intriguing electronic^{9,10} and photonic behaviors.^{11–14}

Beyond graphene,¹⁵ transition metal dichalcogenides¹⁶ have become the focus of extensive research as promising two-dimensional¹⁷ materials for transistor applications. Among them,

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atomically thin molybdenum disulfide (MoS_2)¹⁸ stands out due to its direct optical band gap of 1.8 eV,¹⁹ enabling potential applications in visible-range optoelectronics^{20,21} alongside novel phenomena such as valley polarization,^{22–24} Zeeman splitting,¹⁸ and superconductivity.²⁵ Notably, MoS_2 field-effect transistors (FETs) have enabled the development of photodetectors²⁶ with impressive photoresponsivity of up to 1000 A/W and diverse response times.^{20,27} A remarkable feature is the observation of persistent photoconductivity,^{28–30} where conductivity fails to return to its dark-state value after illumination is turned off. Interestingly, similar device structures have also exhibited significantly lower photoresponsivity, as low as 0.1 A/W.³¹

The varied electrical behavior in MoS_2 devices is fundamentally linked to random disorder^{32–34} and carrier localization, which strongly influence their optoelectronic properties.^{35–38}

In this work, we conduct detailed temperature-dependent electrical transport measurements to investigate the conduction mechanisms and the impact of carrier localization on the optoelectronic transport properties of single-layered MoS_2 transistors.

Our analysis reveals variable-range hopping as the dominant mechanism governing electrical transport in the channel, enabling the determination of the localization length. Interestingly, calculations derived from temperature-dependent optoelectronic transport measurements yield a comparable localization length, demonstrating a strong correlation between these phenomena. Here the findings are presented.

Experiment

Materials

The devices were made from bulk MoS_2 (obtained from 2D Semiconductors Inc. USA) and bulk hexagonal boron nitride, which are grown in a facility in National Institute for Materials Science, Japan.

Device fabrication and measurements

Single-layered MoS_2 ³⁹ was obtained via standard mechanical exfoliation of commercially available bulk crystals. The exfoliated MoS_2 flakes were subsequently transferred^{40,41} onto a few-layered hBN substrate (exfoliated from crystals sourced from NIMS, Japan) on a $\text{SiO}_2/\text{Si}^{++}$ substrate. In this configuration, the heavily doped p-type Si^{++} serves as a global back gate. Few-layered hBN,⁴² a wide-bandgap semiconductor (≈ 6 eV), provides an atomically smooth and defect-sparse insulating interface, mitigating the impact of defects at the SiO_2 -TMD interface on electrical and optoelectronic transport. The surface morphology was characterized by atomic force microscopy (Park Systems NX-20 AFM) (see Supplementary Info).⁴³

Electrical contacts to the MoS_2 were defined using electron-beam lithography^{44–46} and fabricated through thermal evaporation of Cr (5 nm) and Au (50 nm). The device architecture and experimental setup are illustrated in Fig. 1(a). A constant bias voltage was applied to the source (S) terminal, while the drain (D) current (I_{DS}) was measured using a lock-in amplifier across various temperatures. A tunable DC voltage, applied to the p-doped Si^{++} , functioned as the global back gate (V_g). All measurements were conducted in a custom-built cryostat²⁸ under high vacuum conditions (10^{-6} mbar).

Figure 1(b) presents optical image of one of the fabricated devices, where the large purple flake represents the few-layered hBN, and the outline of the MoS_2 flake is indicated by dotted blue lines. The yellow regions correspond to invasive gold contacts deposited on the MoS_2 flake. Prior to the contact fabrication, the flakes were characterized through room-temperature photoluminescence (PL) and Raman spectroscopy (Raman-PL spectrometer, LabRam HR, Horiba Jobin Vyon).

Results and Discussions

We begin to describe our device characterization with the room temperature photoluminescence (PL) emission spectra are presented in Fig. 1(c). The PL peaks were analyzed using Lorentzian fitting to determine their positions. The deconvoluted spectra reveal prominent emission peaks

