

Tunneling valley Hall effects in monolayer $1T'$ -MoS₂ junctions

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(Received 28 October 2025; revised 7 May 2026; accepted 9 July 2026; published 23 July 2026)

The tunneling valley Hall effect (TVHE) provides high-efficiency conversion from charge to valley, which is crucial to valleytronic devices. Recently, TVHE in two-dimensional junctions has attracted increasing attention. Here, we comprehensively study the TVHE and other tunneling Hall effects in monolayer $1T'$ -MoS₂ (TMS) junctions. Monolayer TMS, a representative two-dimensional transition-metal dichalcogenide, hosts gapped and tilted Dirac fermions with spin splitting tunable by an out-of-plane electric field. The tunneling Hall effects for valley and other degrees of freedom reflect the evolution of the unique electronic structure featured by the reversible spin splitting and the topological transition. For the monolayer TMS at zero electric field, the intrinsic valley Hall effect is absent due to the opposite spin Berry curvature in each valley, which makes the TVHE the dominant valley Hall mechanism for valleytronic applications. We further demonstrate the resonant enhancement of TVHE through the transmission pattern and show the electrically tunable high conversion ratio. For the monolayer TMS at nonzero electric field, the TVHE is closely related to the tunneling spin Hall effect due to the valley-spin locking, whose sign and magnitude changes can be used to distinguish the direction of the spin splitting and to provide an indirect signature for the topological transition, respectively. For the tunneling charge Hall effect, a universal conversion ratio is analytically derived and numerically confirmed. This study provides a comprehensive understanding of tunneling Hall effects in monolayer TMS junctions and provides an opportunity for two-dimensional transition-metal dichalcogenides in valleytronics and spintronics.

DOI: [10.1103/fnmp-rtjx](https://doi.org/10.1103/fnmp-rtjx)

I. INTRODUCTION

Electrons in crystalline solids bear various internal degrees of freedom. The efficient control of a certain electron's degree of freedom may bring about a promising field, e.g., electronics or spintronics, based on the charge or spin. Around the momentum extremum of the electronic energy dispersion, the valley index can be endowed to electrons as an additional degree of freedom. To exploit the physics and application prospects of the valley degree of freedom is the aim of valleytronics [1–20], which is a flourishing field following the fabrication of various two-dimensional materials [21–23]. Manipulating the valley polarization is crucial to valleytronics and can be realized principally by using a lot of different external fields, such as optical [6,24–33], electrical [1,4,12,19,34–38], strain [5,7,15,39–42], and magnetic [29,43–56] fields. For realistic applications compatible with the present semiconductor industry, the all-electric valley polarization is highly anticipated [36,57–59].

The valley Hall effect (VHE), implying the valley contrasting Hall currents in the presence of a longitudinal valley-unpolarized current, is an efficient electrical

mechanism to manipulate valley polarization [21]. The VHE was initially proposed in graphene with a gap opening due to the inversion symmetry breaking [2], and the accompanying transverse transport originates from the Berry curvature of the energy band, so it is intrinsic. This intrinsic VHE has been demonstrated in graphene [8–10] and monolayer transition-metal dichalcogenides [11,12,60]. The Berry curvature is inversely proportional to the magnitude of the band gap near the band edge [2,61]. This causes two obstacles to utilizing the intrinsic valley effect in realistic devices. (I) To observe the intrinsic VHE, the fine-tuning of doping density and even the gap value is obligatory [8–12,60], e.g., the VHE becomes invisible if the doping is away from the band edge. (II) The transverse current is usually far less than the longitudinal current since the anomalous velocity driven by the Berry curvature is rather small, i.e., the tiny VHE ratio [11,60], causing the low-efficiency conversion of valley current from charge current. To bypass the obstacles accompanying the intrinsic VHE, it is intriguing to explore a different mechanism for generating the VHE.

In view of the important role played by the tunneling junctions in transistors [62] and spin devices [63], we recently proposed the tunneling VHE (TVHE) driven by the tilted Dirac fermions [64]. The TVHE can realize the high-efficiency conversion of charge current into the valley current, with all-electric tunability and without the obstacles of the intrinsic VHE [64]. At present, the TVHE has inspired some

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interesting studies on the various Hall effects in junctions [65–68] and has attracted increasing attention. Thus, it is a promising direction to study the tunneling Hall effects for valley and other degrees of freedom in more materials.

Looking back at the history of the intrinsic VHE, it was proposed in gapped graphene [2] and then generalized to the two-dimensional transition-metal dichalcogenides [6]. The significance of this generalization comes from the intrinsic inversion symmetry breaking due to the lack of an inversion center in the crystal structure and the strong spin-orbit coupling due to the d orbitals of the heavy metal atoms, which leads to the first observation of the intrinsic VHE in two-dimensional transition-metal dichalcogenides [11]. Two-dimensional transition-metal dichalcogenides have abundant phases; except for the 2H phase for observing the intrinsic VHE [6], another $1T'$ phase was also well-known. $1T'$ transition-metal dichalcogenides, with MoS_2 as a typical example, have been predicted to be a two-dimensional topological insulator [69] and have been experimentally verified [70–74]. The monolayer $1T'$ - MoS_2 (TMS) possesses the tilted but gapped Dirac fermions and is a promising platform for the TVHE [64]. More importantly, the tunable spin splitting by an out-of-plane electric field in monolayer TMS favors the valley-spin locking, which may bring about novel features and easy observation for the TVHE, analogous to those induced by the spin-orbit coupling for the intrinsic VHE in the 2H phase of TMS.

Here, we comprehensively study the tunneling Hall effects for the valley, spin, and charge in monolayer TMS junctions. To consider the typical sandwich-like junctions with the left and right electrodes and the central spacer region, we analytically and numerically reveal the unique features of the tunneling Hall effects there. The tunneling Hall effects induced by the skew transmission reflect the electronic structure of the host material for junctions [64]. For the tilted Dirac fermions, they possess gap opening and tunable valley-spin locking by an out-of-plane electric field in monolayer TMS, in contrast with the simple gapless ones in 8- $Pmmn$ borophene. The monolayer TMS still respects the time-reversal and inversion symmetries and does not host the intrinsic VHE despite the presence of gap opening. Thus, we first briefly discuss the spin and valley resolved Berry curvature and the topological invariant for the electronic structure of the monolayer TMS. Specific to the tunneling Hall effects, we identify three main findings. (I) At zero electric field, the TVHE is the dominant valley Hall mechanism of the monolayer TMS for the valleytronic applications because the intrinsic VHE does not occur due to the opposite spin Berry curvature in each valley. For the TVHE, we study its dependence on multiple parameters with a focus on the resonant enhancement due to the transmission matching and highlight the high conversion ratio. (II) The TVHE is closely related to the tunneling spin Hall effect due to the valley-spin locking, whose sign change corresponds to the reversal of the spin splitting and magnitude change provides the indirect signature for the topological transition, respectively. (III) For the charge degree of freedom, the universal tunneling charge Hall ratio is analytically derived and numerically demonstrated. This study aims to realize the tunneling Hall effects in a realistic monolayer TMS, which is beneficial to the

experimental observation and the novel valleytronic and spintronic applications based on two-dimensional transition-metal dichalcogenides.

II. THEORETICAL FORMALISM

A. Model Hamiltonian of uniform monolayer

In the Cartesian coordinate system X - Y , the Hamiltonian of monolayer TMS under an out-of-plane electric field is [69,75,76]

$$H_\eta(\mathbf{q}) = \begin{bmatrix} \mathbf{h}_{\eta,+}(\mathbf{q}) & \mathbf{0} \\ \mathbf{0} & \mathbf{h}_{\eta,-}(\mathbf{q}) \end{bmatrix}, \quad (1)$$

where the spin- and valley-dependent component is

$$\mathbf{h}_{\eta,s}(\mathbf{q}) = \mathbf{h}_{\eta,s}^1(\mathbf{q}) + \mathbf{h}_{\eta,s}^2(\mathbf{q}) + \mathbf{h}_{\eta,s}^3(\mathbf{q}), \quad (2)$$

with

$$\mathbf{h}_{\eta,s}^1(\mathbf{q}) = (v_1 q_X \tau_2 - v_2 k_Y s \tau_1), \quad (3a)$$

$$\mathbf{h}_{\eta,s}^2(\mathbf{q}) = -\eta k_Y (v_- \tau_0 + v_+ \tau_3), \quad (3b)$$

$$\mathbf{h}_{\eta,s}^3(\mathbf{q}) = (c_E E_z - \eta s \Delta_{\text{so}}) \tau_1. \quad (3c)$$

Here, $\hbar \equiv 1$, $s = \pm 1$ are for the spin-up and spin-down states, $\eta = \pm 1$ represent Λ and Λ' valleys, and τ_1, τ_2, τ_3 are the Pauli matrices of pseudospin and τ_0 is the identity matrix. The first term $\mathbf{h}_{\eta,s}^1(\mathbf{q})$ is similar to the Hamiltonian of monolayer graphene but anisotropic due to the unequal Fermi velocities $v_1 = 3.87 \times 10^5$ m/s and $v_2 = 0.46 \times 10^5$ m/s [69]. The two Dirac points lie at $\pm q_0 = 1.46 \text{ nm}^{-1}$ along the Y axis [69], so $k_Y = q_Y - \eta q_0$ is the wave vector relative to the Dirac points with q_Y the Bloch momentum. The second term $\mathbf{h}_{\eta,s}^2(\mathbf{q})$ leads to the tilt of anisotropic Dirac cones, in which $v_{\pm} = Q_0(m_Y^d \pm m_Y^p)/(2m_Y^d m_Y^p)$ with $m_Y^p = 0.16m_0$ and $m_Y^d = 0.37m_0$ [76]. m_0 is the mass of the free electron. The third term of $\mathbf{h}_{\eta,s}^3(\mathbf{q})$ includes the intrinsic gap $\Delta_{\text{so}} = v_2 q_0$ induced by spin-orbit coupling and the extrinsic gap induced by the electric field $c_E E_z$ with c_E the electric coefficient [76]. For convenience, we define $E_c = \Delta_{\text{so}}/c_E$ and then $\mathcal{E} = E_z/E_c$ is a dimensionless quantity. Obviously, $H_\eta(\mathbf{q}) = H_{-\eta}^*(-\mathbf{q})$ due to time-reversal symmetry. For Eq. (1), the energy dispersion is

$$\varepsilon_\lambda^{\eta,s} = -\eta v_- k_Y + \lambda \sqrt{(s\mathcal{E}\Delta_{\text{so}} - \eta\Delta_{\text{so}} - v_2 k_Y)^2 + v_1^2 q_X^2 + v_+^2 k_Y^2}, \quad (4)$$

and the wave function is

$$\phi_\lambda^{\eta,s}(\mathbf{R}) = \frac{1}{\sqrt{1 + |\alpha_\lambda^{\eta,s}|^2}} \begin{pmatrix} 1 \\ \alpha_\lambda^{\eta,s} \end{pmatrix} e^{i\mathbf{q}\cdot\mathbf{R}}, \quad (5)$$

where $\alpha_\lambda^{\eta,s}$ is

$$\alpha_\lambda^{\eta,s} \equiv \frac{iq_X v_1 - sk_Y v_2 + (\mathcal{E} - \eta s)\Delta_{\text{so}}}{\varepsilon_\lambda^{\eta,s} + \eta k_Y (v_- - v_+)}. \quad (6)$$

