

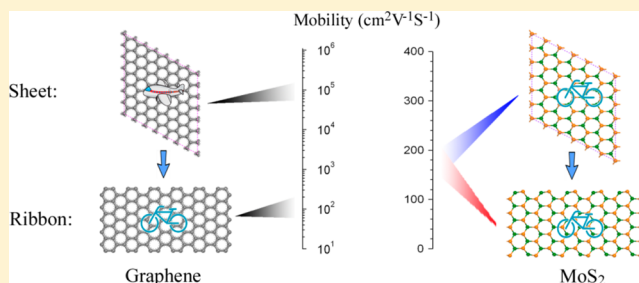
Polarity-Reversed Robust Carrier Mobility in Monolayer MoS₂ Nanoribbons

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S Supporting Information

ABSTRACT: Using first-principles calculations and deformation potential theory, we investigate the intrinsic carrier mobility (μ) of monolayer MoS₂ sheet and nanoribbons. In contrast to the dramatic deterioration of μ in graphene upon forming nanoribbons, the magnitude of μ in armchair MoS₂ nanoribbons is comparable to its sheet counterpart, albeit oscillating with ribbon width. Surprisingly, a room-temperature transport polarity reversal is observed with μ of hole (h) and electron (e) being 200.52 (h) and 72.16 (e) cm² V⁻¹ s⁻¹ in sheet, and 49.72 (h) and 190.89 (e) cm² V⁻¹ s⁻¹ in 4 nm nanoribbon. The high and robust μ and its polarity reversal are attributable to the different characteristics of edge states inherent in MoS₂ nanoribbons. Our study suggests that width reduction together with edge engineering provide a promising route for improving the transport properties of MoS₂ nanostructures.



INTRODUCTION

Two-dimensional (2D) materials are attractive for use in nanoscale electronic and photonic devices as a result of their unique electronic properties.¹ Graphene is by far the most widely studied 2D material due to its massless charge carriers.² However, pristine graphene does not possess a bandgap, a property that is critical for applications in logic transistors to attain a large on/off ratio. Various methods have been proposed to open its bandgap, such as lateral confinement in graphene nanoribbons (GNR). In theory, the carrier mobility (μ) of GNR should be significantly lower than that of a graphene sheet due to the loss of massless Dirac Fermion characteristics.³ In reality, there should be also significant reduction in carrier mobility arising from other factors such as edge disorders and defects in GNRs.^{4–7}

More recently, 2D transition metal dichalcogenides (TMDs), which are composed of atomic layers coupled by van der Waals forces, have gained considerable interest.^{8–11} Unlike graphene, single-layer MoS₂, a member of TMD family, is a semiconductor with a large bandgap, and hence monolayer MoS₂ has been regarded as a promising candidate for field effect transistor (FET) with an on/off ratio exceeding 10⁸ (refs 12 and 13) and highly sensitive photodetectors.¹⁴ For a suspended MoS₂ sheet, the carrier mobility μ is found to be in the range of 0.5–3 cm² V⁻¹ s⁻¹ (ref 15). By improving sample quality,¹⁶ removing absorbates,^{17,18} or depositing atop a high-dielectric layer,¹³ extrinsic scatters such as charged impurities¹⁹ and grain boundaries²⁰ can be partially suppressed,²¹ and the value of μ can be enhanced to around 200 cm² V⁻¹ s⁻¹.²² Recently, one-dimensional (1D) MoS₂ nanoribbons^{23,24} and other TMD materials^{25,26} with a width down to several nanometers were synthesized (using chemical unzipping of nanotubes, or

electron irradiation of sheet). A couple of questions arise promptly: Is there a similar remarkable reduction (several orders of magnitude) of μ in the MoS₂ nanoribbons compared to the MoS₂ sheet, as occurring in graphene? Also, what is the size-dependent behavior of their mobility? Clearly, the answers to these questions are of ultimate importance for their nanoelectronic applications, and it is the subject of the present study.