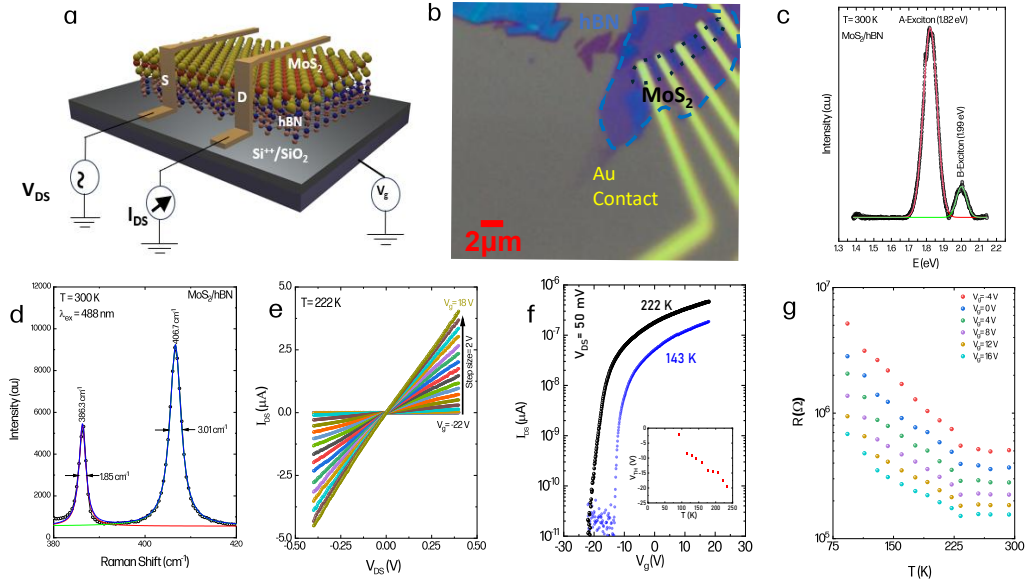


Figure 1: Device Architecture and primary characterizations. (a) Schematic of the MoS₂-hBN device architecture and electrical measurement setup. A constant bias voltage is applied to the source (S) terminal, and the drain (D) current (I_{DS}) is measured using a lock-in amplifier at various temperatures. A tunable DC voltage (V_g) is applied to the p-doped Si⁺⁺, serving as a global back gate. (b) Optical image of the MoS₂-hBN device. The purple flake (outlined in dashed blue) represents the few-layered hBN substrate, with the MoS₂ flake (marked by a black dotted outline) placed on top. Invasive Cr/Au electrical contacts are fabricated on MoS₂ to define a channel length of approximately 2 μm. (c) Room temperature (295 K) photoluminescence (PL) spectra of the device in (b), showing excitonic peaks from MoS₂ at 1.82 eV ($\lambda = 681$ nm) and 1.99 eV ($\lambda = 623$ nm) with a linewidth of 50 meV. The solid purple line represents a Lorentzian fit to the experimental data. (d) Room temperature Raman spectroscopy of the MoS₂/hBN device measured using an excitation of 488 nm. The solid line is the Lorentzian fit to the experimental data which elucidates the prominent Raman active modes as E_{2g} at $(386.3 \pm 0.1) \text{ cm}^{-1}$ and A_{1g} at $(406.7 \pm 0.1) \text{ cm}^{-1}$. The corresponding full-width-half-maxima (FWHM) are found to be $(1.85 \pm 0.08) \text{ cm}^{-1}$ and $(3.01 \pm 0.02) \text{ cm}^{-1}$ respectively. (e) Representative output characteristics (I_{DS} - V_{DS}) at 222 K for gate voltages (V_g) ranging from -22 V to 18 V in 2 V steps. Linearity in the curves indicates the absence of a Schottky barrier at the MoS₂-Au interface, suggesting good device quality. (f) Transfer characteristics (I_{DS} - V_g) at 143 K and 222 K with $V_{DS} = 50$ mV. The transconductance increases for negative V_g , indicating n-type doping of the channel. The negative threshold voltage (V_{TH}) implies the conduction band edge (E_c) lies above the Fermi level at zero V_g , requiring negative V_g to align the Fermi level closer to the conduction band edge. V_{TH} shifts with temperature (Inset: variation of V_{TH} with temperature), decreasing as temperature increases. This behavior reflects a reduction in the energy barrier for electrons entering the conduction band. (g) Temperature dependence of resistivity (semi-log representation) at various gate voltages. Resistances are extracted from linear fits of the output characteristics near zero V_{DS} . The negative temperature coefficient of resistance indicates the semiconducting nature of the MoS₂ layer, with Fermi energy in the band gap at the given V_g . Two distinct regimes are observed: a temperature-sensitive regime $T < 225$ K and a nearly temperature-independent regime $T > 225$ K, indicating different transport mechanisms.

at (1.80 ± 0.05) eV and (1.99 ± 0.02) eV, corresponding to the A and B excitons in MoS₂, with an FWHM of (0.33 ± 0.05) eV and (0.23 ± 0.03) eV respectively. The strong A-exciton feature suggests that the used MoS₂ is indeed single layer, originating from the direct transitions at the K-point in the Brillouin zone.¹⁸ Near the A-exciton, a small hump was observed in at lower energy (1.78 eV), signaling a trion formation and indicating a possibility of an unintentional electron doping.