To define the pseudospin $\bar{\tau}_j \equiv (\phi_\lambda^{\eta,s})^\dagger \tau_j \phi_\lambda^{\eta,s}$, $j \in \{1, 2, 3\}$, $\alpha_\lambda^{\eta,s}$ can be rewritten as

$$\alpha_\lambda^{\eta,s} = \frac{\bar{\tau}_1 + i\bar{\tau}_2}{1 + \bar{\tau}_3},$$

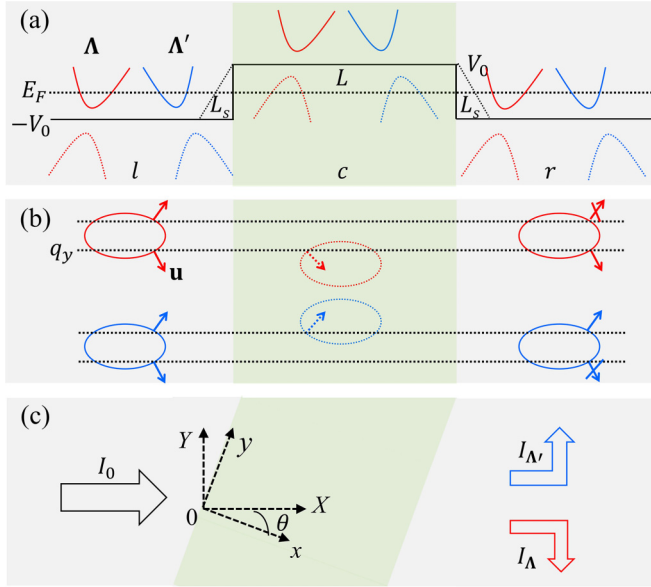


FIG. 1. Schematic monolayer 1T'-MoS₂ junctions and the generation of the tunneling Hall effects. (a) Monolayer 1T'-MoS₂ has two valleys, i.e., Λ (red) and Λ' (blue) ones which are both gapped Dirac cones. The Fermi level and the potential are tuned by a bottom gate and a top gate. Here, $-V_0$ (V_0) is fixed in the middle of the gapped Dirac cones of the left and right electrodes (the central region) and E_F is variable. (b) An npn junction is considered, i.e., E_F lies in the conduction (valence) band of the electrodes (the central region). The constant-energy contours of two valleys are shown. In the Λ valley, states with group velocity $u_y < 0$ are allowed, while in the Λ' valley, states with $u_y > 0$ are allowed. This leads to valley-contrasting skew transmission. (c) The junction defines a rotated coordinate system (x - y) relative to the crystal axes (X - Y). An unpolarized valley current I_0 is incident from the left electrode, due to the skew transmission [panel (b)], the valley-polarized Hall current I_A and $I_{A'}$ occur at the right electrodes, i.e., the tunneling valley Hall effect.

with

$$\bar{\tau}_1 = \frac{-sk_Y v_2 + (\mathcal{E} - \eta s) \Delta_{so}}{\varepsilon_{\pm}^{\eta,s} + \eta v_- k_Y}, \quad (7a)$$

$$\bar{\tau}_2 = \frac{q_X v_1}{\varepsilon_{\pm}^{\eta,s} + \eta v_- k_Y}, \quad (7b)$$

$$\bar{\tau}_3 = \frac{-\eta v_+ k_Y}{\varepsilon_{\pm}^{\eta,s} + \eta v_- k_Y}. \quad (7c)$$

The intimate relationship between the wave function and pseudospin greatly facilitates understanding of transmission governed by pseudospin conservation [77].

B. Longitudinal and transverse transport in junctions

To apply the nonuniform potential on the monolayer TMS, the junction is formed [cf. Figs. 1(a) and 1(c)]. As shown in Fig. 1(c), the junction defines the other Cartesian coordinate system x - y , in which the x axis and the y axis are normal and parallel to the junction interface, respectively. The two Cartesian coordinate systems x - y and X - Y have a

relative rotation denoted by θ . Thus, for an arbitrary vector $\mathbf{A} \equiv (A_x, A_y) \equiv (A_X, A_Y)$, we have

$$A_x = A_X \cos \theta + A_Y \sin \theta, \quad (8a)$$

$$A_y = -A_X \sin \theta + A_Y \cos \theta. \quad (8b)$$

The junction potential $V(x) = V_0$ for $0 \leq x \leq L$ and it is $-V_0$ elsewhere [cf. Fig. 1(a)]. Without loss of generality, the Fermi level E_F is considered in the conduction (valence) band when $V(x) = -V_0$ [$V(x) = V_0$], i.e., an npn junction is considered [cf. Fig. 1(a)]. When electrons are incident from the left region [cf. Fig. 1(a)], the wave function can be expressed as

$$\psi_L^{\eta,s}(x) = \phi_{+,i}^{\eta,s}(x) + r^{\eta,s}(q_y) \phi_{-,r}^{\eta,s}(x), \quad (9a)$$

$$\psi_C^{\eta,s}(x) = a^{\eta,s}(q_y) \phi_{+,a}^{\eta,s}(x) + b^{\eta,s}(q_y) \phi_{-,b}^{\eta,s}(x), \quad (9b)$$

$$\psi_R^{\eta,s}(x) = t^{\eta,s}(q_y) \phi_{+,t}^{\eta,s}(x). \quad (9c)$$

Here, we add the subscript i , r , and t for the incident right-going, reflected left-going, and transmitted right-going states in the left and right electrodes. In addition, a and b are for right-going and left-going states in the central scattering region. Note that the spin-flip scattering does not exist for a scalar potential. This makes Eq. (9) applicable to the single valley with one constant-energy contour at low doping and two constant-energy contours at high doping. Solving the continuity conditions of wave functions in different regions, $\psi_L^{\eta,s}(0) = \psi_C^{\eta,s}(0)$ and $\psi_C^{\eta,s}(L) = \psi_R^{\eta,s}(L)$, gives all scattering coefficients, $r^{\eta,s}(q_y)$, $a^{\eta,s}(q_y)$, $b^{\eta,s}(q_y)$, and $t^{\eta,s}(q_y)$. Because the same left and right electrodes are considered, the transmission probability in the right electrode can be written as

$$T^{\eta,s}(q_y) = |t^{\eta,s}(q_y)|^2, \quad (10)$$

where

$$t^{\eta,s}(q_y) = \frac{(\alpha_n^{\eta,s,\rightarrow} - \alpha_n^{\eta,s,\leftarrow})(\alpha_p^{\eta,s,\rightarrow} - \alpha_p^{\eta,s,\leftarrow}) D_p^{\rightarrow} D_p^{\leftarrow}}{D_n^{\rightarrow} \Omega}, \quad (11)$$

with

$$D_j^{\pm} = \exp(iq_{j,x}^{\eta,s,\pm} L), \quad j \in \{n, p\}, \quad (12a)$$

$$\Omega = \Omega_{\rightarrow} - \Omega_{\leftarrow}, \quad (12b)$$

$$\Omega_{\pm} = (\alpha_p^{\eta,s,\rightarrow} - \alpha_n^{\eta,s,\pm})(\alpha_p^{\eta,s,\leftarrow} - \alpha_n^{\eta,s,\pm}) D_p^{\pm}. \quad (12c)$$

Here, $\alpha_n^{\eta,s,\pm}$ ($\alpha_p^{\eta,s,\pm}$) represent $\alpha_{\lambda}^{\eta,s}$ of the right-going ($\rightarrow$) and left-going ($\leftarrow$) states in the n (p) region, and $q_{n,x}^{\eta,s,\pm}$, $q_{p,x}^{\eta,s,\pm}$ are the longitudinal wave vectors for the invariant q_y and E_F in the transmission events. Using the transmission, we can define the longitudinal and transverse transport coefficients σ_{xx} , σ_{xy} , σ_{xy}^V , and σ_{xy}^S for the longitudinal, the charge Hall, the valley Hall, and the spin Hall conductances, respectively [64]:

$$\sigma_{xx} = \frac{\sigma_0}{4\pi^2} \sum_{\eta=\pm, s=\pm} \int T^{\eta,s}(q_y) dq_y, \quad (13a)$$

$$\sigma_{yx} = \frac{\sigma_0}{4\pi^2} \sum_{\eta=\pm, s=\pm} \int \xi^{\eta,s,\rightarrow}(q_y) T^{\eta,s}(q_y) dq_y, \quad (13b)$$

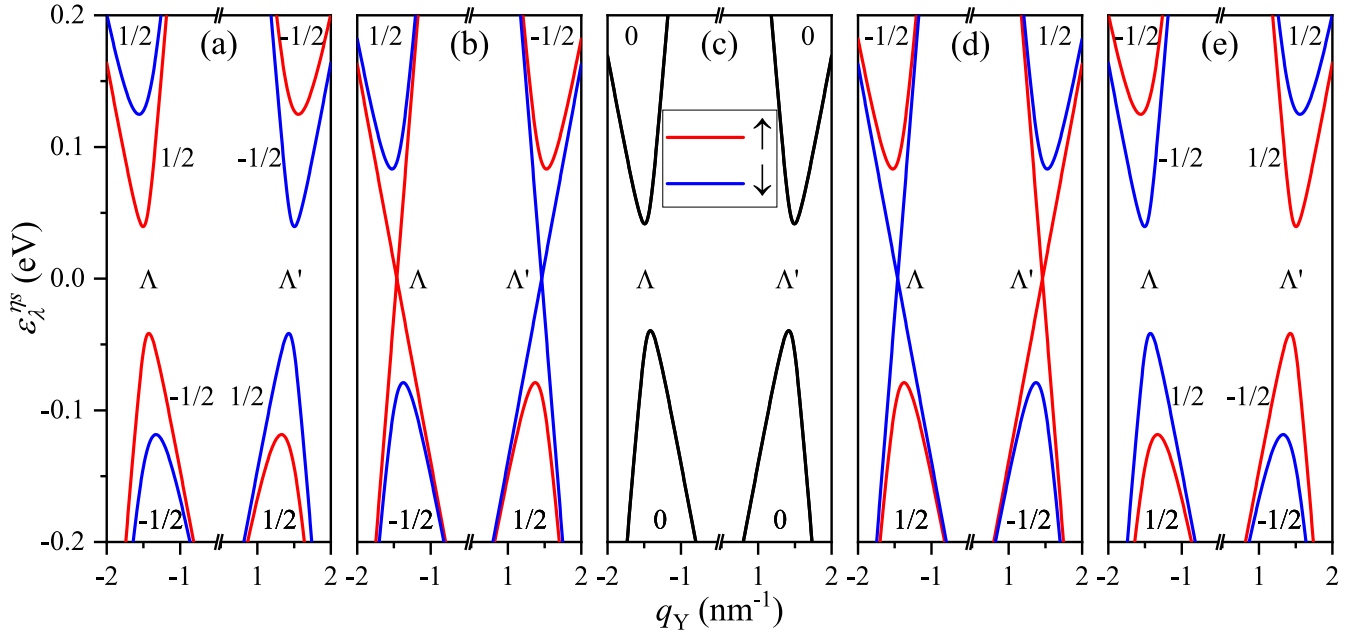


FIG. 2. The evolution of the electronic structure of the monolayer $1T'$ -MoS₂ under an electric field, $\mathcal{E} = -2, -1, 0, 1, 2$ for panels (a)–(e). $\mathcal{E} \neq 0$ induces the reversible spin splitting, which leads to the spin- and valley-polarized bands. And the case of the spin splitting of $\mathcal{E}$ is exactly opposite to that of the $-\mathcal{E}$ case. Upon increasing the magnitude of $\mathcal{E}$, the gap for each valley first closes and then reopens, implying the existence of a topological transition.

