

All-armchair-edged Xenes and optically controlled enhancement-mode transistor

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Two-dimensional semiconductors are promising candidates for next-generation electronics due to their exceptional electrical, optical, and mechanical properties. However, developing enhancement-mode transistors compatible with current semiconductor technologies remains challenging. Here, we introduce a class of two-dimensional semiconductors—all-armchair-edged Xenes—the band gaps of which can be continuously tuned by adjusting the nanoribbon width or applying uniaxial strain. We demonstrate that a single circularly polarized light field induces different band gap variations for spin-up and spin-down electrons, enabling efficient spin filtering. Tensile strain enhances edge-state interactions, significantly increasing the band gap, especially in wider nanoribbons. Based on these findings, we propose an enhancement-mode field-effect transistor controlled solely by either left- or right-circularly polarized light and connected to topological insulator leads. The transistor's threshold parameters, breakdown voltage, and output characteristics can be tailored by adjusting its channel width. Moreover, by adjusting the intensity and chirality of the light, we can selectively generate spin-up or spin-down currents. Using computer vision techniques, we propose a method to accurately reconstruct an all-armchair-edged lattice structure from scanning tunneling microscopy images.

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I. INTRODUCTION

The latest international roadmap for devices and systems (IRDS) predicts that beyond the 2-nm technology node, two-dimensional (2D) materials will replace silicon as the primary channel materials to sustain the progression of Moore's Law [1]. Group IV Xenes include monolayers of silicon, germanium, tin, and lead [2–4]. First-principles calculations confirm the thermodynamic stability of low-buckled Xenes [5]. This buckling promotes the hybridization of the π and σ orbitals, significantly enhancing spin-orbit coupling (SOC) through the

first-order contribution of the intrinsic atomic SOC [6]. Spin-orbit coupling, combined with time-reversal symmetry, locks the spin direction of edge electrons to their momentum, creating topologically protected states that are resistant to backscattering [7–10]. Topological insulators provide a promising solution to the interconnect bottleneck posed by traditional copper interconnects in CMOS technology, as well as to the thermal dissipation challenges in transistors [11–14]. Among topological materials, Xenes are highly compatible with existing semiconductor technologies, potentially reducing both the manufacturing cost and complexity of novel devices [15,16].

Silicene, germanene, stanene, and plumbene have been successfully epitaxially grown on various metallic (111)-terminated surfaces (such as Ag [17–19], Ir [20,21], Pt [22], Au [23], Al [24], Sb [25], Cu [26], $\text{Pd}_{1-x}\text{Pb}_x$ [27]) and nonmetallic substrates (such as ZrB_2 [28], MoS_2 [29,30], Ge [31], Bi_2Te_3 [32], PbTe [33], InSb [34]). Although these experimentally fabricated Xenes undergo various periodic reconstructions due to substrate coupling

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and band hybridization, experimental results have partially confirmed theoretical predictions about their structures and associated properties. Experimental observations have revealed density of states peaks attributed to edge states in silicene [35]. In 2023, quantum spin Hall states and topological phase transitions essential for realizing the topological transistor were observed [36]. Recent experiments have demonstrated Floquet-Bloch band engineering and related electron transport phenomena induced by polarized light in various solid-state materials [37–39].

Field-effect transistors (FETs) are essential in modern electronic devices and are classified as either depletion-mode or enhancement-mode transistors, depending on whether they are in the ON or OFF state without a gate-controlled field [40–42]. This distinction makes each type particularly suitable for specific applications in electronic circuits. Enhancement-mode FETs, which remain cutoff at zero gate voltage, are commonly utilized as switching elements in integrated circuits, whereas depletion-mode FETs serve as load resistors in logic circuits.

Recently, depletion-mode FETs based on zigzag-edged Xenes have garnered considerable research interest [43–50]. The OFF state of a depletion-mode FET is established through two key mechanisms: (1) the opening of a band gap via the breaking of inversion symmetry or time-reversal symmetry, and (2) the creation of a band mismatch resulting from topological phase transitions induced by external fields. Leveraging the first mechanism, a silicene field-effect transistor that operates at room temperature has been successfully fabricated [51]. However, current theoretical and experimental research on enhancement-mode Xene FETs remains scarce. The primary challenges are that (1) pristine armchair Xene, featuring both armchair and zigzag edges, exhibits alternating metallic and insulating states that vary with the width; and (2) the staggered potential induced by the vertical electric field cannot reduce the band gap of armchair Xene, hindering the formation of conductive channels in the ON state.

Herein, we propose an all-armchair-edged Xene structure, where all four edges exhibit armchair configurations [see Fig. 1(a)]. Our analysis shows that the band gap of this structure increases steadily as the ribbon width decreases. Using a tight-binding model, we explore the effects of uniaxial strain on hopping energies, effective spin-orbit coupling, and the band gap. We also apply the Green function method to study the impact of circularly polarized light fields on spin transport properties. Building on these findings, we propose an enhancement-mode transistor controlled by a single circularly polarized light field, and discuss potential experimental methods for its realization. Our results offer a promising approach for designing enhancement-mode transistors based on Xenes, potentially advancing the development of next-generation electronic devices.