In this study, by using first-principles calculations and deformation potential theory, we investigate the intrinsic mobility of a MoS₂ sheet and nanoribbons by means of acoustic phonon scattering mechanism. In stark contrast to graphene, we find that a MoS₂ nanoribbon with width down to 4 nm still has a mobility μ comparable to 2D MoS₂ sheet counterpart, thus showing another important advantage of MoS₂ besides the presence of finite bandgap. More interestingly, due to a different scattering intensity between electron and hole, the transport polarity in nanoribbons is reversed from their sheet counterpart: For sheet, electron and hole μ at room temperature are 72.16 and 200.52 cm² V⁻¹ s⁻¹, respectively; however, electron and hole μ are 190.89 and 49.72 cm² V⁻¹ s⁻¹ for a ribbon with a width of 4 nm. Analysis of electronic band structure shows that in MoS₂ nanoribbons, the nondegraded μ and reversed polarity are contributed by the edge states. Our study opens up the new possibility of tuning the polarity and/or enhancing the mobility by edge engineering in MoS₂ nanostructures.

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■ COMPUTATIONAL DETAILS

In inorganic semiconductors, the coherent wavelength of thermally activated electrons or holes at room temperature is much larger than their lattice constant and is close to that of acoustic phonon modes in the center of first Brillouin zone (FBZ). The electron–acoustic phonon coupling dominates the scattering at low energy regime,^{27,28} which can be effectively calculated by the deformation potential (DP) theory proposed by Bardeen and Shockley.²⁹ On the basis of the effective mass approximation, the DP theory has been extensively applied to study μ in 2D^{30,31} and 1D^{3,32–34} materials with the following forms:

$$\mu_{2D} = \frac{2e\hbar^3 C}{3k_B T |m^*|^2 E_1^2} \quad (1)$$

$$\mu_{1D} = \frac{e\hbar^2 C}{(2\pi k_B T)^{1/2} |m^*|^{3/2} E_1^2} \quad (2)$$

where m^* is the effective mass, T is the temperature. E_1 is the DP constant which denotes the shift of the band edges (conduction band minimum for electrons and valence band maximum for holes) induced by the strain. C is the elastic modulus of a uniformly deformed crystal for simulating the lattice distortion activated by the strain. For the 2D system, the in-plane stiffness $C^{2D} = [\partial^2 E / \partial \delta^2] / S_0$, where E is the total energy of the supercell, δ is the applied uniaxial strain, and S_0 is the area of the optimized supercell. In the present work, all the above quantities are calculated using density functional theory (DFT) with the generalized gradient approximation (GGA), as implemented in the Vienna ab initio simulation package (VASP).³⁵ Spin-restricted calculations are performed using the projector augmented wave method with the Perdew–Burke–Ernzerhof functional (PAW–PBE) and a kinetic energy cutoff of 400 eV. An orthogonal supercell is created for MoS₂ sheet, as shown in Figure 1a. The atomic plane and its neighboring image are separated by a 20 Å vacuum layer. The k -meshes for the sheet and nanoribbons are 10×15 and 1×10 , respectively. All the structures are relaxed until the Hellmann–Feynman forces become less than 0.01 eV/Å.

■ RESULTS

We first investigate the electronic structure and acoustic phonon-limited mobility in monolayer MoS₂. The atomic structure is shown in Figure 1a, where the orthogonal supercell is enclosed with dashed lines, together with the hexagonal primitive cell for comparison. The supercell built in this way allows for an intuitive demonstration of carrier conduction along the armchair (a_{o1}) and zigzag (a_{o2}) directions. The upper right panel shows the FBZ associated with the hexagonal and orthogonal lattice. Figure 2a shows the band structure for the MoS₂ sheet. The K point (fractional reciprocal coordinates: $-1/3, 2/3$) defined in reciprocal lattice of the primitive cell is folded into $(0, 1/3)$ point sitting at the Γ -Y branch in the FBZ of the supercell (see Figure 1a). The middle panel shows the valleys around the conduction band minimum (CBM) and valence band maximum (VBM), where electrons and holes drifting through the K point along the armchair (b_{o1}) and zigzag (b_{o2}) directions are highlighted by the dashed lines. The obtained bandgap of 1.64 eV is consistent with previous DFT studies.^{36,37} Through projecting the contour lines into the 2D k -space, we observe nearly circular lines near the K center as shown in the right panel, indicating a small anisotropic character in band surface and associated electronic properties of low energy-excited carriers. The effective mass m_{ap}^* tensor for charge transport along a_{o1} and a_{o2} directions are calculated by $\hbar^2 [\partial^2 \epsilon(k) / \partial k_\alpha \partial k_\beta]^{-1}$, which indeed reveals a similar value for holes (0.57 m_e along a_{o1} direction and 0.60 m_e along a_{o2} direction) and electrons (0.46 m_e along a_{o1} direction and 0.48