$$\sigma_{yx}^V = \frac{\sigma_0}{4\pi^2} \sum_{\eta=\pm, s=\pm} \int \eta \zeta^{\eta,s,\rightarrow}(q_y) T^{\eta,s}(q_y) dq_y, \quad (13c)$$

$$\sigma_{yx}^S = \frac{\sigma_0}{4\pi^2} \sum_{\eta=\pm, s=\pm} \int s \zeta^{\eta,s,\rightarrow}(q_y) T^{\eta,s}(q_y) dq_y. \quad (13d)$$

Generally, all conductances depend on the parameters (E_F, V_0, L, θ), but they are not shown explicitly for brevity. Here, $\sigma_0 = -e^2/\hbar = -2.434 \times 10^{-4}$ S is the reduced conductance. The velocity ratio is defined as

$$\zeta^{\eta,s,\rightarrow}(q_y) = \frac{u_y^{\eta,s,\rightarrow}(q_y)}{u_x^{\eta,s,\rightarrow}(q_y)},$$

where $u_x^{\eta,s,\rightarrow}$ ($u_y^{\eta,s,\rightarrow}$) is the longitudinal (transverse) component of the electronic group velocity $\mathbf{u}^{\eta,s,\rightarrow} = (u_x^{\eta,s,\rightarrow}, u_y^{\eta,s,\rightarrow})$ with $\rightarrow$ denoting the right-going states. In addition, $\mathbf{u}^{\eta,s,\leftarrow}$ is the electronic group velocity of left-going states. Furthermore, to assess the conversion efficiency, the charge, valley, and spin Hall ratios are defined as $\Theta = \sigma_{xy}/\sigma_{xx}$, $\Theta^V = \sigma_{xy}^V/\sigma_{xx}$ and $\Theta^S = \sigma_{xy}^S/\sigma_{xx}$, respectively.

III. RESULTS AND DISCUSSIONS

The top and bottom gates may induce an out-of-plane electric field in the monolayer TMS, which brings about the evolution of its electronic structure. Figure 2 shows the band evolution under the electric field $\mathcal{E} = -2, -1, 0, 1, 2$ for Figs. 2(a)–2(e). Because $\mathcal{E} = E_z/E_c$ with $E_c = \Delta_{so}/c_E \approx 1.42$ V/nm [76], the range $\mathcal{E} = -2, -1, 0, 1, 2$ corresponds to physical electric fields $E_z \approx -2.8, -1.4, 0, 1.4, 2.8$ V/nm. We note that electric fields on the order of ≈ 1 V/nm are experimentally accessible in dual-gated van der Waals heterostructures, particularly using high-quality dielectric layers

such as hBN, for which the breakdown field can be up to 2.1 V/nm in a 3-nm-thick sample [78]. Therefore, the values $|E_z| \approx 1$ V/nm correspond to realistic experimental conditions. The larger values $|E_z| \approx 2$ V/nm used in our paper are primarily intended to clearly illustrate the evolution of the band structure. The monolayer at zero electric field is a well-known topological insulator for $\mathcal{E} = 0$, for which the topological transition exists due to $\mathcal{E} \neq 0$. To show the topological transition, Eq. (2) can be rewritten into the form $\sim \mathbf{d} \cdot \boldsymbol{\tau}$ near the Dirac points, and then the corresponding Berry curvature can be analytically given as

$$\Omega_{\lambda}^{\eta,s}(q_X, k_Y) = \frac{-\lambda \eta v_1 v_+ (\mathcal{E} - \eta s)}{2 \Delta_{so}^2 \left[(\mathcal{E} - \eta s - s \frac{v_2 k_Y}{\Delta_{so}})^2 + \frac{(v_1^2 q_X^2 + v_+^2 k_Y^2)}{\Delta_{so}^2} \right]^{3/2}}. \quad (14)$$

In particular, the spin Berry curvature in each valley is opposite at $\mathcal{E} = 0$. This highlights the importance of TVHE for the applications of the monolayer TMS in valleytronics. Furthermore, the momentum integral of $\Omega_{\lambda}^{\eta,s}$ gives the spin- and valley-resolved Chern number:

$$C_{\lambda}^{\eta,s} = \sum_{(q_X, k_Y)} \Omega_{\lambda}^{\eta,s}(q_X, k_Y) = \frac{\lambda \eta s}{2} \text{sgn}(s\mathcal{E} - \eta). \quad (15)$$

Obviously, $\mathcal{E} = \pm 1$ is the phase boundary, consistent with the gapless electronic structure in Figs. 2(b) and 2(d). The Chern number is shown for each band in Fig. 2, except for Fig. 2(c), which is spin-degenerate, but its spin-resolved Chern number is also given by $C_{\lambda}^{\eta,s}$, e.g., it is $\pm 1/2$ for the conduction band $\lambda = +1$ with $s = \mp 1$. Using the Chern number for each band, one can define the spin Chern number $C_{\lambda}^s = (\sum_{\eta} C_{\lambda}^{\eta,+} - \sum_{\eta} C_{\lambda}^{\eta,-})/2$ and the valley Chern

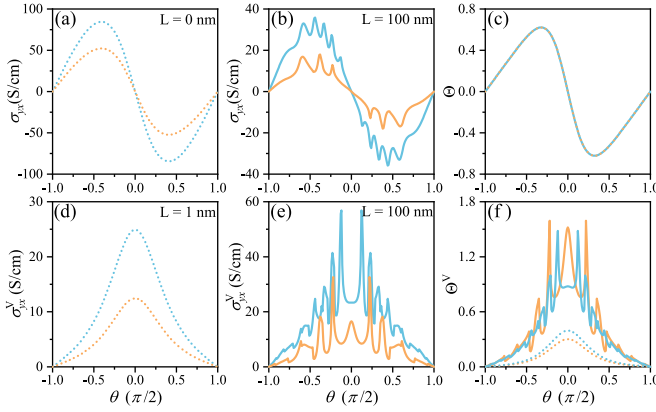


FIG. 3. Tunneling charge and valley Hall conductances for monolayer $1T'$ -MoS₂ junctions. (a), (b) Tunneling charge Hall conductance σ_{yx} as a function of the junction direction θ for $L = 0$ and 100 nm, respectively. (c) Tunneling charge Hall ratio Θ as a function of θ for parameters as in panels (a) and (b). (d), (e) Tunneling valley Hall conductance σ_{yx}^V as a function of θ for $L = 1$ nm and 100 nm, respectively. (f) Tunneling valley Hall ratio Θ^V as a function of θ for the parameters as in panels (d) and (e). Here, with $\mathcal{E} = 0$, $E_F = 0$, $V_0 = 0.07$ eV for the orange lines and $V_0 = 0.1$ eV for the blue lines.

number $C_\lambda^\eta = (\sum_s C_\lambda^{+,s} - \sum_\eta C_\lambda^{-,s})/2$, respectively. As a result, $(|C_\lambda^s|, |C_\lambda^\eta|) = (1, 0)$ for $-1 < \mathcal{E} < 1$ and $(|C_\lambda^s|, |C_\lambda^\eta|) = (0, 1)$ otherwise; this implies the phase transition from the topological insulator to band insulator or quantum valley insulator by tuning the electric field across $\mathcal{E} = \pm 1$. The tunneling Hall effects of the TMS junctions are determined by the electronic structure. In light of the evolution of the electronic structure with the electric field $\mathcal{E}$, we begin our discussions from the case $\mathcal{E} = 0$ to that of $\mathcal{E} \neq 0$.

A. $\mathcal{E} = 0$ case

In this case, the TVHE and tunneling charge Hall effect are discussed since the tunneling spin Hall effect is quenched by the spin-degenerate bands.

1. Universal tunneling charge Hall ratio Θ

To consider the general junction θ , Fig. 3 shows the tunneling charge and valley Hall conductances for the $1T'$ -MoS₂ junctions. The junction direction θ is tunable by the incident unpolarized charge current. In Fig. 3(a), the junction width is intentionally chosen as $L = 0$, i.e., essentially for a uniform monolayer TMS (with E_F in the conduction band). As long as $\theta \neq n\pi/2$ with n an integer, the tunneling charge Hall conductance is finite and has a form $\sigma_{yx} \sim \sin \theta \cos \theta$, which is as expected from the anisotropic and tilted Dirac fermions of uniform monolayer TMS. By using a finite L , Fig. 3(b) shows that σ_{yx} exhibits a series of peaks caused by the resonant tunneling across the monolayer TMS junction. This resonant enhancement also exists for the other conductances and will be explained in detail for the TVHE later. Two values of V_0 are considered, higher V_0 leads to higher σ_{yx} since more electrons participate in the transport process. Remarkably, although σ_{yx} has a strong dependence on the L and V_0 , the charge Hall ratio Θ for different L and V_0 does not exhibit the features of

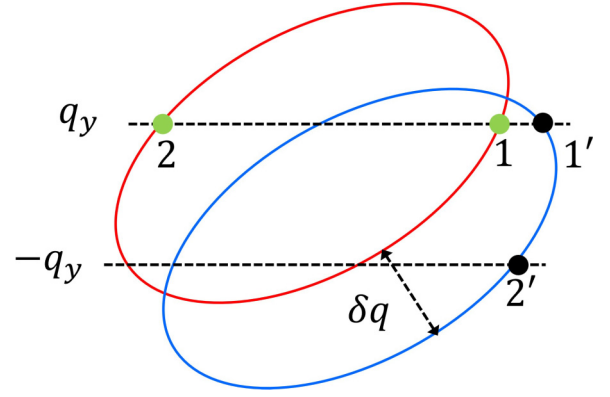


FIG. 4. The constant-energy contours of two valleys in the right electrodes. Two constant-energy contours are ellipses and away from each other along their semiminor axis, in which the red (blue) one is for the $\eta = +$ ($\eta = -$) valley with the spacing δq . The conserved momentum q_y picks up the states on the contours, e.g., two green (black) dots on the $\eta = +$ ($\eta = -$) contour.

resonant tunneling and coalesces into a single curve, as shown by Fig. 3(c), i.e., universal Θ behavior.