II. MODEL AND METHODS

A. Tight-binding model for uniaxially strained Xenes

The Hamiltonian of all armchair-edged Xene, considering the effects of weak uniaxial strain along different directions, can be expressed as follows [52,53]:

$$H = - \sum_{\langle ij \rangle \sigma} t_n(R_n) c_{i\sigma}^\dagger c_{j\sigma} + \frac{i\lambda_{\text{SO}}(R_n)}{3\sqrt{3}} \sum_{\langle\langle ij \rangle\rangle \sigma \bar{\sigma}} v_{ij} c_{i\sigma}^\dagger S_{\sigma \bar{\sigma}}^z c_{j\bar{\sigma}} + \frac{i\lambda_{\Omega}}{3\sqrt{3}} \sum_{\langle\langle ij \rangle\rangle \sigma \bar{\sigma}} v_{ij} c_{i\sigma}^\dagger c_{j\bar{\sigma}}. \quad (1)$$

Here, the operators $c_{i\sigma}^\dagger$ and $c_{j\sigma}$ denote the creation and annihilation operators for electrons with spin σ at the i th and j th sites. The summations $\sum_{\langle ij \rangle}$ and $\sum_{\langle\langle ij \rangle\rangle}$ represent interactions over nearest-neighbor and next-nearest-neighbor sites. The first term describes electron hopping between nearest-neighbor atoms, characterized by the transfer energy $t_n(R_n) = t_0 (1 - \beta(\delta R_n/R_n^0))$ [54–57], where t_0 and $\beta = (\partial \ln t_n / \partial \ln R_n)|_{R_n=R_n^0}$ are the hopping energy without strain and the Grüneisen parameter, respectively, and the quantity $\delta R_n = R_n - R_n^0$ with $R_n^0 = |\vec{R}_n^0|$ represents the change in bond length due to deformation. As shown in Fig. 1(a), in the absence of strain, the bond vectors between an arbitrary atom and its three nearest neighbors can be expressed as $\vec{R}_1 = a(\frac{\sqrt{3}}{2}, \frac{1}{2}, \cot \phi)$, $\vec{R}_2 = a(-\frac{\sqrt{3}}{2}, \frac{1}{2}, \cot \phi)$, and $\vec{R}_3 = a(0, -1, \cot \phi)$, with lattice constant a . Under uniaxial strain, the deformed vectors are obtained via $\vec{R}_n = (1 + \vec{\epsilon})\vec{R}_n^0$. The strain tensor in the lattice coordinate system is given by

$$\vec{\epsilon} = \epsilon \begin{bmatrix} \cos^2 \theta - v_{\parallel} \sin^2 \theta & (1 + v_{\parallel}) \sin \theta \cos \theta & 0 \\ (1 + v_{\parallel}) \sin \theta \cos \theta & \sin^2 \theta - v_{\parallel} \cos^2 \theta & 0 \\ 0 & 0 & -v_{\perp} \end{bmatrix}. \quad (2)$$

Here, ϵ denotes the magnitude of the strain, and θ is the angle between the applied strain and the x axis, as shown in Fig. 2(a). The in-plane Poisson ratio, $v_{\parallel}$, and the out-of-plane Poisson ratio, $v_{\perp}$, characterize the material's deformation within and perpendicular to the plane.

B. Effective spin-orbit coupling with strain effects

The second term in Eq. (1) describes the effect of effective SOC on next-nearest-neighbor electron hopping, where v_{ij} represents the position-dependent Haldane phase factor, and S^z denotes the z component of the Pauli matrix. The effective SOC, λ_{SO} , is related to the intrinsic SOC strength, ξ_0 ; the energy difference, Ω , between s and p orbitals; and the hopping integrals between these orbitals, namely, Slater-Koster parameters $V_{ss\sigma}$, $V_{sp\sigma}$, $V_{pp\sigma}$, and $V_{pp\pi}$. Additionally, it is influenced by the orientation angle,