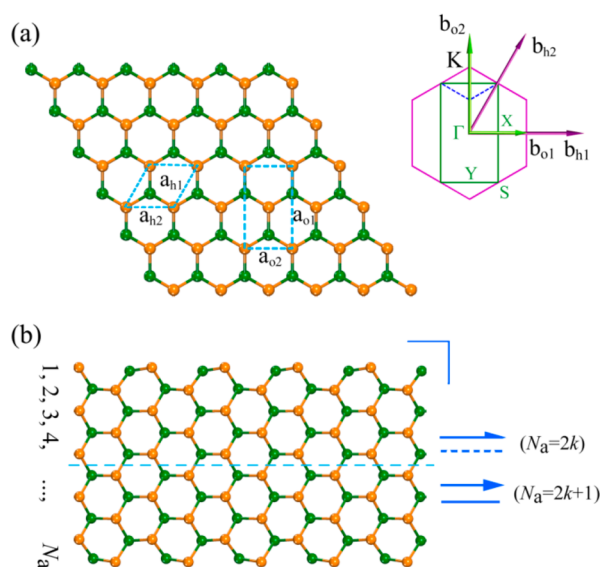


Figure 1. Atomic structure model of monolayer MoS₂ sheet and nanoribbons. (a) Atomic structure model of MoS₂ monolayer. The dashed lines represent the hexagonal primitive cell (defined by a_{h1} and a_{h2}) and the orthogonal supercell (defined by a_{o1} and a_{o2}). The upper right panel plots the FBZ associated with the two lattices. The blue dashed line shows the folding of the K point in FBZ of the hexagonal lattice into FBZ related to the orthogonal lattice. (b) Atomic structure and nomenclature of armchair MoS₂ nanoribbons. The symmetry elements such as the 2-fold rotation (screw) axis represented by the blue \rightarrow and \rightarrow , and mirror (glide) planes represented by the blue — and dashed line, are shown for $N_a = 2k+1$ ($N_a = 2k$), respectively, where k is an integer. For all the ribbons, there is a mirror plane (represented by the blue right angle symbol, top right of (b)) parallel to the ribbon plane.

m_e along a_{o2} direction). Our results are consistent with previous estimation of 0.64 and 0.48 m_e for holes and electrons, respectively.³⁸

Figure 2b shows the variation of total energy (E) with uniaxial strain (δ) applied along a_{o1} and a_{o2} directions, respectively. The in-plane stiffness C^{2D} is obtained through fitting the energy-strain curves. The two curves are nearly identical as shown in Figure 2b, and the difference in C^{2D} along the two directions is small (127.44 and 128.16 N/m for a_{o1} and a_{o2} directions, respectively). By assuming a finite thickness ($t_0 = 0.65$ nm) for 2D MoS₂ sheet, the three-dimensional (3D) Young's modulus can be estimated as $C^{3D} = C^{2D} / t_0$, amounting to 196.1 and 197.2 GPa, respectively, in good agreement with the experimental value (270 ± 100 GPa).^{39,40} Figure 2c shows the shift of band edges as a function of strain along a_{o1} direction, and a similar result for a_{o2} is also observed (data not shown). Through dilating the lattice along a_{o1} and a_{o2} directions, the DP constant E_1 is then calculated as $dE_{edge} / d\delta$, equivalent to the slope of the fitting lines, where E_{edge} is the energy of the conduction (valence) band edge.

On the basis of the obtained E_1 , C^{2D} , and m^* , and using eq 1, the acoustic phonon-limited mobility at room temperature (300 K) and the relaxation time ($\tau = \mu m^* / e$) are calculated and compiled in Table 1. The obtained electron mobility is 72.16 (a_{o1} direction) and 60.32 $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$ (a_{o2} direction), respectively. For holes, the mobility is about 3 times larger than that of electrons, with a value of 200.52 (a_{o1} direction) and 152.18 $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$ (a_{o2} direction), respectively. The calculated electron mobilities are in good agreement with experimental