To derive the universal Θ , the key is to simplify the expressions of σ_{yx} , which can be performed through the intuitive physical picture. Figure 4 shows the constant-energy contours of two valleys, the simplification is realized through the replacement of the states of the black dot 1' by the black dot 2', and then the replacement of the states of the black dot 2' by the green dot 2. As a result, the calculations of the tunneling conductances only require the information of a single valley, e.g., $\eta = +$ in our simplification (cf. two green dots in Fig. 4). The simplification benefits from the time-reversal symmetry, which enforces $T^{\eta,s}(q_y) = T^{-\eta,-s}(-q_y)$ and $\mathbf{u}^{\eta,s,\rightarrow}(q_y) = -\mathbf{u}^{-\eta,-s,\leftarrow}(-q_y)$. As a result, the tunneling charge Hall ratio is given as (cf. Appendix A)

$$\Theta = \frac{(\gamma^2 - 1) \sin \theta \cos \theta}{\gamma^2 \sin^2 \theta + \cos^2 \theta}, \quad (16)$$

where $\gamma^2 = (v_2^2 + v_+^2 - v_-^2)/v_1^2$. This demonstrates that Θ is independent of the barrier length (L) and height (V_0), and even the Fermi level E_F . Several comments follow: (I) Θ may be finite only when $\gamma^2 \neq 1$. Typically, $\Theta = 0$ in graphene for the isotropic Dirac cones. (II) Equation (16) is also applicable to the uniform system (i.e., $V_0 = 0$), where it is an anisotropic effect and is well known [cf. Ref. [79] and the discussion following Eq. (9) in Ref. [80]]. However, even in anisotropic systems, Θ may not exist when $\gamma^2 = 1$ shown by Eq. (16), in contrast with the conventional expectation [80]. (III) Θ is the monotonic function of γ^2 , its magnitude increases with increasing γ^2 and is a periodic function of θ with the period π . This universal Θ behavior is first found for the gapless tilted Dirac fermions [64] (e.g., in $8-Pmmn$ borophene), and here it is further generalized to the gapped tilted Dirac fermions (in monolayer TMS in this study).

2. Tunneling valley Hall effect

Turn to the TVHE, which is the dominant valley Hall mechanism for the valleytronic applications of monolayer

TMS since there is no intrinsic VHE. For the two valleys coupled by time-reversal symmetry, the velocity textures are not independent, and they satisfy (cf. Fig. 4)

$$\zeta^{+,s,\vec{\epsilon}}(q_y) = \zeta^{-,s,\vec{\epsilon}}(q_y + \delta q_y), \quad (17)$$

where

$$\delta q_y = 2 \left| \frac{\eta v_- \varepsilon_\lambda^{\eta s} + v_2 (s\mathcal{E} - \eta) \Delta_{so}}{v_+^2 + v_-^2 - v_-^2} \right| \cos \theta. \quad (18)$$

When $V_0 = 0$, i.e., in the uniform system,

$$\sigma_{yx}^V \propto \int dk_y \zeta^{+,s,\rightarrow}(q_y) - \int dk_y \zeta^{-,s,\rightarrow}(q_y) = 0, \quad (19)$$

which is in contrast with the finite σ_{yx} there. Once the junction is formed [cf. Fig. 1(b)], the incident electrons of two valleys will experience different skew transmission due to the momentum mismatch. For the Λ valley (red), the electronic states with the group velocity $u_y < 0$ ($u_y > 0$) are allowed (forbidden) for transmission. For the Λ' valley (blue), the skew transmission is reversed for the electronic states with the group velocity $u_y < 0$ ($u_y > 0$). Actually, the skew transmission of the Λ valley is related to that of the Λ' valley through time-reversal symmetry, i.e., $T^{\eta,s}(q_y) = T^{-\eta,-s}(-q_y)$. As a result, an unpolarized valley current I_0 incident from the left electrode generates the valley-polarized Hall currents I_Λ and $I_{\Lambda'}$, which occur at the right electrode, as shown by Fig. 1(c), i.e., TVHE.

To quantitatively examine the TVHE in monolayer TMS junctions, Figs. 3(d)–3(f) are plotted. When L is small, the tunneling valley Hall conductance is mainly determined by the doping of the incident states in the left electrode. Once the junction is formed, even the width L is very small, σ_{yx}^V becomes finite and rather sizable when comparing Fig. 3(a) with Fig. 3(d). This means that the uniform system can be regarded as a critical case of the junctions at which $\sigma_{yx}^V = 0$ due to Eq. (19). In Fig. 3(e), some peaks occur for σ_{yx}^V . The peaks of σ_{yx}^V originate from the resonant transmission due to the propagation of right-going and left-going states and their matching with L . To explain this point, we first present the resonant condition for the junctions based on the anisotropic material (i.e., monolayer TMS here):

$$(q_x^{\eta,s,\rightarrow} + q_x^{\eta,s,\leftarrow})L = 2\pi m. \quad (20)$$

Here, $q_x^{\eta,s,\rightarrow}$ ($q_x^{\eta,s,\leftarrow}$) is the longitudinal component of momentum for the right-going (left-going) states, and m is an integer. To consider two typical junction directions, i.e., $\theta = 0$ and $\theta = \pi/4$, Figs. 5(a) and 5(b) shows σ_{yx}^V and σ_{xx} as the function of the barrier length L , respectively. Clearly, the peaks of σ_{yx}^V and σ_{xx} are from the resonant transmission, as shown in Figs. 5(c) and 5(d). The tunneling valley Hall ratio $\Theta^V = \sigma_{yx}^V / \sigma_{xx}$ shown in Fig. 3(f) and Figs. 5(e) and 5(f) has giant magnitude compared with about 10^{-3} for the intrinsic valley Hall ratio [11,60]. Furthermore, Θ^V is tunable by the parameters (E_F , V_0 , L , θ), e.g., by V_0 and θ in Fig. 3(f) and by L in Figs. 5(e) and 5(f). More importantly, Θ^V can be enhanced resonantly, which is in contrast with the parameter-independent behavior of the universal Θ . A large TVHE is also present in the smooth junction, as evinced by the tight-binding model calculations (cf. Appendix C).

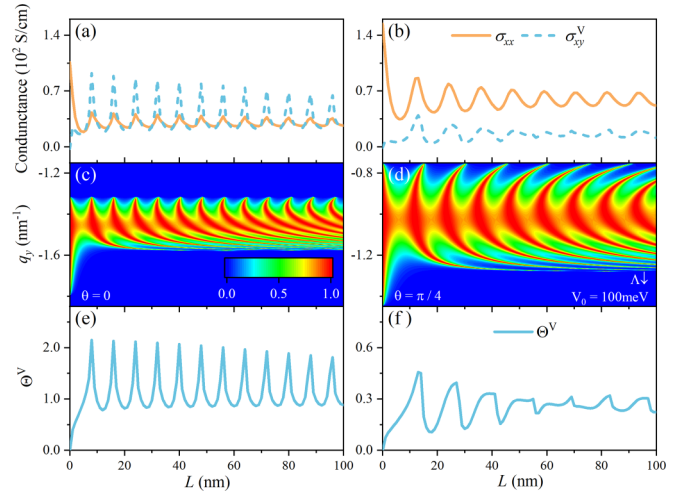


FIG. 5. The underlying mechanism of resonant enhancement for transport in monolayer $1T'$ -MoS₂ junctions. (a), (b) Longitudinal and tunneling valley Hall conductances are shown as functions of barrier length L . (c), (d) Transmission probability is shown as a function of barrier length L and q_y . (e), (f) Tunneling valley Hall ratio is shown as a function of barrier length L . Here $V_0 = 100$ meV and $\mathcal{E} = 0$, the junction rotation angles $\theta = 0$ in panels (a) and (c), (e) and $\theta = \pi/4$ in panels (b) and (d), (f).

B. $\mathcal{E} \neq 0$ case

When $\mathcal{E} \neq 0$, the spin splitting of electronic structure occurs; each band becomes spin- and valley-polarized and the spin-polarization for $\mathcal{E}$ case is exactly opposite to that of $-\mathcal{E}$ case. For the considered npn junction, the position of E_F define two regimes, i.e., one constant-energy contour for a low doping valley and two constant-energy contours for a high doping valley. For these two regimes, the universal charge Hall ratio retains unchanged since the spin-flip scattering does not exist for the scalar scattering potential (cf. the spin-independent derivations for Θ in Appendix A). In this section, we focus on the TVHE and the tunneling spin Hall effect.

1. One constant-energy contour

As shown in Fig. 2, there are two conduction bands in each valley due to $\mathcal{E}$ -induced spin splitting. When E_F is lower than the bottom of the second conduction band, there is only one constant-energy contour in a single valley where the electronic states of the monolayer TMS are fully valley- and spin-polarized, i.e., valley-spin locking. The longitudinal transport of valley-spin locking states in junctions has been proposed to be implemented in valley-spin valves [81]. But the transverse transport of valley-spin locking states and its potential in devices has not been studied. To focus on the tunneling valley and spin Hall effects, according to the definition [cf. Eq. (13)], the valley Hall conductances are the same for $\pm\mathcal{E}$, whereas the spin Hall conductances are reversed for $\pm\mathcal{E}$ as dictated by the electronic structure [cf. Figs. 2(a), 2(e) and Figs. 2(b), 2(d)]. So $\sigma_{xy}^V = \sigma_{xy}^S$ for $\mathcal{E} > 0$ and $\sigma_{xy}^V = -\sigma_{xy}^S$ for $\mathcal{E} < 0$. Then, we only need to show the tunneling spin Hall effects, cf. Fig. 6. Figures 6(a)–6(d) show the tunneling spin Hall conductance and ratio, respectively. As expected, the tunneling spin Hall conductance can be manipulated by

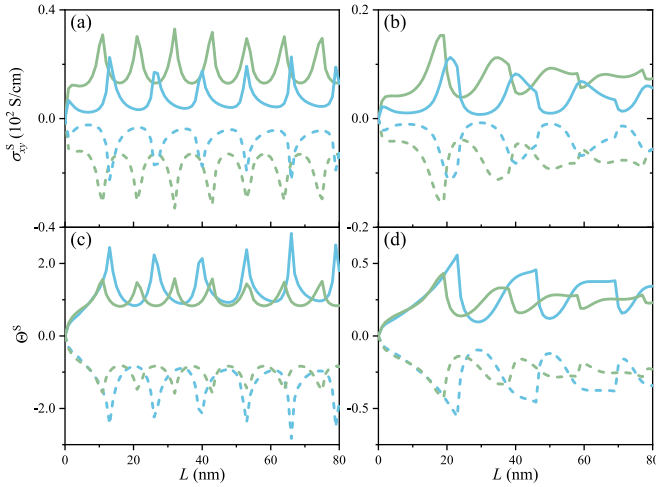


FIG. 6. Tunneling spin Hall effect as a function of the barrier length L by using different electric fields, $\mathcal{E} = \pm 1$ (green) and ± 2 (blue). (a), (b) Tunneling spin Hall conductances. (c), (d) Tunneling spin Hall ratio. The spin conductances and ratio are positive (negative) for $\mathcal{E} > 0$ ($\mathcal{E} < 0$) denoted by the solid (dashed) lines. Two junctions are considered: $\theta = 0$ in panels (a) and (c) and $\theta = \pi/4$ in panels (b) and (d). Here, $E_F = 0$ and $V_0 = 70$ meV.