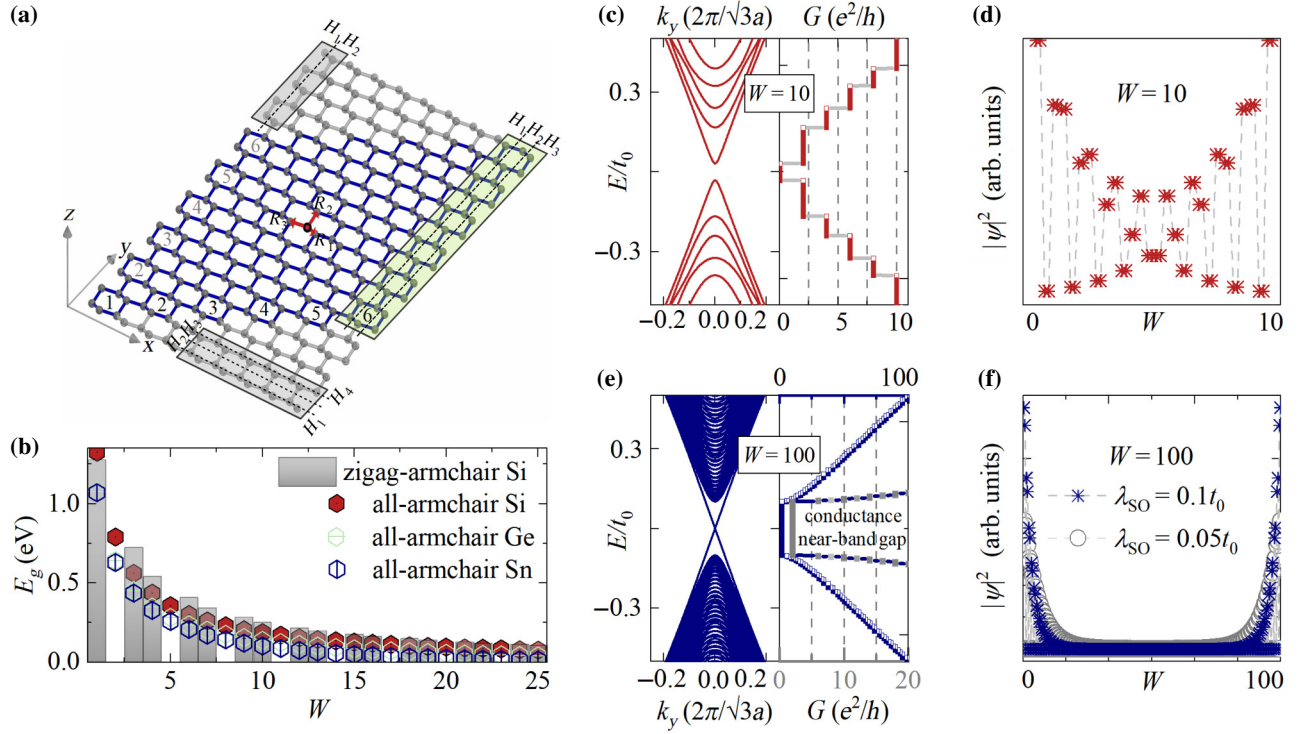


FIG. 1. (a) Three-dimensional schematic of an all-armchair-edged Xene with a width of $W = 6$. Gray bonds indicate the atoms removed, and the green-highlighted region represents the unit cell. (b) Band gap magnitude, E_g , as a function of nanoribbon width, W . Column chart represents zigzag-armchair-edged silicene, while the scatter plot represents all-armchair-edged silicene, germanene, and stanene. Electronic band structure and conductance as functions of electron energy, E , for all-armchair-edged Xene nanoribbons with widths (c) $W = 10$ and (e) $W = 100$. Squared wave function of states near the Fermi level for ribbon widths (d) $W = 10$ and (f) $W = 100$. Electron energy is expressed in units of nearest-neighbor hopping energy, t_0 , with the spin-orbit coupling strength set to $\lambda_{SO} = 0.1t_0$.

ϕ , between the atomic bond and the z axis. The relationship is expressed as follows [58]:

$$\lambda_{SO} = \frac{\xi_0}{9} \Omega^2 \left(\frac{V_{pp\pi} - V_{pp\sigma}}{V_{sp\sigma}^4} \right)^2 \times \frac{\cot^2 \phi}{1 + \cos^2 \phi \left(\frac{V_{pp\pi} - V_{pp\sigma}}{V_{sp\sigma}} \right)^2 \left(1 + \frac{9}{4} \sin^2 \left(\frac{\Omega}{V_{sp\sigma}} \right) \right)}. \quad (3)$$

For low-buckled silicene, germanene, and stanene, the values of ϕ are found to be 101.7° , 106.5° , and 107.1° , respectively. It is noteworthy that the application of tension strain can reduce the ϕ angle. When the strain reaches an intensity of $\varepsilon = 1/\nu_\perp$, the buckled structure transitions to a planar configuration. Under weak strain ($\varepsilon \ll 1$), since $\cot^2 \phi \approx \cos^2 \phi \ll 1$, and considering the effects of strain on the orientation angle and hopping integrals, Ω^2 in Eq. (3) is replaced with $\Omega^2 \left[1 + 2\beta \left(\frac{1}{3} \sum_{n=1}^3 \delta R_n / R_0 \right) \right] / R_n^0$ and $\cot^2 \phi$ in Eq. (3) is replaced with $\cot^2 \phi ((1 - \nu_\perp \varepsilon) / (1 + \varepsilon))^2$. This yields the

relationship for the effective spin-orbit coupling strength, $\lambda_{SO}(R_n)$, as a function of strain.

C. Next-nearest-neighbor interactions induced by circularly polarized light

The third term in Eq. (1) arises from the Haldane interaction induced by off-resonant circularly polarized light [59–61]. In hexagonal lattice systems, such light introduces an additional phase factor, $e^{iA_{ij}(t)}$, affecting the electron hopping energy, t , between lattice sites. This phase, given by $A_{ij}(t) = (e/\hbar)(\mathbf{r}_i - \mathbf{r}_j) \cdot \mathbf{A}(t)$, depends on the electron's path and the electromagnetic potential, $\mathbf{A}(t) = [\pm A \sin(\Omega t), A \cos(\Omega t)]$. Here, A denotes the amplitude of the electromagnetic potential, while Ω represents the frequency of the light field. The positive sign corresponds to right circularly polarized light, whereas the negative sign indicates left circularly polarized light, reflecting their respective angular momentum quantum numbers. Under the off-resonant condition, $\hbar\Omega \gg t_0$, where the high-frequency approximation is valid, and for $\Lambda^2 \ll 1$, where the Bessel function rapidly converges and higher-order