The room temperature Raman spectroscopy of one of the devices is shown in Fig.1(d). The experimental data show standard Raman characteristics of MoS₂ on hBN, the in-plane E_{2g} mode $((386.3 \pm 0.1) \text{ cm}^{-1})$ and out-of-plane A_{1g} mode $((406.7 \pm 0.1) \text{ cm}^{-1})$. The difference between these two prominent Raman features came out as 20.4 cm^{-1} . The Raman spectra of the extension of the same MoS₂ flake on the silicon wafer, gives a difference of 18 cm^{-1} , as expected for the monolayer MoS₂.⁴⁷ Following the correlative plot of the positions of A_{1g} and E_{2g} as described in reference,⁴⁸ we further estimate the strain present in the system as -0.26% . The negative sign suggests a compressive strain.

The electrical transport properties are characterized through the output characteristics of (I_{DS} - V_{DS}) the MoS₂ field-effect transistor, as shown in Fig. 1(e). Measurements were conducted at $T = 222 \text{ K}$ for gate voltages (V_g) ranging from -22 V to 18 V in 2 V steps. The linear output characteristic curves suggest ohmic behavior across all V_g , indicating the absence of Schottky barriers at the contacts and confirming the high quality of the device. These further enables the extraction of resistance from the Ohmic representation. The decreasing slope suggest an increase in resistance as V_g decreases. In Fig. 1(f), the transfer characteristics (I_{DS} - V_{DS}) of the device (presented in a semi-logarithmic scale) are shown, measured at $T = 222 \text{ K}$ and 143 K for a source-drain voltage of $V_{DS} = 50 \text{ mV}$ over the range of V_g from -30 V to 30 V . At large negative V_g , I_{DS} remains nearly zero until V_g approaches approximately -20 V , which acts as a threshold voltage (V_{TH}) where it begins to increase. Conduction begins in the negative V_g regime, indicating that the MoS₂ films are intrinsically n-type.⁴⁹ The charge carrier density (n) can be evaluated using the similar prescription described earlier.^{50,51} The doping concentration is

evaluated as $1 \times 10^{12} \text{ cm}^{-2}$ [See Supplementary information]. As the temperature (T) increases, the threshold voltage (V_{TH}) decreases monotonically (inset of Fig. 1(f)), reflecting a shift of the Fermi level toward the conduction band. This shift reduces the energy barrier for electrons to enter the conduction band. The on-off ratio of the device is approximately 10^5 , highlighting its reasonably well performance. The electron field-effect mobility (μ) was determined using the relation $\mu = (L/W)C_{ox}^{-1}V_{DS}^{-1} \left(\frac{dI_{DS}}{dV_G} \right)$,⁵¹ where the oxide capacitance is modeled as a series combination of the capacitances of 300 nm SiO_2 and 20 nm hBN.⁵⁰ At room-temperature μ comes out to be $8 \text{ cm}^2/\text{Vs}$, and is consistent with typical values for back-gated MoS_2 devices.^{19,51}

In Fig. 1(g), the temperature (T) dependence of the device resistance (R) is plotted for various V_g . The high channel resistance (approximately $1 \text{ M}\Omega$ typical for MoS_2), does not allow us to perform four-terminal measurements due to the internal impedance of the lock-in amplifier. Instead, the two-terminal resistance was determined from linear extrapolations of the I_{DS} - V_{DS} curves at different V_g and T . The resistance increases as the temperature decreases, indicating the semiconducting nature of the device for all V_g . The negative temperature coefficient of resistance further suggests that the Fermi energy remains within the band gap at the given V_g .