$\mathcal{E}$; reversing the conductance sign by applying $\pm \mathcal{E}$ (cf. the solid lines vs the dashed lines in Fig. 6) and increasing the conductance magnitude by increasing $|\mathcal{E}|$ (cf. the green lines vs the blue lines in Fig. 6). Note that the tunneling longitudinal $\sigma_{xx} > 0$. The dependence on $\mathcal{E}$ of the tunneling spin Hall effect is general and exists for any junction direction, cf. Fig. 6 for $\theta = 0$ in the left column vs $\theta = \pi/4$ in the right column. As two by-products of the tunneling spin Hall conductance, the sign can identify two opposite spin splittings, i.e., $\sigma_{xy}^S(\mathcal{E} > 0) > 0$ and $\sigma_{xy}^S(\mathcal{E} < 0) < 0$, and the magnitude should be used to distinguish the different topological phases, e.g., the magnitude change from $(\mathcal{E} < 1)$ to $(\mathcal{E} > 1)$ for fixing V_0 and E_F due to the gap closing and reopening. These topological transitions are associated with the evolution of the doping with the electric field $\mathcal{E}$. To consider the same Fermi level E_F in Fig. 2, the doping is maximal at the critical field $|\mathcal{E}| = 1$ for the topological transition, see Figs. 2(b) and 2(d). As a result, the tunneling spin Hall conductance should show a peak at $\mathcal{E} = 1$ or $\mathcal{E} = -1$. Figure 7 shows the tunneling

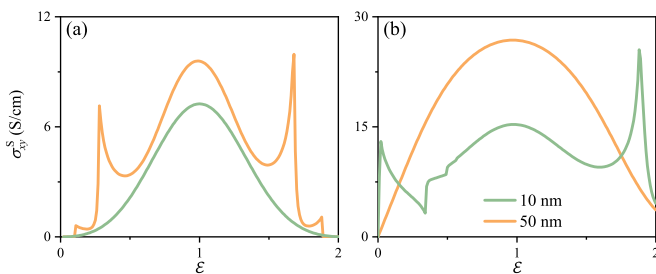


FIG. 7. Tunneling spin Hall conductances as a function of electric fields $\mathcal{E}$ by considering different barrier lengths L . (a) $V_0 = 41$ meV and (b) $V_0 = 70$ meV. There are always peaks at $\mathcal{E} = 1$ for the topological transition beyond the shifting resonant peaks. Here, $E_F = 0$.

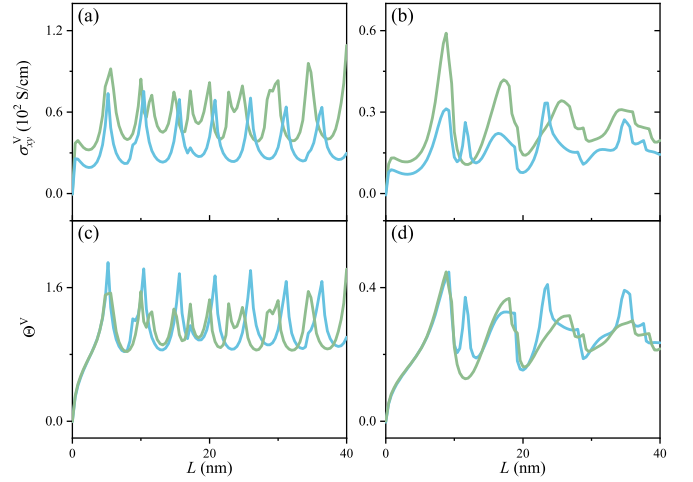


FIG. 8. Tunneling valley Hall effect as a function of the barrier length L by using different electric fields, $\mathcal{E} = \pm 1$ (green) and ± 2 (blue). (a), (b) Tunneling valley Hall conductances. (c), (d) Tunneling valley Hall ratio. The spin conductances and ratio for $\mathcal{E} > 0$ ($\mathcal{E} < 0$) are denoted by the solid (dashed) lines. The solid and dashed lines exactly overlap. Two junctions are considered: $\theta = 0$ in panels (a) and (c) and $\theta = \pi/4$ in panels (b) and (d). Here, $E_F = 0$ and $V_0 = 150$ meV.

spin Hall conductance as a function of the electric field $\mathcal{E}$ by considering different barrier lengths L and different V_0 . For different barrier lengths L and different V_0 , there are resonant peaks, shifting along the axis of $\mathcal{E}$ with the change of L or V_0 . In contrast, the peaks at $\mathcal{E} = 1$ are stationary and always occur, which is actually due to the topological transition. Therefore, the stationary conductance peaks located at $\mathcal{E} = \pm 1$ are distinguished from ordinary resonant peaks. Since $\mathcal{E} = \pm 1$ corresponds to the bulk gap-closing points where the spin- and valley-resolved Chern numbers change [cf. Eq. (15)], these stationary conductance peaks serve as indirect signatures of the topological phase transition.

2. Two constant-energy contours

As shown in Fig. 2, tuning E_F into the second conduction band, there are two constant-energy contours in a valley. The electronic states on the two constant-energy contours are both spin-polarized but along opposite directions. As a result, two constant-energy contours have a summed (subtracted) contribution to the tunneling valley (spin) Hall effect. Figure 8 shows the TVHE by considering two constant-energy contours for the high-doping valleys. According to the definition, $\mathcal{E}$ can only manipulate the magnitude of valley Hall conductances, which are always positive, as shown in Fig. 8. Near some values of L , the double peaks [e.g., cf. $L = 18$ nm and 24 nm in Fig. 8(a)] occur due to the algebraic sum of the resonant enhancement from two constant-energy contours. The double peaks also exist in the tunneling valley Hall ratio [cf. Fig. 8(c)], but they are blurred in the tilted junction with $\theta \neq 0$ [cf. Figs. 8(b) and 8(d) for $\theta = \pi/4$] due to the less sharp resonant enhancement.

Figure 9 shows the tunneling spin Hall effect by considering two constant-energy contours for the high-doping valleys. Due to the subtracted contribution of two constant-energy

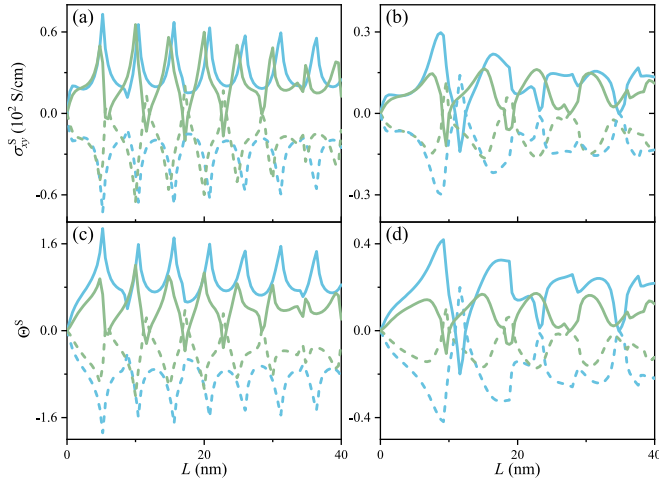


FIG. 9. Tunneling spin Hall effect as a function of the barrier length L by using different electric fields, $\mathcal{E} = \pm 1$ (green) and ± 2 (blue). (a), (b) Tunneling spin Hall conductances. (c), (d) Tunneling spin Hall ratio. The spin conductances and ratio are positive (negative) for $\mathcal{E} > 0$ ($\mathcal{E} < 0$) denoted by the solid (dashed) lines. Two junctions are considered: $\theta = 0$ in panels (a) and (c) and $\theta = \pi/4$ in panels (b) and (d). Here, $E_F = 0$ and $V_0 = 150$ meV.

contours, the antidouble peaks for the tunneling spin Hall effect [e.g., cf. $L = 18$ nm and 24 nm in Figs. 9(a) and 9(c)] occur, even reversing the sign for the unidirectional electric field [cf. the solid lines for $\mathcal{E} > 0$ or the dashed lines for $\mathcal{E} < 0$ in Figs. 9(a) and 9(c)]. For a tilted junction with $\theta = \pi/4$ in Figs. 9(b) and 9(d), the antidouble peaks are also blurred by the not sharp resonant enhancement.

IV. CONCLUSIONS

To conclude, we have comprehensively studied the tunneling Hall effects for the valley and other degrees of freedom in monolayer $1T'$ -MoS₂ junctions. The tunneling Hall effects, which respect time-reversal symmetry such as the nonlinear Hall effect [82–84] and the Magnus Hall effect [80], are attracting increasing attention. The tilted Dirac fermions play a key role in the tunneling Hall effects, which are gapped and spin-splitting in monolayer $1T'$ -MoS₂, in contrast with those in 8-*Pmmn* borophene [64]. The gap opening and the spin splitting, both controlled by an out-of-plane electric field, together lead to the topological transition. The unique electronic structure of the monolayer $1T'$ -MoS₂ shows itself in the tunneling Hall effects. At zero electric field, the tunneling valley effect is the dominant valley Hall mechanism for the valleytronic applications based on monolayer $1T'$ -MoS₂, since there is no intrinsic valley Hall effect, despite the presence of gap opening. The tunneling valley Hall effect can be tuned by the multiple parameters, for which the resonant enhancement due to the transmission matching appears, leading to an electrically tunable high tunneling valley ratio. Due to the valley-spin locking induced by the nonzero electric field, the tunneling spin Hall effect differs by a sign from the tunneling valley Hall effect at low doping. And the sign and magnitude changes of the tunneling spin Hall effect correspond to the reversal of the spin splitting and the topological transition,

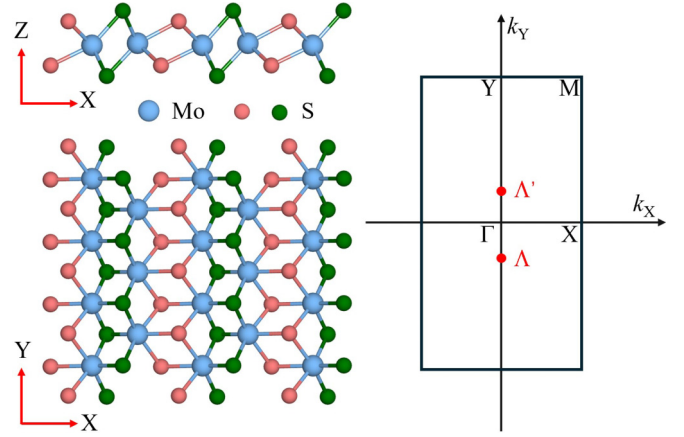


FIG. 10. Lattice structure of the monolayer $1T'$ -MoS₂ in direct space (left panel) and the corresponding Brillouin zone in reciprocal space (right panel).

respectively. In particular, we obtain a universal conversion ratio for the tunneling charge Hall effect, as that in 8-*Pmmn* borophene [64], which is independent of the gap opening and spin splitting. As a result, we provide a complete understanding of tunneling Hall effects in monolayer $1T'$ -MoS₂ junctions and expect their experimental observation in realistic two-dimensional transition-metal dichalcogenides, which can then be used in valleytronic and spintronic devices.