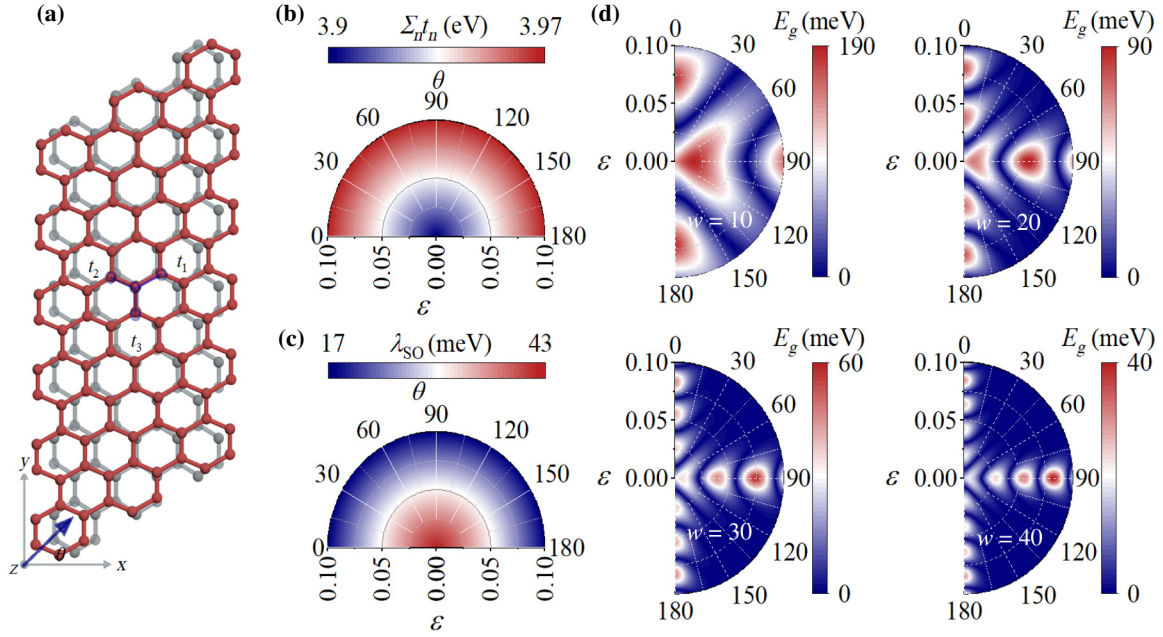


FIG. 2. (a) Top-view comparison of uniaxially strained (red) and unstrained (gray) all-armchair-edged Xene. Applied tension, indicated by the blue arrow, forms an angle of $\theta = \pi/4$ with the x axis. (b) Total hopping energy, $\sum_n t_n$, and (c) effective spin-orbit coupling, λ_{SO} , as functions of strain direction, θ , and strain strength, ε . (d) Variation of the band gap, E_g , with strain direction, θ , and magnitude, ε , for all-armchair-edged Xene with widths $W = 10, 20, 30$, and 40 .

terms are negligible, the approximate effective Hamiltonian can be expressed as the next-nearest-neighbor interaction in Eq. (1). For left-handed circularly polarized light, the light parameter, λ_Ω , is given by $\lambda_\Omega \propto -\Lambda^2/\Omega < 0$, while for right-handed light, $\lambda_\Omega \propto +\Lambda^2/\Omega > 0$, where the light intensity is characterized by $\Lambda = eaA/\hbar$.

D. Spin-dependent electron transport

The spin-dependent current through all armchair-edged Xene can be expressed in the form of the Landauer-Büttiker formula as [62,63]

$$I_\sigma = \frac{e}{h} \int T_\sigma(E) [f_L(E) - f_R(E)] dE. \quad (4)$$

Here, $f_\alpha(E) = [e^{(E-\mu_\alpha)/k_B T} + 1]^{-1}$ represents the Fermi-Dirac distribution function for the left ($\alpha = L$) and right ($\alpha = R$) leads, where T is the equilibrium temperature and μ_α is the electrochemical potential. The chemical potentials of the leads can be adjusted by the applied bias voltage, V_{bias} , leading to $\mu_L = -\mu_R = eV_{\text{bias}}/2$.

By employing the Green function technique, the spin-dependent electron transmission coefficient, $T_\sigma(E)$, is given by [64–67]

$$T_\sigma(E) = \text{Tr}[\Gamma_{L\sigma} \mathbf{G}_\sigma^r(E) \Gamma_{R\sigma} [\mathbf{G}_\sigma^r(E)]^\dagger]^{-1}. \quad (5)$$

Here, $\mathbf{G}_\sigma^r(E)$ represents the retarded Green function of the entire system, while $\Gamma_{L\sigma}$ and $\Gamma_{R\sigma}$ are the linewidth functions that characterize the coupling between the central

scattering region and the left or right leads. The retarded Green function is defined as $\mathbf{G}_\sigma^r(E) = [E\mathbf{I} - \mathbf{H}_0 - \Sigma_{L\sigma}^r - \Sigma_{R\sigma}^r]^{-1}$. Additionally, the linewidth function, $\Gamma_{L\sigma}$, can be expressed as $\Gamma_{L\sigma} = i(\Sigma_{L\sigma}^r - [\Sigma_{L\sigma}^r]^\dagger)$. In this context, the Hamiltonian matrix of the central scattering region, $\mathbf{H}_0$, can be constructed based on Eq. (1) and the unit cell shown in Fig. 1(a). The self-energy function describing the coupling between the leads and the central region are given by $\Sigma_{\alpha\sigma}^r(E) = \mathbf{H}_\alpha \mathbf{g}_{\alpha\sigma}^r(E) \mathbf{H}_\alpha^\dagger$, where the surface Green function, $\mathbf{g}_{\alpha\sigma}^r(E)$, can be obtained using the transfer matrix method [68] or the Green function method [69]. Based on the calculated current, the linear conductance, G , can be determined by $G = \lim_{\Delta V \rightarrow 0} \Delta I / \Delta V$. The spin polarization of the electrons is defined as $P = (I_\uparrow - I_\downarrow) / (I_\uparrow + I_\downarrow) = (G_\uparrow - G_\downarrow) / (G_\uparrow + G_\downarrow)$, where $I_\uparrow$ and $I_\downarrow$ (or $G_\uparrow$ and $G_\downarrow$) represent the currents (or conductances) for spin-up and spin-down electrons, respectively.

In the theoretical calculations of transport properties and band structure under the influence of light fields, the off-resonant light field is treated as a periodically driven perturbation. This perturbation modifies the band structure through virtual photon absorption processes, which, in turn, alters the system's Hamiltonian and impacts the transport properties [60,61]. Additionally, when applying the Landauer-Büttiker formalism, the effect of the bias is incorporated into the Fermi distribution function, whereas the light field's effects are captured by adjusting the effective Hamiltonian. As a result, a self-consistent treatment of both the bias and the light field is not considered.

III. RESULTS AND DISCUSSION

A. 2D semiconductor with a width-tunable band gap

For Xenes with both zigzag and armchair edges, calculations based on tight-binding models or the $\mathbf{k} \cdot \mathbf{p}$ approximation indicate that the band structure along the armchair edge alternates between metallic and insulating states, depending on the nanoribbon width [Fig. 1(b), column chart]. By selectively removing atoms at approximately 30° to the zigzag edge [indicated by the region with gray bonds in Fig. 1(a)], a Xene sheet with four armchair edges is formed. The boundary conditions for all-armchair-edged Xenes differ from those of zigzag-armchair-edged Xenes, as shown in the rectangular areas of Fig. 1(a). In the zigzag-armchair-edged system, the Hamiltonian matrix for the unit cell is divided into an even number of submatrices, whereas the all-armchair-edged system's Hamiltonian matrix decomposes into an odd number of $2W$ -dimensional submatrices ($H_{\text{cell}} = H_1 \oplus H_2 \oplus H_3$).