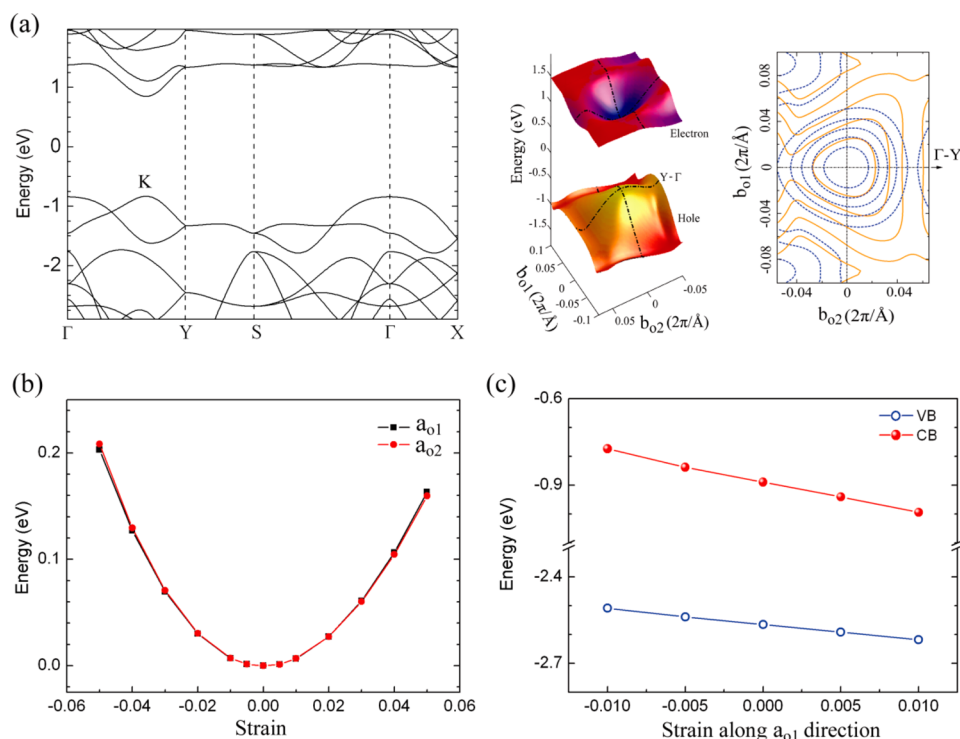


Figure 2. Electronic properties of monolayer MoS₂ sheet. (a) Band structure for monolayer MoS₂ sheet in the orthogonal supercell (left panel). The surface plots of valleys around VBM and CBM are shown in the middle panel. The dash-dotted lines represent carriers drifting along the \mathbf{b}_{01} (armchair) and \mathbf{b}_{02} (zigzag) directions through the K point, which is set to (0,0). The right panel is the contour plot of the valleys in the 2D k -space, which reveals a small anisotropic behavior near the K point for both hole (orange solid lines) and electron (blue dotted lines). The two dotted lines crossing the K point are the in-plane projection of dash-dotted lines in the middle panel. (b) Energy-strain relationship along \mathbf{a}_{01} and \mathbf{a}_{02} directions. (c) Shifts of conduction band and valence band under uniaxial strain along \mathbf{a}_{01} direction.

Table 1^a

carrier type	E_1 (eV)	C^{2D} (N/m)	m^* (m_e)	τ (fs)	μ ($\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$)
e(\mathbf{a}_{01})	-10.88	127.44	0.46	18.89	72.16
h(\mathbf{a}_{01})	-5.29	127.44	0.57	64.73	200.52
e(\mathbf{a}_{02})	-11.36	128.16	0.48	16.58	60.32
h(\mathbf{a}_{02})	-5.77	128.16	0.60	51.83	152.18

^aDeformation potential E_1 , in-plane stiffness C^{2D} , effective mass m^* , relaxation time τ , and mobility μ for electron (e) and hole (h) along \mathbf{a}_{01} and \mathbf{a}_{02} directions in 2D monolayer MoS₂ sheet at 300 K.

values.^{15–20} Our study shows that the hole mobility is about 3-fold larger than the electron mobility. Although there is no directly experimentally measured value of hole mobility in monolayer MoS₂, a recent indirect measurement based on the Hall effect for thin flake MoS₂ indicated that the hole mobility is twice the value of the electron mobility.⁴¹ According to our calculation, the larger hole mobility for monolayer MoS₂ originates from the smaller deformation potential constant E_1 of the valence band compared with that of the conduction band. It should be noted that the synthesized MoS₂ samples, due to the presence of impurity and defects, tend to be unintentionally extrinsically doped and normally show n-type conduction with more abundant carriers of electrons than holes. In the present work, we focus on the intrinsic transport properties of MoS₂ and determine the transport polarity by the mobility difference between electrons and holes, as adopted in previous studies.^{3,42}