The data in Fig. 1(g) further exhibit a crossover from a strongly temperature-dependent regime at low temperatures ($T \leq 225 \text{ K}$) to a weakly temperature-dependent regime at higher temperatures ($T > 225 \text{ K}$). In disordered electronic systems, low-temperature electrical transport is governed by a variable range hopping (VRH) mechanism, where electrons hop between spatially distant localized states. Unlike thermally activated transport where the charge carriers crossover the barrier, VRH mechanism predicts a distinct temperature dependence of the conductivity, described by^{52–56}

$$\sigma = \sigma_0(T) \exp[-(T_0/T)^{(\frac{1}{d+1})}] \quad (1)$$

where d is the dimensionality and T_0 is the correlation energy scale, associated with the degree of disorder. The conductivity pre-factor (σ_0) depends on T as T^{-p} , where $p \approx 0.8 - 1$.⁵⁷ The VRH mechanism highlights the critical role of disorder and carrier localization in determining transport behavior at low T . We analyzed the low- T conductivity data of our devices within the framework

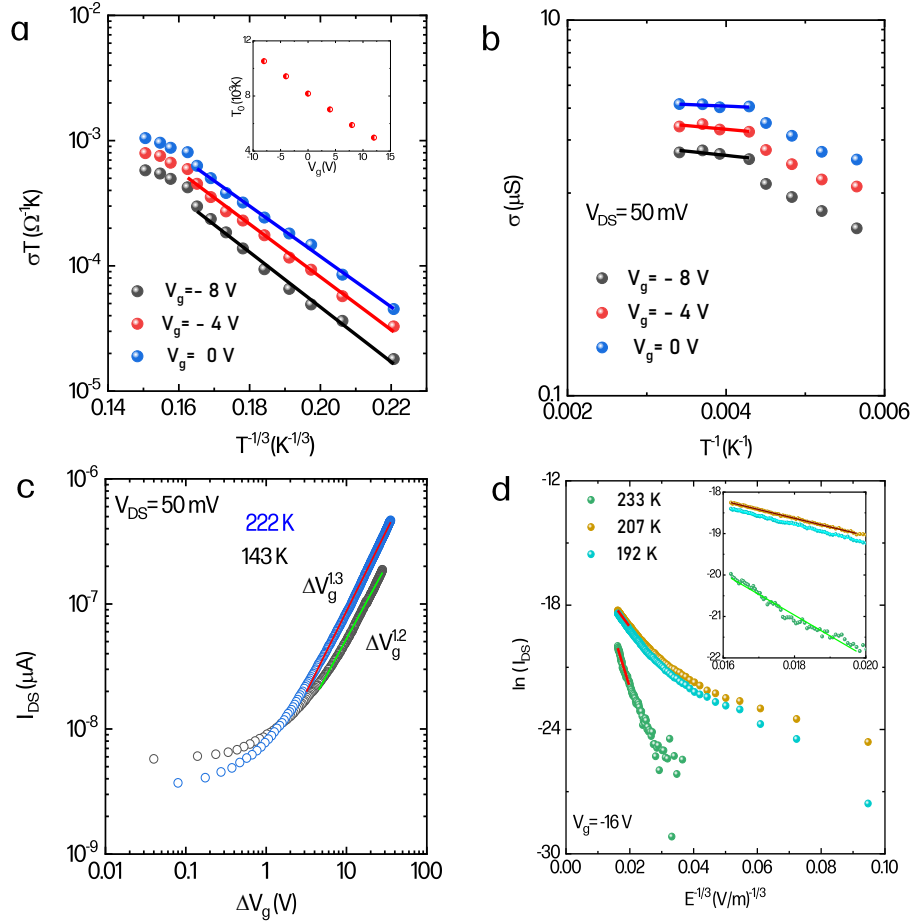


Figure 2: Analysis of the electrical transport. (a) Semi-logarithmic representation of the channel conductivity with $T^{-1/3}$ measured for three representative V_g at $V_{DS}=50$ mV. The linear fit in the low-T regime, suggests conduction through the Mott's variable range hopping (VRH) mechanism, where the electrons hop between localized states, following equation 1. (Inset: The gate voltage variation of the fitting parameter T_0 which connects to the localization energy and length. (b) The temperature dependence of the conductivity in an Arrhenius representation indicating the almost T-independent conductivity at higher temperatures. The calculated activation energy from the Arrhenius fit comes out as 0.03 eV. (c) The effective gate voltage (δV_g) dependence of the source-drain current measured using 50 mV source-drain voltage at two representative temperature 143 K and 222 K in double-logarithmic representation. The linearity of the plot at higher ΔV_g , suggest a power law behavior. The extracted exponent comes around 1.2; suggesting scattering occurs from screened Coulomb impurity. (d) Non-linear transport showing I_{DS} as a function of $E^{-1/3}$ (in semi-logarithmic representation) for three representative temperatures. (Inset:) The slope of the linear part at high electric fields yields the parameter E_{VRH} .