The band gap of all-armchair-edged Xenes does not show periodic oscillation. Instead, as illustrated by the scatter plot in Fig. 1(b), these systems behave as two-dimensional semiconductors with a quasicontinuously tunable band gap. The band gap is inversely proportional to both the nanoribbon width, W , and the effective spin-orbit coupling strength, λ_{SO} . For narrow systems, the band gap reaches several hundred meV [Figs. 1(b), 1(c)]. Narrow all-armchair Xenes exhibit semiconductorlike behavior in both their band structure and conductance. In contrast, wider systems [Fig. 1(e)] show a closed band gap, with the conductance of all-armchair Xene nanoribbons displaying a series of nonzero quantized values, $4(e^2/h)(W + 1/2)$.

In all armchair-edged Xenes, the band gap does not arise from the breaking of inversion symmetry, unlike other two-dimensional materials, such as hexagonal boron nitride (*h*-BN), black phosphorus, and transition metal dichalcogenides. The Hamiltonian matrix, H_{cell} , for this structure, detailed in Eq. (1) and Fig. 1(a), remains invariant under the inversion operation, $UH_{\text{cell}}U^{-1} = H_{\text{cell}}$, which interchanges the diagonal elements of H_{cell} while preserving the off-diagonal hopping terms. The formation of the band gap in all armchair-edged Xenes is mainly determined by the spatial distribution of electronic states, which varies monotonically with the nanoribbon width.

Figures 1(d) and 1(f) display the squared wave functions of states near the Fermi level for nanoribbons with widths $W = 10$ and $W = 100$, respectively. In wider all-armchair-edged Xene nanoribbons [$W = 100$, Fig. 1(f)], electronic states are uniformly distributed, enabling free electron movement and resulting in metallic behavior. Conversely, in narrower nanoribbons [$W = 10$, Fig. 1(d)], electron states are unevenly distributed with significant real-space wave function overlap, which leads to band gap formation. Additionally, under identical size conditions, systems with lower effective spin-orbit coupling,

λ_{SO} , exhibit increased wave function overlap, as indicated by the gray lines in Fig. 1(f). Consequently, all-armchair silicene exhibits a larger band gap compared to germanene and stanene.

B. Effects of uniaxial strain on the electronic band structure

The low-buckled hexagonal lattice structure of Xenes makes them highly sensitive to interface strain, which arises from lattice mismatch or differences in thermal expansion coefficients between the substrate and the two-dimensional material. In the tight-binding approximation, the electronic band structure is primarily determined by the hopping energy, t_n , and the effective spin-orbit coupling, λ_{SO} . As illustrated in Fig. 2(a), applying uniaxial strain alters both the degree of buckling and the bond lengths between lattice sites. Moreover, Eqs. (2) and (3) demonstrate that both t_n and λ_{SO} are dependent on the strain direction, θ , and the strength, ε . Therefore, by adjusting the magnitude and direction of the strain, one can effectively modulate the electronic structure and transport properties of all-armchair-edged Xenes.

Figure 2(b) illustrates that the total hopping energy, $\sum_n t_n = t_1 + t_2 + t_3$, depends monotonically on the applied uniaxial strain, ε , for any strain direction, θ . Specifically, for $\varepsilon > 0$, the total hopping energy exceeds $3t_0$, whereas for $\varepsilon < 0$, it is less than $3t_0$. In contrast, the individual hopping parameters, t_n , vary nonuniformly with both strain strength, ε , and direction, θ . Under tensile strain, for $\theta \in (0, \pi/2)$, t_1 is smaller than t_2 , while for $\theta \in (\pi/2, \pi)$, t_1 is larger than t_2 . The condition $t_1 = t_2$ is achieved only at $\theta = 0$, $\theta = \pi/2$, and $\theta = \pi$. To maximize the band gap, it is essential to ensure that $t_1 = t_2 > t_3$. Therefore, when the strain direction is aligned with $\theta = 0$, $\pi/2$, or π , and the strain intensity, ε , is appropriately adjusted, the band gap of all-armchair-edged Xene nanoribbons can be significantly increased. As illustrated in Fig. 2(d), applying strain in the direction of $\theta = \pi/2$, the maximum band gaps for germanene nanoribbons with widths $W = 10, 20, 30$, and 40 are 186, 92, 58, and 40 meV, respectively. This application of strain results in increases of approximately 35%, 62%, 102%, and 160% in the band gaps.

Xenes possess noncoplanar lattice structures, and the bond angle, ϕ , between atomic bonds and the vertical axis decreases under tensile strain. For example, freestanding germanene initially has a bond angle of $\theta = 106.5^\circ$. When the strain reaches $\varepsilon \approx 0.2$, ϕ decreases to 90° , triggering a structural transition from a low-buckled to a planar configuration. According to Eq. (3), the effective SOC strength is angle dependent. A decreasing ϕ causes the p_z^A orbitals to become orthogonal to the p_x^B and p_y^B orbitals. Therefore, as illustrated in Fig. 2(c), tensile strain leads to a reduction in the effective SOC strength of Xenes.