ACKNOWLEDGMENTS

This work was supported by the Science Challenge Project (Grant No. TZ2025017), the NSFC (Grants No. 12174019 and No. 12274019), and an NSAF grant in NSFC with Grant No. U2230402. S.H.Z. is also supported by the Fundamental Research Funds for the Central Universities (010-63263119). We acknowledge computational support provided by the Beijing Computational Science Research Center (CSRC) and Hefei Advanced Computing Center.

DATA AVAILABILITY

The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

APPENDIX A: LATTICE STRUCTURE AND BRILLOUIN ZONE OF MONOLAYER $1T'$ -MoS₂

Here, Fig. 10 presents the lattice structure of the monolayer $1T'$ -MoS₂ in direct space (left panel) and its Brillouin zone in reciprocal space (right panel). The high-symmetry points are highlighted in the Brillouin zone, particularly the Λ and Λ' points, which host the Dirac cones.

APPENDIX B: UNIVERSAL CHARGE HALL ANGLE

Due to time-reversal symmetry, $T^{\eta,s}(q_y) = T^{-\eta,-s}(-q_y)$ and $\mathbf{u}^{\eta,s,\rightarrow}(q_y) = -\mathbf{u}^{-\eta,-s,\leftarrow}(-q_y)$, the longitudinal conductance and charge Hall conductance can be rewritten as

$$\sigma_{xx} = 2 \sum_s \int T^{s,\eta}(k_y) dk_y, \quad (\text{B1})$$

and

$$\sigma_{yx} = \frac{\sigma_0}{4\pi^2} \sum_{\eta=\pm 1, s=\pm 1} \int \frac{u_y^{s,\eta,\rightarrow}(q_y)}{u_x^{s,\eta,\rightarrow}(q_y)} T^{s,\eta}(q_y) dq_y \quad (\text{B2a})$$

$$= \frac{\sigma_0}{4\pi^2} \sum_s \int \left(\frac{u_y^{\eta,s,\rightarrow}}{u_x^{\eta,s,\rightarrow}} + \frac{u_y^{\eta,s,\leftarrow}}{u_x^{\eta,s,\leftarrow}} \right) T^{s,\eta}(q_y) dq_y, \quad (\text{B2b})$$

respectively. As a result, the calculation of σ_{yx} only requires the information of an arbitrary valley. Here and later, the superscript for the group velocity $\mathbf{u} = (u_x, u_y) = (u_X, u_Y)$ is omitted unless it is necessary. Utilizing the coordinate transformation for the group velocity, we have

$$u_x = u_X \cos \theta + u_Y \sin \theta, \quad (\text{B3a})$$

$$u_y = -u_X \sin \theta + u_Y \cos \theta. \quad (\text{B3b})$$

To assume ϕ ($\bar{\phi}$) as the azimuthal angle of $\mathbf{u}$ in the coordinate system x - y (X - Y), then the component ratio of the group velocity is

$$\frac{u_y}{u_x} = \tan \phi \quad (\text{B4a})$$

$$= \frac{-v_X \sin \theta + v_Y \cos \theta}{v_X \cos \theta + v_Y \sin \theta} \quad (\text{B4b})$$

$$= \frac{\tan \bar{\phi} - \tan \theta}{1 + \tan \bar{\phi} \tan \theta}, \quad (\text{B4c})$$

with

$$\tan \bar{\phi} = \frac{v_Y}{v_X}. \quad (\text{B5})$$

In the X - Y coordinate system, the group velocity is defined as the gradient of the energy dispersion $\mathbf{u} = \nabla \varepsilon_{\lambda}^{\eta s}$ and its components are

$$v_X = \frac{\partial \varepsilon_{\pm, \eta s}}{\partial q_X} = \frac{q_X v_1^2}{\varepsilon_{\eta s} + \eta v_- q_Y}, \quad (\text{B6a})$$

$$v_Y = \frac{\partial \varepsilon_{\pm, \eta s}}{\partial q_Y} = -\eta v_- + \frac{q_Y (v_2^2 + v_+^2) + v_2 (\eta - s \mathcal{E}) \Delta_{so}}{\varepsilon_{\lambda}^{\eta s} + \eta v_- q_Y}. \quad (\text{B6b})$$

So one can obtain

$$\tan \bar{\phi} = \frac{v_Y}{v_X} = \frac{-\eta \gamma_2 \epsilon + \gamma^2 q_Y + \gamma_1^2 k_0 (\eta - s \mathcal{E})}{q_X}, \quad (\text{B7})$$

where

$$\gamma_1 \equiv \frac{v_2}{v_1}, \quad \gamma_2 \equiv \frac{v_-}{v_1}, \quad (\text{B8a})$$

$$\gamma^2 \equiv \frac{v_2^2 + v_+^2 - v_-^2}{v_1^2}, \quad (\text{B8b})$$

$$\epsilon \equiv \frac{\varepsilon_{\lambda}^{\eta s}}{v_1}. \quad (\text{B8c})$$

In the x - y coordinate system, we replace $\tan \bar{\phi}$ in the expression of $\tan \phi$:

$$\frac{v_y}{v_x} = \tan \phi = \frac{\tan \bar{\phi} - \tan \theta}{1 + \tan \bar{\phi} \tan \theta}, \quad (\text{B9a})$$

$$= \frac{q_x A_0 + q_y A_1 + B_0 \cos \theta}{q_x A + q_y A_0 + B_0 \sin \theta}, \quad (\text{B9b})$$

where

$$A_0 \equiv (\gamma^2 - 1) \sin \theta \cos \theta, \quad (\text{B10a})$$

$$A \equiv \gamma^2 \sin^2 \theta + \cos^2 \theta, \quad (\text{B10b})$$

$$A_1 \equiv \gamma^2 \cos^2 \theta + \sin^2 \theta. \quad (\text{B10c})$$

$$B_0 \equiv [\gamma_1^2 k_0 (\eta - s \mathcal{E}) - \eta \gamma_2 \epsilon - \eta \gamma^2 k_0], \quad (\text{B10d})$$

To recover the superscript of the group velocity, the prefactor of the integrand of σ_{yx} is

$$\frac{u_y^{\eta,s,\rightarrow}}{u_x^{\eta,s,\rightarrow}} + \frac{u_y^{\eta,s,\leftarrow}}{u_x^{\eta,s,\leftarrow}} = \frac{q_x^{\rightarrow} A_0 + q_y A_1 + B_0 \cos \theta}{q_x^{\rightarrow} A + q_y A_0 + B_0 \sin \theta} + \frac{q_x^{\leftarrow} A_0 + q_y A_1 + B_0 \cos \theta}{q_x^{\leftarrow} A + q_y A_0 + B_0 \sin \theta}. \quad (\text{B11})$$

Furthermore, it is crucial to derive the longitudinal component of momentum $q_x^{\rightarrow}$ ($q_x^{\leftarrow}$) for the right-going (left-going) states on the constant-energy contour of an arbitrary valley, which are together determined by the conserved momentum q_y along the junction interface and the energy dispersion $\varepsilon_F \equiv E_F + V_0 = \varepsilon_{\lambda}^{\eta s}$ in the electrodes. Utilizing the coordinate transformation for the momentum, we have

$$q_x = q_X \cos \theta - q_Y \sin \theta, \quad (\text{B12a})$$

$$q_y = q_X \sin \theta + q_Y \cos \theta. \quad (\text{B12b})$$

Thus, we obtain a quadratic equation with one unknown for q_x :

$$A q_x^2 + 2B q_x + C = 0, \quad (\text{B13})$$

where

$$B = B_0 \sin \theta + A_0 q_y, \quad (\text{B14a})$$

$$C = A_1 q_y^2 + 2B_0 \cos \theta q_y + \Gamma^2 k_0^2 + 2\gamma_2 k_0 \epsilon_F - \epsilon_F^2, \quad (\text{B14b})$$

with

$$\Gamma^2 = \mathcal{E} \gamma_1^2 - \gamma_2^2 + \gamma_3^2, \\ \epsilon_F = \varepsilon_F / v_1, \quad \gamma_3 \equiv \frac{v_+}{v_1}.$$

Obviously, $q_x^{\leftarrow}$ and $q_x^{\rightarrow}$ are related to each other through the Vieta's theorem:

$$q_x^{\leftarrow} + q_x^{\rightarrow} = \frac{B}{A}, \quad (\text{B15a})$$

$$q_x^{\leftarrow} q_x^{\rightarrow} = \frac{C}{A}. \quad (\text{B15b})$$

As a result, we can simplify the expression for the prefactor of the integrand of σ_{yx} , which is

$$\frac{u_y^{\eta,s,\rightarrow}}{u_x^{\eta,s,\rightarrow}} + \frac{u_y^{\eta,s,\leftarrow}}{u_x^{\eta,s,\leftarrow}} \quad (\text{B16a})$$

$$= \frac{2(A_1 q_y + B_0 \cos \theta) - 2B(A_1 q_y + B_0 \cos \theta) - 2B^2 A_0/A + 2A_0 C}{AC - B^2} \quad (\text{B16b})$$

$$= \frac{2A_0}{A} \frac{AC - B^2}{AC - B^2} \quad (\text{B16c})$$

$$= \frac{2(\gamma^2 - 1) \sin \theta \cos \theta}{\gamma^2 \sin^2 \theta + \cos^2 \theta}. \quad (\text{B16d})$$

Finally, the charge Hall ratio is analytically derived:

$$\Theta = \frac{\sigma_{yx}}{\sigma_{xx}} = \frac{(\gamma^2 - 1) \sin \theta \cos \theta}{\gamma^2 \sin^2 \theta + \cos^2 \theta}, \quad (\text{B17})$$

which is universal and applicable to the uniform monolayer and junctions of $1T'$ -MoS₂.

APPENDIX C: THE COMPLEMENTARY CALCULATIONS BASED ON THE TIGHT-BINDING HAMILTONIAN

1. Tight-binding Hamiltonian in momentum space

For the monolayer $1T'$ -MX₂, where M = (W, Mo) and X = (S, Te, Se), the energy bands closest to the Fermi level are primarily contributed by the $d_{x^2-y^2}$ and d_{z^2} orbitals of the M atom, as well as the p_x orbital of the X atom. The tight-binding (TB) Hamiltonian $H_0(\mathbf{k})$ is given by [85,86]

$$H_{11,33} = \mu_d + 2d_3 \cos(k_X a) + 2d_1 \cos(k_Y b), \quad (\text{C1a})$$

$$H_{22,44} = \mu_p + 2p_2 \cos(k_X a) + 2p_1 \cos(k_Y b), \quad (\text{C1b})$$

$$H_{12} = -2it_2 \sin(k_Y b), \quad (\text{C1c})$$

$$H_{13} = d_2 e^{-ik_X a} (1 + e^{ik_Y b}), \quad (\text{C1d})$$

$$H_{14} = t_1 (1 - e^{ik_Y b}) + t_3 (e^{-ik_Y b} - e^{2ik_Y b}), \quad (\text{C1e})$$

$$H_{23} = -t_1 (1 - e^{ik_Y b}) - t_3 (e^{-ik_Y b} - e^{2ik_Y b}), \quad (\text{C1f})$$

$$H_{24} = p_3 (1 + e^{ik_Y b}), \quad (\text{C1g})$$

$$H_{34} = -2it_2 \sin(k_Y b), \quad (\text{C1h})$$

$$H_E = \text{diag}(c_E E_z, 0, -c_E E_z, 0), \quad (\text{C1i})$$

in the orbital basis $(d_{\mathbf{k}M_1}, p_{\mathbf{k}X_3}, d_{\mathbf{k}M_2}, p_{\mathbf{k}X_2})$. Here, $d_{\mathbf{k}M_1}$ and $d_{\mathbf{k}M_2}$ denote the d -orbital states on the sublattices M_1 and M_2 , respectively, while $p_{\mathbf{k}X_3}$ and $p_{\mathbf{k}X_2}$ represent the p -orbital states on the sublattices X_3 and X_2 , E_z describes the effect of the perpendicular electric field, and c_E is the electrical

coefficient. The lattice constants $a = 0.3173255$ nm and $b = 0.5722851$ nm.