of the two-dimensional ($d = 2$) Mott variable-range hopping (VRH) model, as shown in Fig. 2(a). The ordinate is represented as σT , accounting for the T -dependent pre-factor of the conductivity, for three representative gate voltages (V_g). The experimental data exhibit excellent agreement with the two-dimensional Mott-VRH transport model, indicating that electronic transport in this system occurs through a broad band of localized states.⁵² From the fit, we extracted the characteristic parameter T_0 , found to be approximately 10^4 K (with an estimated error of 10 K), which decreases monotonically with increasing V_g [see inset Fig. 2(a)].⁵⁷ The energy scale T_0 holds significant implications, as it is directly related to the density of states near the Fermi energy ($N(E_F)$) and the localization length (ξ) via the relation $T_0 = \frac{\beta}{k_B N(E_F) \xi^2}$,^{54,57} where $\beta \approx 14$ is a numerical constant. Using a typical weakly varying value of $N(E_F)$ of $10^{14} \text{ eV}^{-1} \text{ cm}^{-2}$,^{51,54,57} the localization length (ξ) is estimated to be approximately 5 nm, which approaches the effective Bohr radius of hydrogen-like centers in MoS_2 .^{51,54} One of the standard sources of defects in MoS_2 is sulfur vacancies, which were created unintentionally during the fabrication process. In a perfect monolayer of MoS_2 , each Mo atom is surrounded by six S atoms (in a trigonal prismatic coordination). A sulfur vacancy occurs when one or more sulfur atoms are missing from this lattice. The sulfur vacancies are energetically stable in MoS_2 and shown theoretically to create localized states within the bandgap.^{54,58} These values of T_0 and the corresponding ξ are consistent with those reported in the literature.⁵⁷ Considering that the MoS_2 device is fabricated on a defect-free, atomically flat hBN substrate, we attribute the localized states to bulk defects within the MoS_2 rather than interface-induced defects. In the high-temperature regime ($T > 250$ K), as shown in Fig. 2(b), the conductivity exhibits a marginal temperature dependence. Analyzing this behavior in an Arrhenius representation,⁵³ we find that the conductivity (σ) follows the relation $\sigma = \sigma_0 \exp(-E_0/k_B T)$, indicating a simple thermally activated transport mechanism, where E_0 represents the activation barrier. The fit yields an activation energy of $E_0 = (0.030 \pm 0.008) \text{ eV}$, which is an order of magnitude smaller than the MoS_2 -Au contact barrier. This finding suggests that the electrical transport observed in Fig. 2(a) primarily originates from the channel rather than transmission at the contact barrier. Due to the electron-rich nature of the metal contact, it

induces n-type doping in the adjacent region of MoS₂, shifting the local Fermi level toward the conduction band edge. Although the MoS₂/metal interface may generate additional defect states, this analysis focuses on their collective impact on carrier transport rather than specific interfacial origins. Within the MoS₂ channel, bulk defect states enable hopping-mediated electron transport, particularly when band-like transport is inhibited by localization effects. While ohmic behavior is observed macroscopically, localized band bending near contacts and potential metal-induced gap states (MIGS) can modulate the local density of states. This subtly influences carrier injection efficiency and spatial carrier distribution, thereby affecting defect-mediated transport. Crucially, MIGS are expected to be orders of magnitude smaller than bulk defects—consistent with observed ohmic characteristics—as their dominance would preclude such behavior.

Some previous studies have also indicated that, in ultra-thin MoS₂, localized states arise due to random potential fluctuations caused by trapped charges at the MoS₂-SiO₂ interface, with reduced screening owing to the significant band gap of MoS₂.⁵¹ To investigate the nature of carrier scattering by defects, we analyze the conductivity at different V_g and relatively higher temperatures (T), where electronic wavefunctions are nearly extended.

In two-dimensional semiconducting systems with a parabolic band structure, charge impurity scattering leads to $\sigma \propto n^2$ for bare Coulomb impurities or $\sigma \propto n$ for screened Coulomb impurities, where n represents the carrier density.^{51,59} In our device, the dependence of σ on the effective gate voltage ($\Delta V_g = V_g - V_{TH} \propto n$) is shown in Fig. 2(c) on a double logarithmic scale. The linearity of the plot indicates that σ follows a power-law dependence on ΔV_g or n . The extracted exponent, ranging from 1.2 to 1.3, suggests that scattering is dominated by screened charged impurities.