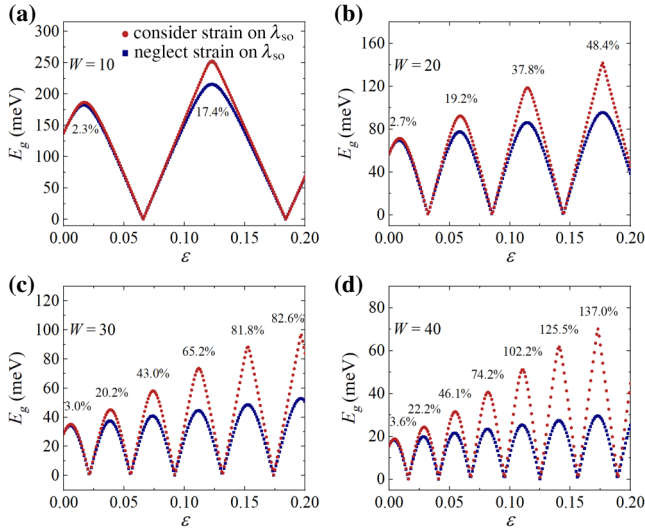


FIG. 3. Band gap, E_g , as a function of strain magnitude, ε , for all armchair-edged Xene with widths (a) $W = 10$, (b) $W = 20$, (c) $W = 30$, and (d) $W = 40$ at a strain direction of $\theta = 0.5\pi$. Red dotted lines account for the effect of strain on the effective spin-orbit coupling, λ_{SO} , while the blue lines do not take this effect into consideration.

From the analysis presented in Fig. 1, we observe that a reduction in spin-orbit coupling strengthens edge-state interactions, leading to an increased band gap. Consequently, as illustrated in Figs. 3(a)–3(d), the influence of strain on spin-orbit coupling significantly increases the band gap. This phenomenon is more pronounced in wider nanoribbons. For example, within the strain range $0 < \varepsilon < 0.2$, the band gap of nanoribbons with width $W = 10$ increases by approximately 17.4% compared to cases neglecting strain-induced spin-orbit coupling. For $W = 40$, the increase is around 137%. Notably, for wider nanoribbons, even at lower strain levels, accounting for strain's effect on spin-orbit coupling results in a significant band gap increase. The band gap enlargement caused by variations in spin-orbit coupling strength approaches the influence of hopping energy. This highlights the importance of considering strain's impact on spin-orbit coupling, particularly for wider nanoribbons.

C. Spin filtering induced by single circularly polarized light

The electron band structure can be effectively modified through virtual photon absorption when subjected to circularly polarized light, provided the off-resonant condition, $\hbar\Omega \gg t_0$, is met. Under these conditions, the overlap integral of the wave functions at the armchair edges is proportional to $e^{-W|\sigma\lambda_{SO}-\lambda_{\Omega}|}$. Additionally, for left-circularly polarized light, $\lambda_{\Omega} < 0$, whereas for right-circularly polarized light, $\lambda_{\Omega} > 0$. Consequently, when right-handed (left-handed) light is applied, the overlap integral for spin-down

(spin-up) electron states continuously decreases. In contrast, the overlap integral for spin-up (spin-down) electron states initially increases, reaches a maximum when $\lambda_{SO} = \lambda_{\Omega}$, then slightly decreases back to its initial value when $\lambda_{SO} = 2\lambda_{\Omega}$, and subsequently continues to decrease. This asynchronous modulation of the coupling strength of edge states allows circularly polarized light with specific angular momentum to selectively control the band structure of spin-up or spin-down electrons. Figures 4(a)–4(c) illustrate the energy bands and conductance for spin-up and spin-down electrons under varying intensities of right circularly polarized light. As shown in Fig. 4(a), within the intensity range $\lambda_{\Omega} < \lambda_{SO}$, the coupling of edge states for spin-up electrons is enhanced, causing a continuous increase in the band gap. Conversely, the coupling for spin-down electrons diminishes, leading to a monotonic decrease in the band gap [Fig. 4(b)]. This disparity induces a significant splitting between the energy bands of the two spin orientations, resulting in distinct spin-up and spin-down conductance plateaus [Fig. 4(c)]. Notably, to emphasize the light-field effect, the conductance in Fig. 4(c) was calculated under uniform circularly polarized light across both the source and drain electrodes and the central scattering region.

Based on the above analysis, as shown in Fig. 4(d), the application of either left-handed or right-handed circularly polarized light enables all-armchair Xenes to selectively filter spin-up or spin-down electrons, achieving complete (100%) spin polarization. Importantly, this complete spin polarization occurs without requiring external electric or magnetic fields. Additionally, the band gap of all-armchair Xenes can be adjusted by changing the nanoribbon width, providing precise control over the energy window for light-induced spin filtering. Analysis of the three plots in Fig. 4(d) indicates that the energy range for 100% spin polarization ($P = 1$) varies significantly with the ribbon width, W . In narrower nanoribbons, the band gap near the Fermi level remains pronounced, even under high-intensity light. Conversely, increasing the ribbon width under the same lighting conditions reduces the band gap, facilitating complete spin polarization at the Fermi level.

Figure 5 demonstrates the impact of uniaxial strain on spin polarization, P , in nanoribbons of varying widths W . As shown in Fig. 4(d), in the absence of tensile strain ($\varepsilon = 0$), light-induced spin splitting reaches its maximum when $\lambda_{\Omega} = \lambda_{SO}$. Beyond this point, increasing the light field does not further expand the energy range for spin filtering. However, the application of uniaxial strain alters the strength of spin-orbit coupling and wave function overlap, significantly widening the energy window for spin filtering. As indicated in the blue regions of Figs. 5(a)–5(d), for nanoribbons with widths of $W = 10, 20, 30$, and 40 , an appropriate strain nearly doubles the energy window that supports 100% spin filtering.