To account for spin-orbit coupling (SOC), we need to use the spinful basis $(d_{\mathbf{k}M_1\sigma}, p_{\mathbf{k}X_3\sigma}, d_{\mathbf{k}M_2\sigma}, p_{\mathbf{k}X_2\sigma})$, which leads to the full Hamiltonian $H(\mathbf{k})$:

$$H(\mathbf{k}) = \sigma_0 \otimes H_0(\mathbf{k}) + H_{\text{SOC}}(\mathbf{k}), \quad (\text{C2})$$

where

$$\begin{aligned} H_{\text{SOC}} = & [(\lambda_{d1} \sigma_z + \lambda_{d2} \sigma_y) \sin(k_Y b)] \tau_3 (s_0 + s_3)/2 \\ & + [(\lambda_{p1} \sigma_z + \lambda_{p2} \sigma_y) \sin(k_Y b)] \tau_3 (s_0 - s_3)/2 \\ & - i\lambda_{t5} \sigma_y (1 + e^{ik_Y b}) (\tau_1 + i\tau_2) s_1/2 + S_+ + S_- + \text{H.c.}, \end{aligned} \quad (\text{C3})$$

with

$$\begin{aligned} S_{\pm} = & \pm [i(\lambda_{t1} \sigma_z + \lambda_{t3} \sigma_y) + (\lambda_{t2} \sigma_z + \lambda_{t4} \sigma_y) e^{\pm ik_X a}] \\ & \otimes (\tau_0 \mp \tau_3) (s_1 + is_2)/4. \end{aligned} \quad (\text{C4})$$

Here, λ_i is the SOC strength and σ , τ , and s are Pauli matrices acting on spin, sublattice, and orbital degrees of freedom, respectively. The parameters in $H_0(\mathbf{k})$ and H_{SOC} are presented in the Tables I and II. Two key notes are as follows: (1) $H(\mathbf{k})$ is renormalized for favoring the numerical calculations through omitting the difference of atomic vectors in the unit cell, i.e., $H(\mathbf{k})$ is actually in the unit-cell basis instead of the original form in the atomic basis [85,86]. (2) The different potentials are applied along the X direction, which avoids the intervalley scattering and keeps k_Y a good quantum number.

The TB Hamiltonian $H(\mathbf{k})$ captures the gapped and tilted Dirac dispersion in the Dirac cones, but the linear regime of $H(\mathbf{k})$ is rather narrow ≈ 100 meV [85] compared with the 1 eV of graphene [87]. The low-energy continuum model of the TB Hamiltonian can be mapped to the used low-energy Hamiltonian [cf. Eq. (1)] in the text. Due to the field-dependent gaps, the fitting parameters vary for different

TABLE I. TB Model Parameters (eV).

μ_d	μ_p	d_1	d_2	d_3	p_1
-1.00772	0.922436	0.524631	-0.27021	0.180134	-0.52972
p_2	p_3	t_1	t_2	t_3	
0.011201	-0.25881	0.016205	0.127180	-0.35440	

TABLE II. SOC Parameters (eV).

λ_{d1}	λ_{d2}	λ_{p1}	λ_{p2}	λ_{t1}
-0.00482	0.018456	0.039409	0.155553	-0.00232
λ_{t2}	λ_{t3}	λ_{t4}	λ_{t5}	
0.002479	0.182737	-0.01615	0.083867	

TABLE III. Low-energy model fitting parameters ($\mathcal{E} = 0$).

v_1	v_2	v_+	v_-	k_0 (1/nm)	offset (eV)
2.2300	0.3894	2.8695	1.2899	1.7871	-0.0039

electric fields. For three typical electric fields: (1) When $\mathcal{E} = 0$ or $c_E E_z = 0$, the fitted parameters are given by Table III. (2) When $\mathcal{E} = 1$ or $c_E E_z = 0.103$ eV, the fitted parameters are given by Table IV. (3) When $\mathcal{E} = 2$ or $c_E E_z = 0.206$ eV, the fitted parameters are given by Table V. In Tables III–V, the offset represents a rigid shift of the entire band, and the units for the velocity parameters are 10^5 m/s.

2. Tight-binding Hamiltonian in real space

Because k_y is a good number, we can perform the partial Fourier transform for the k_x , then the corresponding real-space Hamiltonian for $H(\mathbf{k})$ with SOC is

$$\begin{aligned} \bar{H}(k_y) = \sum_m [\hat{\mathbf{c}}_m^\dagger(k_y)(\sigma_0 \otimes H_0(k_y) + H_{\text{SOC},0}(k_y))\hat{\mathbf{c}}_m(k_y) \\ + \hat{\mathbf{c}}_{m+1}^\dagger(k_y)(\sigma_0 \otimes H_x + H_{\text{SOC},x})\hat{\mathbf{c}}_m(k_y) + \text{H.c.}] \end{aligned} \quad (\text{C5})$$

in the basis

$$\begin{aligned} \hat{\mathbf{c}}_m^\dagger = \{c_{m,1,\uparrow}^\dagger, c_{m,2,\uparrow}^\dagger, c_{m,3,\uparrow}^\dagger, c_{m,4,\uparrow}^\dagger, c_{m,1,\downarrow}^\dagger, \\ c_{m,2,\downarrow}^\dagger, c_{m,3,\downarrow}^\dagger, c_{m,4,\downarrow}^\dagger\}. \end{aligned}$$

Here, $\hat{\mathbf{c}}_m^\dagger(k_y)$ is the eight-component spinor creation operator at the m th unit cell along X , with orbitals (1–4) for $(d_{\mathbf{k}M_1}, p_{\mathbf{k}X_3}, d_{\mathbf{k}M_2}, p_{\mathbf{k}X_2})$ and $(\uparrow, \downarrow)$ for the spin index. $H_0(k_y)$ is the 4×4 intracell hopping matrix, H_x is the 4×4 nearest-neighbor hopping matrix along $+X$ ($\Delta m = +1$), $H_{\text{SOC},0}(k_y)$ is the 8×8 intracell onsite SOC matrix, $H_{\text{SOC},x}$ is the 8×8 nearest-neighbor SOC matrix along $+x$ ($\Delta m = +1$).

Specifically, the intracell onsite matrix $H_0(k_y)$ (4×4) is

$$H_0(k_y) = \begin{bmatrix} F_{11} & F_{12} & 0 & F_{14} \\ F_{12}^* & F_{22} & F_{23} & F_{24} \\ 0 & F_{23}^* & F_{11} & F_{12} \\ F_{14}^* & F_{24}^* & F_{12}^* & F_{22} \end{bmatrix}, \quad (\text{C6})$$

with the elements given by (all parameters are real)

$$F_{11} = \mu_d + 2d_1 \cos(k_y b), \quad (\text{C7a})$$

$$F_{22} = \mu_p + 2p_1 \cos(k_y b), \quad (\text{C7b})$$

$$F_{12} = -2it_2 \sin(k_y b), \quad (\text{C7c})$$

$$F_{14} = t_1(1 - e^{iky b}) + t_3(e^{-iky b} - e^{2iky b}), \quad (\text{C7d})$$

$$F_{23} = -F_{14}, \quad (\text{C7e})$$

$$F_{24} = p_3(1 + e^{iky b}). \quad (\text{C7f})$$

TABLE IV. Low-energy model fitting parameters ($\mathcal{E} = 1$).

v_1	v_2	v_+	v_-	k_0 (1/nm)	offset (eV)
2.3436	0.4521	2.7933	1.3635	1.7827	-0.0127

TABLE V. Low-energy model fitting parameters ($\mathcal{E} = 2$).

v_1	v_2	v_+	v_-	k_0 (1/nm)	offset (eV)
2.4203	0.3667	2.7292	1.4754	1.7879	-0.0182

The nearest-neighbor hopping matrix H_x (4×4 , $\Delta m = +1$) is

$$H_x = \begin{bmatrix} d_3 & 0 & 0 & 0 \\ 0 & p_2 & 0 & 0 \\ d_2(1 + e^{-iky b}) & 0 & d_3 & 0 \\ 0 & 0 & 0 & p_2 \end{bmatrix}. \quad (\text{C8})$$

The intracell onsite SOC matrix $H_{\text{SOC},0}(k_y)$ (8×8) is

$$H_{\text{SOC},0}(k_y) = H_{\text{SOC},1} + H_{\text{SOC},2} + H_{\text{SOC},3} + M_{4,\text{onsite}} + M_{5,\text{onsite}}, \quad (\text{C9})$$

where

$$H_{\text{SOC},1} = [(\lambda_{d1}\sigma_z + \lambda_{d2}\sigma_y) \sin(k_y b)] \tau_3 \frac{s_0 + s_3}{2}, \quad (\text{C10a})$$

$$H_{\text{SOC},2} = [(\lambda_{p1}\sigma_z + \lambda_{p2}\sigma_y) \sin(k_y b)] \tau_3 \frac{s_0 - s_3}{2}, \quad (\text{C10b})$$

$$H_{\text{SOC},3} = -i\lambda_{t5}\sigma_y(\tau_1 + i\tau_2) \frac{s_1}{2} - i\lambda_{t5}\sigma_y(\tau_1 + i\tau_2) \frac{s_1}{2} e^{iky b}, \quad (\text{C10c})$$

$$M_{4,\text{onsite}} = -i(\lambda_{t1}\sigma_z + \lambda_{t3}\sigma_y) \frac{(\tau_0 + \tau_3)(s_1 + is_2)}{4}, \quad (\text{C10d})$$

$$M_{5,\text{onsite}} = i(\lambda_{t1}\sigma_z + \lambda_{t3}\sigma_y) \frac{(\tau_0 - \tau_3)(s_1 + is_2)}{4}. \quad (\text{C10e})$$

The nearest-neighbor SOC matrix $H_{\text{SOC},x}$ (8×8 , $\Delta m = +1$) is

$$H_{\text{SOC},x} = M_{4,\text{jump}}^\dagger + M_{5,\text{jump}}, \quad (\text{C11})$$

with

$$M_{4,\text{jump}} = -i(\lambda_{t2}\sigma_z + \lambda_{t4}\sigma_y) \frac{(\tau_0 + \tau_3)(s_1 + is_2)}{4}, \quad (\text{C12a})$$

$$M_{5,\text{jump}} = i(\lambda_{t2}\sigma_z + \lambda_{t4}\sigma_y) \frac{(\tau_0 - \tau_3)(s_1 + is_2)}{4}. \quad (\text{C12b})$$

Given $\bar{H}(k_y)$, the junction potential can be incorporated into the onsite term, irrespective of the junction profile (sharp or smooth). Consequently, the transport properties of the junction can be readily computed using the Kwant software [88].