The hopping mechanism has an additional manifestation: field-assisted motion of charge carriers between localized states.⁶⁰ This results in non-linear transport characteristics and a transition to temperature-independent conductivity beyond a threshold electric field. Under the application of a sufficiently large electric field, electrons can gain energy to transition from lower-energy states to higher-energy states. Once the critical electric field is exceeded, the carriers

acquire enough energy to overcome the thermal barrier, rendering the conductivity independent of temperature.

Within the framework of the Mott variable-range hopping (VRH) model, the dependence of resistivity on the applied electric field can be expressed as;^{52,55,60}

$$\rho \propto \exp(E_c/E)^{\frac{1}{3}} \quad (2)$$

The critical field, E_c , is related to the localization length (ξ) and the correlation energy (T_0) via the relationship $\xi = k_B T_0 / e E_c$.⁶¹ In Fig. 2(d), we show the variation of I_{DS} with $E^{-1/3}$ in a semi-logarithmic representation. Below the critical field, the transport exhibits Ohmic behavior (as shown in Fig. 1(d)) and remains strongly temperature-dependent, consistent with a phonon-assisted hopping mechanism.⁶²

Since $E_c(T)$ is temperature-dependent and decreases as T is lowered, non-linear current-voltage characteristics become more pronounced at lower temperatures. At the same time, the channel resistance can become significantly high. The value of E_c was extracted from the linear fit of the data in the low-field regime. As shown in the inset of Fig. 2(d), the least-squares fit yields a critical field E_c of approximately 10^8 V/m (with an estimated error of 10^2 V/m). Using the relationship $\xi = k_B T_0 / e E_c$, the localization length ξ is estimated to be around 8 nm, similar to what has been observed from the Mott's T-dependent VRH fit. Additionally, a rough estimation of the average hopping length, $r = \xi(T_0/T)$, at 100 K gives a value in the order of 100 nm.

We extended our study from electrical transport to optoelectronic measurements, performing time-resolved photo-current relaxation experiments across various temperatures. For these experiments, light of wavelength 660 nm was illuminated for a 20 s and kept off subsequently for the same time until it was turned on again. In Fig. 3(a), the time dependence of I_{DS} under optical illumination (660 nm, $P = 1294$ fW μm^{-2}) is shown at $V_g = -16$ V for three representative temperatures. Upon illumination, I_{DS} increases from its dark state value (I_{OFF}), indicating positive photoconductance, and reaches a higher steady-state value (I_{ON}). This behavior arises from