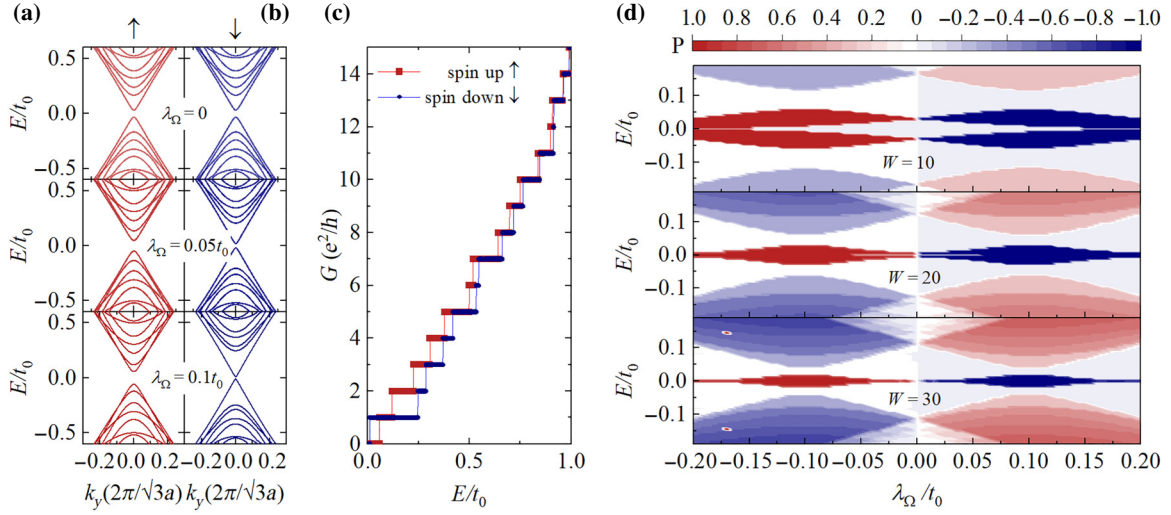


FIG. 4. (a) Band structures of spin-up electrons in all-armchair-edged Xene at various light field intensities: $\lambda_\Omega = 0$, $\lambda_\Omega = 0.05t_0$, and $\lambda_\Omega = 0.1t_0$. (b) Corresponding band structures for spin-down electrons at $\lambda_\Omega = 0$, $\lambda_\Omega = 0.05t_0$, and $\lambda_\Omega = 0.1t_0$. (c) Conductance, G , as a function of electron energy, E , for all-armchair-edged Xene with $\lambda_\Omega = 0.1t_0$. (d) Spin polarization, P , of all-armchair-edged Xene nanoribbons as functions of circularly polarized light field strength, λ_Ω , and electron energy, E , for ribbon widths of $W = 10, 20$, and 30 . Regions where $\lambda_\Omega < 0$ and $\lambda_\Omega > 0$ correspond to left-handed and right-handed circularly polarized light, respectively. Electron energy is expressed in units of the nearest-neighbor hopping energy, t_0 , with the spin-orbit coupling strength set to $\lambda_{SO} = 0.1t_0$.

D. Enhancement-mode transistor controlled by a single light field

We propose an enhancement-mode transistor controlled solely by a light field. As shown in Fig. 6(a), the device channel consists of all-armchair-edged germanene (high-lighted area), while the left and right electrodes are coupled with zigzag-edged germanene, which exhibit edge states. The operational mechanism of the all-armchair-edged

germanene-based transistor is as follows: in the absence of light, the intrinsic band gap inhibits electron transport, thus maintaining the transistor in the OFF state. The ON state is achieved by applying a light field that reduces the band gaps of either spin-up or spin-down electrons, facilitating the formation of a conductive channel.

The source-drain voltage in integrated circuit transistors is selected based on variations in manufacturing processes, design specifications, and operating conditions. For example, low-power FETs employed in mobile devices and other energy-efficient applications typically utilize source-drain voltages on the order of tens of millivolts. In contrast, high-performance processors and graphics processing units typically operate with source-drain voltages in the range of hundreds of millivolts. By adjusting the channel width, the band gap of all-armchair Xenenes can be tuned, thereby allowing the customization of the transistor's operating voltage, output characteristics, and transfer properties to meet specific application requirements.

Figures 6(b) and 6(c) display the drain output current for optically controlled transistors with channel widths of $W = 10$ and $W = 20$, respectively, under varying source-drain voltages and input optical field intensities. The comparison indicates that channel width variations significantly affect the transistor's optical response. In narrow-channel transistors [Fig. 6(b)], an increased band gap markedly enhances breakdown voltage and thermal stability. When the optical field intensity exceeds the threshold—defined as the light intensity required to form a conductive channel between source and drain, thereby switching the transistor from the cutoff to the conducting

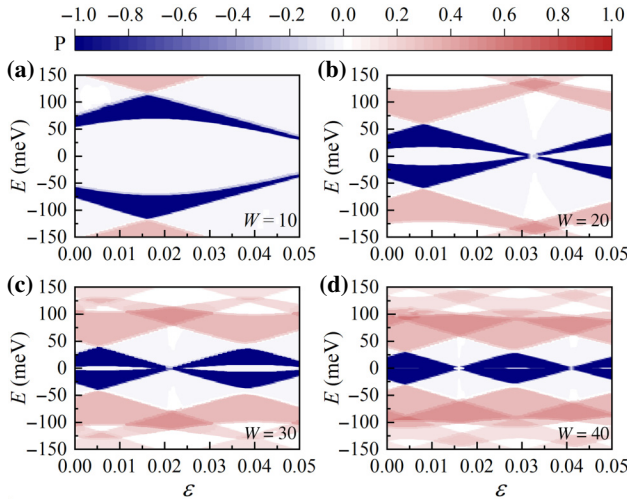


FIG. 5. Spin polarization, P , as functions of strain strength, ε , and electron energy, E , for all armchair-edged germanene nanoribbons with widths of (a) $W = 10$, (b) $W = 20$, (c) $W = 30$, and (d) $W = 40$. Light field intensity is set to $\lambda_\Omega = \lambda_{SO}$ and the strain direction is $\theta = 0.5\pi$.