3. The numerical calculations based on TB model for the tunneling valley Hall effect

Using the numerical calculations based on the TB model, two cases are considered to demonstrate the tunneling valley Hall effect (TVHE), i.e., the case of sharp junctions and the case of smooth junctions.

For the case of sharp junctions, Fig. 11(f) shows the longitudinal conductance σ_{xx} and the valley Hall conductance σ_{xy}^V for three typical electric fields, $\mathcal{E} = 0, 1, 2$. The first row is calculated based on the TB model, while the second row is calculated based on analytical derivations for the low-energy

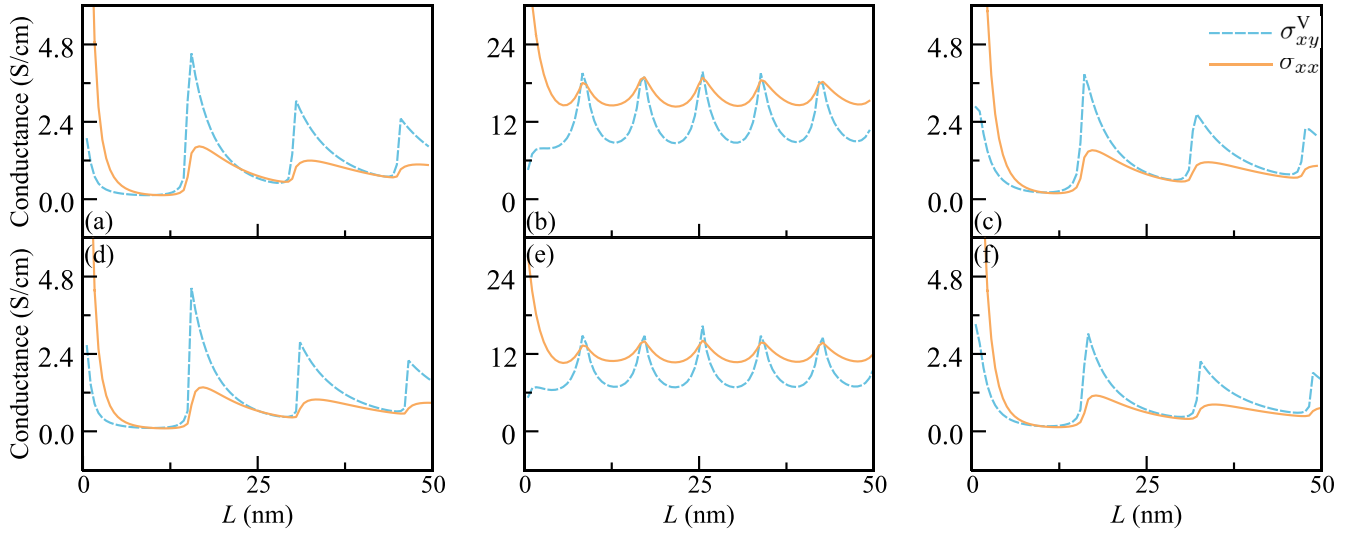


FIG. 11. The valley Hall conductance σ_{xy}^V and longitudinal conductance σ_{xx} . (a)–(c) calculated by using TB model. (d)–(f) calculated by using the low-energy model with the fitting parameters in Tables III–V. Three electric fields are considered: (a), (d) $\mathcal{E} = 0$, (b), (e) $\mathcal{E} = 1$, and (c), (f) $\mathcal{E} = 2$. Here, $E_F = 0$ and $V_0 = 50$ meV.

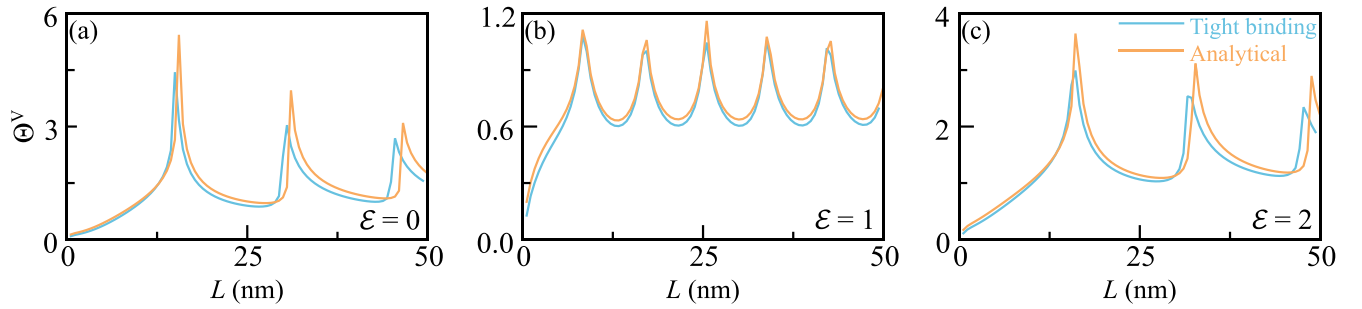


FIG. 12. The valley Hall ratio Θ^V corresponding to Fig. 11. The blue (orange) lines are for TB (low-energy) model.

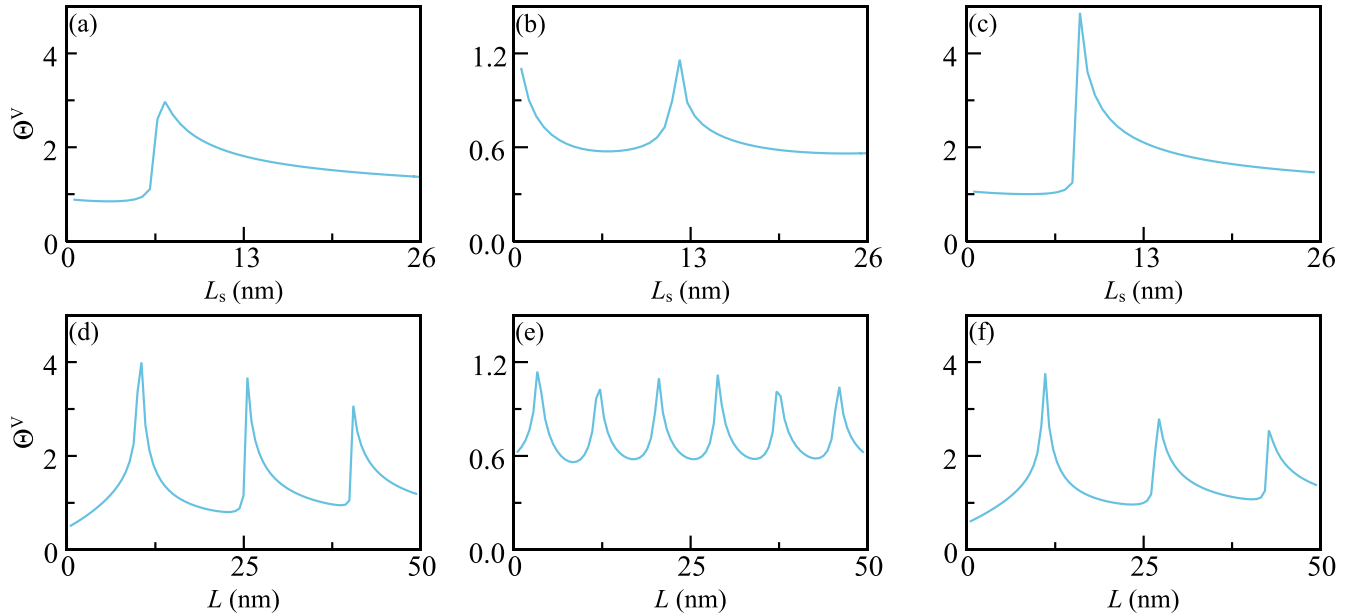


FIG. 13. The valley Hall ratio Θ^V in the smooth junctions. (a)–(c) Θ^V as the function of L_s with the fixing $L = 25$ nm. (d)–(f) Θ^V as the function of L with the fixing $L_s = 5.5$ nm. Three electric fields are considered: (a), (d) $\mathcal{E} = 0$, (b), (e) $\mathcal{E} = 1$, and (c), (f) $\mathcal{E} = 2$. Here, $E_F = 0$ and $V_0 = 50$ meV.

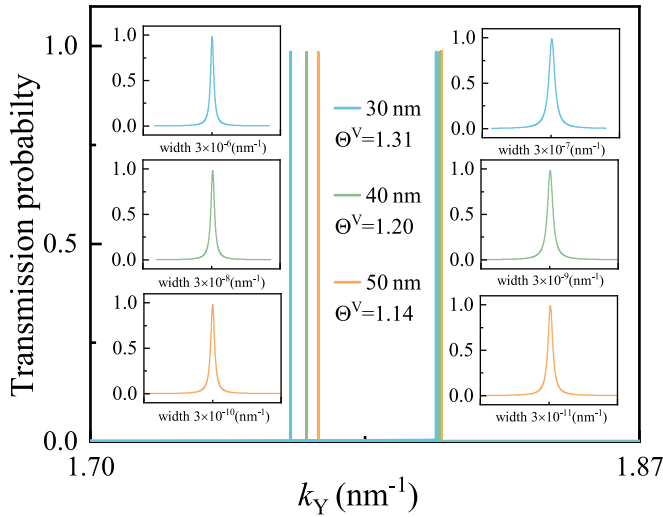


FIG. 14. The transmission and Θ^V in the smooth junction for three different long L_s . Here, $E_F = 0$, $V_0 = 50$ meV, $\mathcal{E} = 0$, and $L = 25$ nm.

model [i.e., Eq. (1)] with the fitting parameters [cf. Tables III–V]. The two calculations agree with each other very well and both show the resonant enhancement of σ_{xx} and σ_{xy}^V , as shown in Fig. 5(a) in the text. Furthermore, the consistency of the two models is verified by Fig. 12, which shows the corresponding valley Hall ratio.

For the case of smooth junctions, the analytical derivations based on the low-energy model are not applicable. Using the TB model, the influence of the smooth regions on the TVHE can be taken into account. In addition to the barrier length L , two linear smooth regions, i.e., one from n to p and the other from p to n with the same length L_s , are considered [cf. Fig. 1(a)]. Figure 13 shows the valley Hall ratio Θ^V in smooth junctions. Θ^V is tunable by L , L_s , and $\mathcal{E}$. On one hand, resonant enhancement always exists. On the other hand, Θ^V can be as large as 100%, which is beneficial for converting the charge current into the valley current. In addition, as L_s increases, Θ^V approaches a constant [cf. the first row of Fig. 13]. This behavior is attributed to the filtering or collimation effect of the smooth junction [89], which leads to very sharp resonant peaks and makes numerical calculations difficult for long L_s [cf. Fig. 14].

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