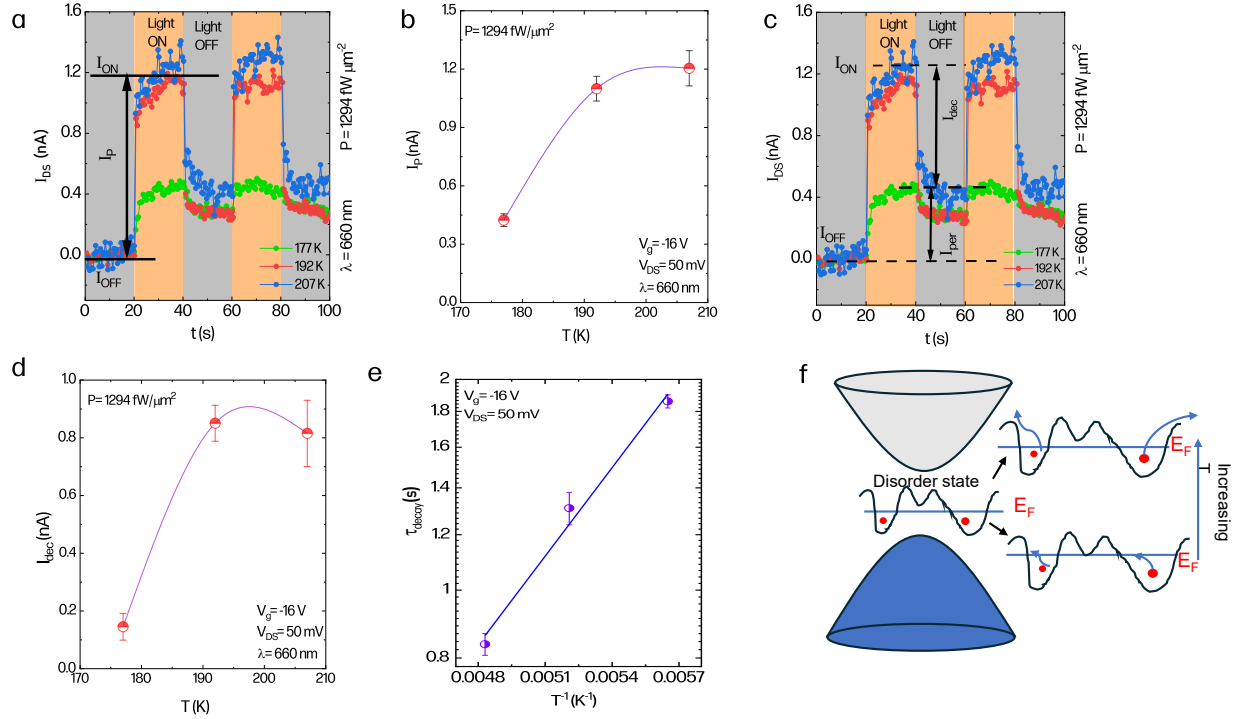


Figure 3: **Optoelectronic transport of MoS₂ on hBN FET device.** (a) Time-resolved photocurrent relaxation dynamics measured at three representative temperatures. Dark current (I_{OFF}) and maximum illuminated current (I_{ON}) define the photocurrent $I_P = I_{ON} - I_{OFF}$. Upon light cessation, I_{DS} exhibits exponential decay toward I_{OFF} but fails to fully recover, indicating persistent photoconductivity. (b) Temperature-dependent photocurrent evolution. The rise in I_P with increasing temperature correlates with enhanced electron delocalization due to thermal energy. (c) I_{dec} is defined as the magnitude of the current that drops once the light is turned off. Eventually, $I_P = I_{dec} + I_{per}$. (d) Temperature variation of the I_{dec} . Higher temperatures amplify the decaying current component, reflecting greater delocalization of trapped electrons. (e) The decay time of I_{DS} , when the light is off, (τ_{decay}), decreases with increasing temperature, suggestive of the faster delocalization time scale, signaling faster detrapping as thermal energy reduces the effective barrier for electron release. (f) Schematic depicting the phenomena described in (a)-(e). Localized states (traps) create potential barriers that confine electrons. Elevated temperatures enable thermal excitation, allowing electrons to surmount these barriers and delocalize.

the dissociation of excitons in MoS₂, driven by the built-in electric field, which injects additional electrons into the channel while holes are trapped in deep defect states. We define the change of source-drain current (photo-current, I_P) as $I_P = I_{ON} - I_{OFF}$. The increase in I_P with temperature (Fig. 3(c)) indicates that thermal energy adds to electron-hole dissociation. Since MoS₂ is intrinsically n-doped, the photogenerated electrons contribute to an increased electron density in the channel, resulting in positive photoconductance (I_{DS} increases under optical illumination). While the time required to build the photocurrent, response time, appears independent of temperature—likely constrained by measurement electronics—a closer examination reveals that, for the same optical intensity and V_g , it (response time, defined as the time to reach 10% to 90% of I_P) increases with rising temperature. This observation can be attributed to the enhanced FET mobility of the devices as the T is increasing. The device showed an impressive average responsivity of 700 A/W at 660 nm. When optical excitation is turned off, the photo-excited electrons are expected to recombine with the holes, returning the current to its dark-state value (I_{OFF}). Since the process of the charge recombination is statistical in nature, the current is expected to exhibit an exponential decay. While it does exhibit such a behavior initially, it fails to fully return to I_{OFF} and instead stabilizes at a higher value, indicating a persistence behavior. This suggests that, in the absence of optical excitation, the number of recombining charge carriers is insufficient to restore the system to its dark state, likely due to the trapping of carriers in localized defect states.

The observed photoconductivity in our device is reversible over multiple illumination cycles. This reversibility and absence of significant photo-fatigue are consistent with previous reports.²⁰ Moreover, the atomically flat hBN provides an inert environment, reducing the density of charge traps at the interface and reduce the photo-induced degradation mechanisms. No measurable shift in device characteristics (such as threshold voltage or dark current) was observed over time, supporting the device's photo-stability.

The persistent current (I_{per}) is defined as the difference from the dark current (I_{OFF}), while the decay current (I_{dec}) represents the component of the current that diminishes from I_{ON} .