We next investigate μ of MoS₂ nanoribbons. It is well-known that the edge states exist in MoS₂ nanoflakes and dominate their catalytic performance.⁴³ However, the role of edge states

in the dynamics of carriers is still unclear. As the zigzag MoS₂ nanoribbons are metallic,^{44,45} here we only consider the semiconducting armchair MoS₂ nanoribbons, which are classified by the number of Mo–S dimer lines (N_a) across the ribbon width, as shown in Figure 1b. A series of armchair nanoribbons with width ranging from $7 \leq N_a \leq 25$ (from 1.1 to 4.0 nm) are calculated. For the 1D case, the stretching modulus is defined as $C^{1D} = [\partial^2 E / \partial \delta^2] / L_0$, where the uniaxial strain δ is applied along the ribbon direction, and L_0 is the lattice constant of the optimized ribbon. Figure 3a shows that C^{1D} increases continuously with N_a . Assuming a finite width (W_0) of the optimized ribbon, the effective C^{2D} for these ribbons can be obtained as C^{1D} / W_0 , ranging between 88.9 and 114.8 N/m (see Supporting Information). Compared with the 2D sheet, the phonon spectrum of nanoribbons broadens toward the high-frequency region due to phonon mode quantization and occurrence of edge phonon modes, giving rise to the softening of the lattice modes and the reduction in the elastic modulus.

Figure 3b shows the DP constant E_1 due to the quasi-static deformation of the ribbon. It is seen that $|E_1|$ of hole is about 2 times larger than that of electron. An opposite trend is true for the 2D sheet where the electron tends to experience stronger acoustic phonon scattering (Table 1). It should be noted that with a further increase in the width of the ribbon, the values of $|E_1|$ for hole and electron are not converged to those of the 2D sheet. This is due to a dramatic difference in the character of frontier orbitals between nanoribbons and sheet, which will be discussed below.

Figure 3c,d present the effective masses for electron and hole in the nanoribbons. The electron effective mass increases gradually and then levels off to a value of around 1.2 m_e for N_a

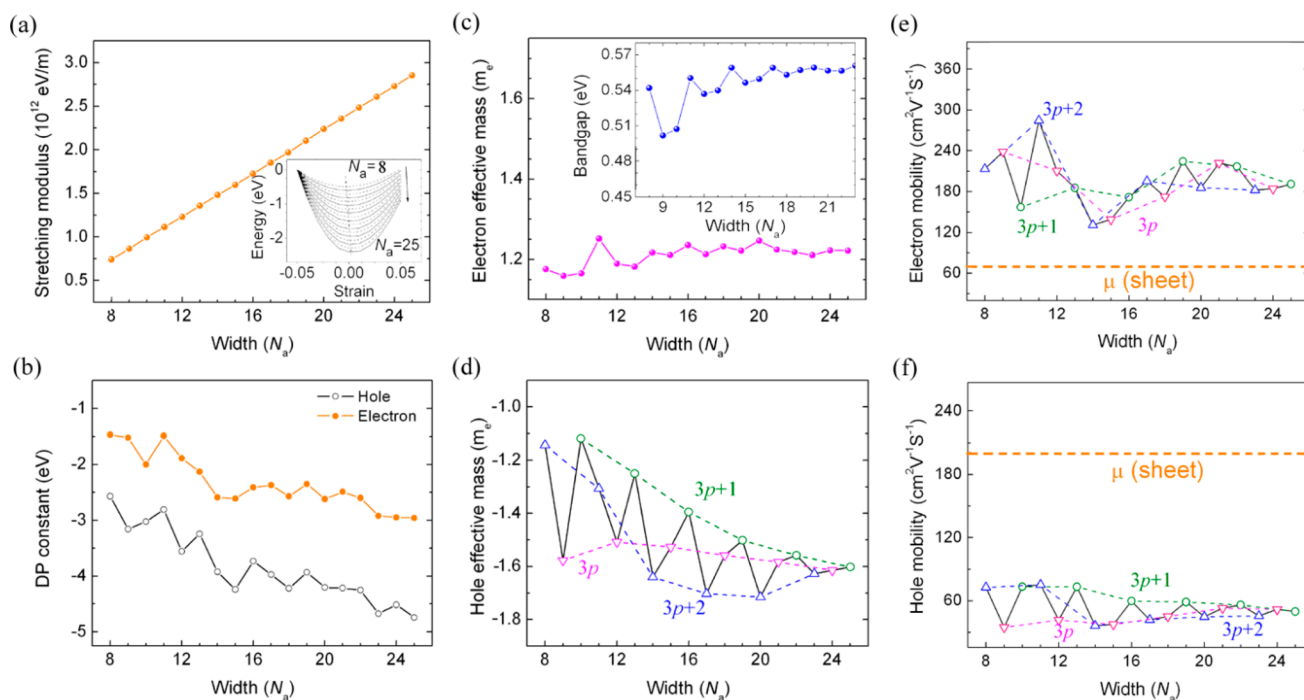


Figure 3. Electronic properties of monolayer MoS₂ nanoribbons as a function of width: (a) stretching modulus, (b) deformation potential constant, (c) electron effective mass, (d) hole effective mass, (e) electron mobility, and (f) hole mobility for MoS₂ armchair nanoribbons as a function of the ribbon width. The mobility is derived at room temperature (300 K). The inset of (a) shows the relationship between total energy and uniaxial strain along the ribbon direction. The inset of (c) shows the variation of bandgap with ribbon width.

> 15 (see Figure 3c). Interestingly, for hole, the effective mass shows a strong oscillation where three distinct families ($3p$, $3p + 1$, and $3p + 2$) of the ribbons can be clearly identified (see Figure 3d). We also calculate the bandgap (Figure 3c inset) of the MoS₂ nanoribbons where the bandgap value also oscillates initially and then converges to a constant value of 0.56 eV, consistent with previous work.⁴⁴ Similar behavior is well-known in the armchair GNR, where a width-dependent oscillation of bandgap occurs.² However, in GNR, there is no appreciable width-dependence of effective mass, and the electrons and holes possess almost the same effective mass.³³ The oscillating behavior in the effective mass of MoS₂ nanoribbons can be explained by the symmetric characteristics of frontier orbitals, which will be discussed shortly. In addition, for wide MoS₂ nanoribbons ($N_a > 20$), the holes have a much larger effective mass (1.6 m_e) than electrons (1.2 m_e). This is in contrast to the 2D sheet, which shows a similar effective mass between holes and electrons (Table 1).

The room temperature μ for ribbons is shown in Figure 3e,f. The mobility initially oscillates with the width of the nanoribbons and then levels off to a value (for $N_a > 23$) of around 190.89 and 49.72 $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$ for electrons and holes, respectively. For holes, there are three families of the ribbons showing smooth trends with the $3p + 1$ family having the largest μ . For electrons, a larger μ is observed, which arises from the much smaller DP constant and the generally smaller effective mass compared with those of holes. In Figure 3e,f, μ in 2D sheet, represented by the horizontal dashed orange line, is also plotted for comparison. Surprisingly, a reversal of transport polarity is observed in μ when the 2D monolayer sheet is cut into the 1D nanoribbon. In the monolayer MoS₂ sheet, the holes show a 3-fold larger mobility than the electrons, whereas this polarity is reversed in nanoribbons. Our results may account for the depletion-to-enhancement mode transition

recently observed in FET based on MoS₂ nanoribbons (the channel width from 2 μm down to 60 nm).⁴⁶ It was shown that through solely reducing the width of the ribbons, the transport characteristic of the FET changes clearly from depletion mode to enhancement mode. In traditional bulk semiconducting devices, this mode transition can only be achieved by chemical doping. However, stable chemical doping in monolayer channel is generally difficult. Our predicted polarity tunability of carriers in single-layer MoS₂ through cutting nanoribbons, together with proper edge engineering, provides a promising avenue to enhance the performance of nanoelectronics devices.

It is well-known that the μ of the graphene sheet is reduced upon cutting into nanoribbons.^{4,5,33} The carrier mobility (μ) of graphene reduces dramatically (to less than 200 $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$ (refs 4 and 5) from $\sim 10^7 \text{cm}^2 \text{V}^{-1} \text{s}^{-1}$ (refs 47 and 48)) upon the width reduction. A first-principles study revealed a strongly width-dependent oscillating behavior in carrier mobility.³³ Studies based on a full band approach⁴⁹ and acoustic phonon scattering estimation⁵⁰ predicted a significant reduction in carrier mobility of GNRs. With decreasing the GNR width, the carrier mobility can be further decreased according to the inverse mobility-gap relationship proposed theoretically recently,³ showing at least a 3-order lower mobility of wide-gap GNRs than nearly zero-gap graphene. Through considering both 1D and 2D MoS₂, our present work reveals that the mobility of MoS₂ nanoribbons is comparable to or even larger than that of monolayer MoS₂ sheet. The width-insensitive carrier mobility is another appealing feature of MoS₂ for applications in nanoscale electronics and photonics devices.