Consequently, the total photoresponse is expressed as $I_P = I_{per} + I_{dec}$, as illustrated in Fig. 3(c). The persistence can be destroyed by applying a higher V_g , which pushes the Fermi level into the conduction band, rendering the channel metallic and facilitating the release of trapped charges.

With increasing T , the magnitude of the decay current (I_{dec}) rises, resulting in a reduction of the persistent current (I_{per}), as shown in Fig. 3(d). Persistent photoconductivity is commonly observed in graphene-TMD heterostructured phototransistors, often attributed to charge trapping at the graphene-TMD interface.^{50,63} While such behavior is rare in TMD-based FETs, previous observations¹⁹ have linked it to surface trap states at the SiO₂-TMD interface. In the present study, however, the MoS₂ FETs are fabricated on atomically flat hBN, a defect-free insulating substrate. Consequently, the observed persistent photocurrent is attributed to trap states intrinsic to the MoS₂ channel.

The recovery time (τ_{decay} , defined as the time required for the current to decrease from 10% I_{dec} to 90% I_{dec}) decreases with increasing T , as shown in Fig. 3(e). The increase in the recovery rate (τ_{decay}^{-1}) with temperature suggests that trapped charges are being delocalized by overcoming the localization energy. A semi-logarithmic plot of τ_{decay} versus $1/T$ reveals an activated behavior following $\tau_{decay} = \tau_0 \exp\left(\frac{E_d}{k_B T}\right)$,^{50,64} where E_d represents the detrapping energy scale. A linear fit to the experimental data yields a detrapping energy of (86.000 ± 0.001) meV. In 2D semiconductors like MoS₂, trap energies can vary widely depending on the nature of the defects and the material's quality. While 86 meV is on the higher end for typical trap energies in 2D materials, it is plausible in systems with deeper traps or specific defect structures and not uncommon in the broader context of semiconducting materials.

We further attempt to estimate the localization length (ξ) using an empirical relation, $\xi = \frac{\hbar v_f}{E_d}$, where v_f is the Fermi velocity of carriers in MoS₂, and $\hbar$ is the reduced Planck's constant. This calculation yields $\xi \approx 7$ nm, in good agreement with values obtained from transport measurements based on the variable-range hopping transport. For this estimation, we adopted a Fermi velocity of $v_f = 10^6$ m/s for electrons in MoS₂, as reported in recent scanning tunneling spectroscopy experiments.^{65,66} While this calculation remains an approximation—given that the Fermi velocity

should ideally be derived from the Fermi energy or other band structure parameters—the result aligns well with empirical expectations. Although we agree that a direct calculation of the localization length from the optoelectronic measurements is challenging, combining theoretical insights with experimental data can provide valuable indirect evidence of localization effects and potentially estimate localization lengths through more sophisticated analysis.

The physical processes described above are illustrated in Fig. 3(f). Disordered states, attributed to the sulfur vacancies in the mid-gap region, act as traps for charges near the Fermi energy, preventing recombination. As temperature increases, thermal energy aids in overcoming the detrapping energy, facilitating recombination and reducing the persistent photo current implying these two processes have close connections.

Other alternatives to the mechanism could be achieved from the machine-learned interatomic potentials (MLIPs), such as those discussed in,⁶⁷ simulating large-scale systems like monolayer MoS₂. MLIPs offer near-DFT accuracy while maintaining molecular dynamics (MD)-level efficiency, enabling simulations that span extended length and time scales, which is essential for exploring realistic device environments and defect-driven processes.

Conclusion

In conclusion, we fabricated a single-layered MoS₂ FET device on a few-layered hBN substrate, serving as an atomically clean and defect-free insulating surface. Low-temperature electrical transport measurements revealed that electrons hop between localized states in MoS₂, generating the observed source-drain current. The localization length, estimated using the Mott variable-range hopping model, was found to be approximately 5 nm.

Optoelectronic transport measurements conducted on the same device demonstrated temperature-dependent persistent photoconductivity, attributed to the trapping of charge carriers in localized states. The observed negative temperature dependence of the detrapping time allowed us to estimate the localization length as 7 nm, further underscoring the significant influence of defect

induced carrier localization on the optoelectronic transport properties of two-dimensional MoS₂.

Supporting Information

The Supporting Information is available free of charge at. The atomic force microscopy (AFM) images of the fabricated devices. The Raman spectroscopy of the MoS₂ layer on SiO₂. The technique to estimate the intrinsic carrier density of the MoS₂ channel.

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