DISCUSSION

To understand the staggering behavior of the effective mass and μ with width in MoS₂ nanoribbons, we analyze the spatial distribution of frontier orbitals. Since all the nanoribbons have a

similar electronic character, the $N_a = 12$ nanoribbon is chosen as a representative for analysis. Figure 4 shows that the ribbon

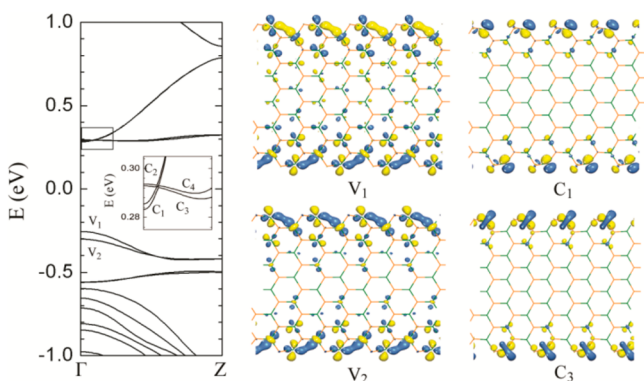


Figure 4. Band structure and frontier orbitals of MoS₂ nanoribbons with $N_a = 12$. The Fermi level is set to zero. The inset in the left panel is a close-up view of the conduction band. The right panels present the frontier orbitals at the Γ point.

is a direct bandgap semiconductor. A wealth of edge states are clearly distributed between -0.5 to 1 eV within the bulk bandgap of MoS₂. Two valence bands, labeled as V_1 and V_2 , and two conduction bands, labeled as C_1 and C_2 , are identified (inset of Figure 4), where all of them have a parabolic character. In addition, two relatively flat bands (C_3 and C_4) are located slightly above the C_1 and C_2 bands. Atomic orbital analysis shows that all these states are mainly composed of Mo $4d$ manifolds: V_1 with in-plane $d_{x^2-y^2}$ and d_z^2 orbitals; C_1 with out-of-plane d_{xy} orbital; and C_3 with d_z^2 orbital. The V_2 , C_2 , and C_4 states are geometrically the same with V_1 , C_1 , and C_3 , respectively, except for a phase difference.

It is interesting to compare the width-dependent behavior between GNR and MoS₂ nanoribbons. For the GNR, the frontier orbitals extend well over the whole ribbon and the μ shows a variation of 2–3 orders of magnitude with width.³³ In contrast, in the case of MoS₂, the presence of edges in nanoribbons leads to the formation of plenty of in-gap states (edge states), and low-energy carriers tend to preferentially populate these states. Therefore, the edge issue is critically important for the performance of electronic and optoelectronic devices made of MoS₂. For MoS₂ nanoribbons, despite evident edge coupling for narrow ribbons, all the states are mainly localized at edges, thus the μ tends to be less sensitive to width. The carriers at edges of sub-10 nm ribbons show a comparable μ with that in MoS₂ sheet. Because of the similar electronic structure, further rigorous study is needed to explore whether the similar characteristics of nondegraded mobility may exist in other TMD family members.

It should be noted that in the present work, the intrinsic mobilities are derived by assuming that the defects and dopants are absent in the monolayer. However, in reality, perturbation arising from structural disorders and environmental adsorbates are inevitable. Previous studies have shown that the isomeric and heteroatomic effects play a significant role in affecting the magnitude and anisotropic character of carrier mobilities in organic molecules,^{51,52} and the van der Waals interaction and the hydrogen bonding between the molecules and lattice host can modulate the mobility as well.¹⁷ In principle, the effects of these weak intermolecular interactions, which are normally accompanied by strong electron–phonon coupling, can be treated by the Marcus–Hush theory.^{53,54}

According to group theory, the electronic eigenstates at Γ point can be classified as the irreducible representation (IR) of the corresponding little group. The MoS₂ nanoribbons have a C_{2v} symmetry (Figure 1). In Table 2, we list the symmetrical

Table 2^a

	8	9	10	11	12	13	14	15
V_1	B_1	B_1	A_1	B_1	B_1	A_1	B_1	B_1
V_2	A_1	A_1	B_1	A_1	A_1	B_1	A_1	A_1

^aAssignment of irreducible representation of C_{2v} group to V_1 and V_2 frontier orbitals at Γ for MoS₂ armchair nanoribbons ($N_a = 8–15$).

characteristics for V_1 and V_2 states at Γ . Both states can be assigned to an A_1 (B_1) IR showing an even (odd) characteristic of the orbital under mirror or glide operation. Interestingly, there is an alternating sequence of the IR character of the states with respect to width of the ribbon. The $3p + 1$ family, which has the smallest hole effective mass and the largest hole mobility, shows an A_1 character. The $3p$ and $3p + 2$ families have a B_1 character. The staggering oscillatory behavior of hole effective mass and mobility can thus be attributed to the different symmetric characteristics of the edge states, which result in different carrier–phonon coupling. As expected, the conduction bands (virtual orbitals) are generally more difficult to be described theoretically than the valence bands (occupied orbitals).⁵⁵ Although the DP constant derived from the shifts of CBM and VBM tends to be less affected by this issue, the curvature of the CBM may not be accurately described by the DFT used here. Therefore, there is no clear ordering behavior in effective mass and mobility for electrons.

Finally, we demonstrate that the spatial distribution and orbital composition of the edge states in the MoS₂ nanoribbons dominate the carrier mobility. For a nanoribbon with $N_a = 12$, the V_1 band is a $d_{x^2-y^2}$ and d_z^2 hybridized state extending along the edge direction, whereas the C_1 level with d_{xy} orbital plane is more localized and perpendicular to the ribbon plane. Therefore, the V_1 level tends to shift more under elastic deformation along the ribbon direction according to eq 2, thus leading to a larger DP constant and a smaller mobility for hole compared with those for electron populating at the C_1 level. This indicates that the carrier mobility of MoS₂ nanoribbons can be modulated by tuning the distribution of edge states through edge engineering (for example, chemical functionalization). For GNR, the edges are stabilized by passivation of hydrogen atoms due to a strong C–H bond, thus largely impeding adsorption of other molecules. However, for MoS₂ nanoribbons, H-passivated edges are less stable, because the H atoms tend to be desorbed from the edges due to the relatively weaker S–H and Mo–H bonds.⁵⁶ The H-free edges in MoS₂ allow more flexibility in functionalizing the edges through anchoring external atoms or molecules. This can in turn affect the distribution of edge states and may decrease the scattering, thus promoting the mobility. On the other hand, the unsaturated S–Mo heteropolar bonds at the ribbon edges may be chemically accessible to other atoms like oxygen, where oxygen sources can be introduced and controlled by using chemical vapor deposition.⁵⁷ The selective chemical affinity of the edges highlights the importance of the edge functionalization on MoS₂ nanostructures and its influence on the electronic properties of MoS₂.

SUMMARY

In conclusion, we have studied the acoustic phonon-limited carrier mobility for both monolayer MoS₂ sheet and nanoribbons. In contrast to graphene, where a remarkable reduction of carrier mobility occurs in nanoribbons, we find that the carrier mobility in MoS₂ nanoribbons is comparable to their MoS₂ sheet counterpart. This feature renders MoS₂ an ideal material for use in nanoelectronics without losing the mobility upon width reduction. Moreover, we find that the spatial distribution and orbital composition of the edge states dominate the dilation behavior of conducting bands. As the edge states are less sensitive to the width variation and persist in the gap of MoS₂ sheet, our study suggests that edge engineering by chemical functionalization or strain in MoS₂ nanostructures can be an effective avenue to tune the transport property. It is expected that the robustness of mobility in ultranarrow MoS₂ nanoribbons can lead to a wide range of applications in nanoelectronic devices.

ASSOCIATED CONTENT

Supporting Information

Irreducible representation of C_{2v} group, stretching modulus of MoS₂ nanoribbons, band structure obtained by HSE06 calculation, strain effect on the effective mass of MoS₂ nanoribbons. This material is available free of charge via the Internet at <http://pubs.acs.org>.

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Notes

The authors declare no competing financial interest.

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