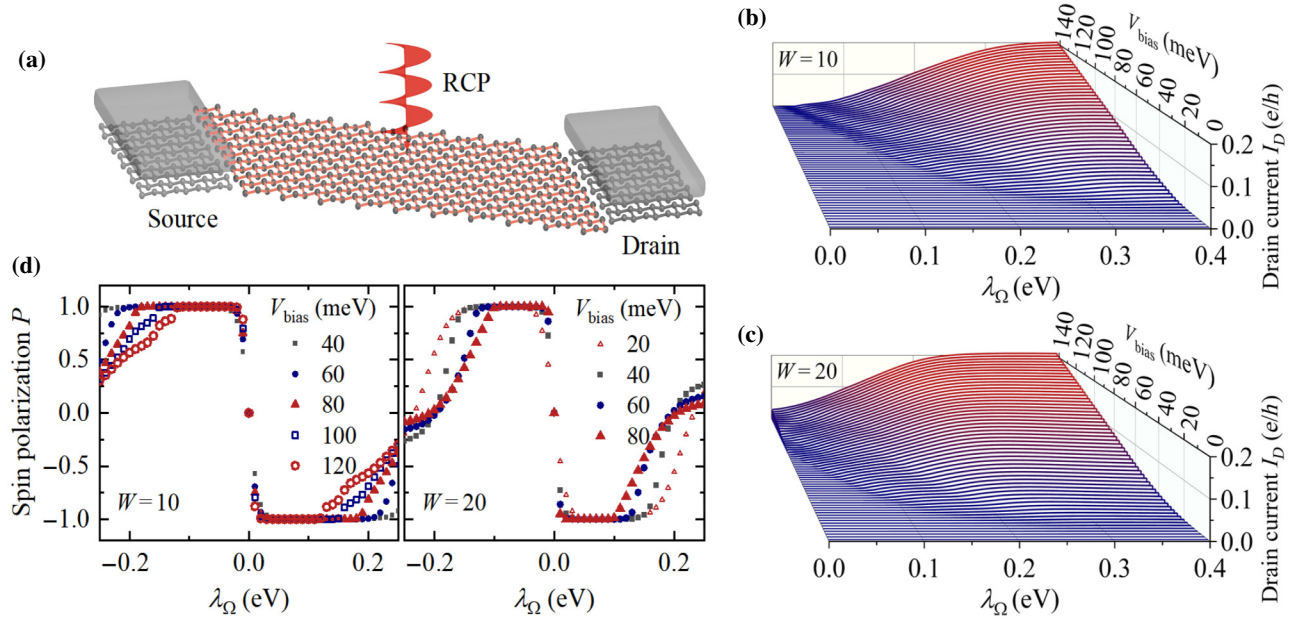


FIG. 6. (a) Schematic of the single optical-field-controlled transistor. Red region indicates the all-armchair-edged germanene channel illuminated by right-handed circularly polarized (RCP) light, while the gray region represents the zigzag-edged electrodes. Variation of the output current, I , with light field intensity, λ_Ω , for channel widths of (b) $W = 10$ and (c) $W = 20$, with a bias voltage, V_{bias} , ranging from 0 to 140 meV. (d) Spin polarization, P , as a function of λ_Ω for channel widths of $W = 10$ and $W = 20$, respectively, under varying bias voltages, V_{bias} .

state—the output current shows an approximately linear relationship with source-drain voltage over a broad spectrum of optical intensities. Conversely, the wide-channel transistor [Fig. 6(c)] requires a lower optical field intensity to position the conduction band within the bias window, which results in a significantly reduced threshold optical parameter.

When the optical field parameter satisfies $\lambda_\Omega > (E_g - \mu)/2$, the optical energy is sufficient to close the electronic band gap, causing the drain current to saturate and become independent of further increases in optical field intensity. Furthermore, the all-armchair-edged Xene phototransistor demonstrates the capability to generate and control spin-polarized currents. As illustrated in Fig. 6(d), unlike conventional transistors, the all-armchair-edged Xene transistor can output either a fully spin-polarized current ($P = 1$) or a nonpolarized charge current ($P = 0$), only depending on the optical field parameter, λ_Ω .

Although a ballistic transport model was employed to illustrate the system's behavior under ideal conditions, phonon scattering significantly influenced the I - V characteristics. When electron-phonon interactions are incorporated, two modifications to the Hamiltonian are required. First, phase factors, $e^{-(\lambda_q/\omega_q)^2}$, associated with the phonon frequency, ω_q , and electron-phonon coupling, λ_q , must be introduced into the nearest- and next-nearest-neighbor terms. Second, the on-site energy at each lattice site must be renormalized by subtracting λ_q^2/ω_q . Consequently,

phonon scattering primarily reduces electron transmission, leading to a decrease in the drain current. Nonetheless, the light-induced switching effect modulated by the single optical field remains operative under these conditions.

E. Computer vision-based extraction of lattice structures from STM images

(1) **Image processing:** Convert the original scanning tunneling microscopy (STM) image into grayscale to reduce computational complexity and emphasize essential details. Apply the contrast limited adaptive histogram equalization algorithm to enhance local contrast and suppress noise by equalizing small image blocks. Binarize the enhanced grayscale image to highlight key features, facilitating accurate feature extraction and target recognition. Figure 7(a) displays the processed silicene STM image.

(2) **Contour extraction and centroid calculation:** Detect continuous foreground or background areas [black regions in Fig. 7(a)] in the binarized images to construct contours based on point connectivity. Identify contours within the lattice regions, as highlighted by blue boxes in Fig. 7(b). Compute spatial moments $M_{pq} = \sum_x \sum_y x^p y^q f(x, y)$, where $f(x, y)$ represents the pixel value at point (x, y) and p and q denote moment orders. For binary images, set $f(x, y) = 1$ for foreground pixels and $f(x, y) = 0$ for background pixels. Calculate the centroid coordinates (c_x, c_y) using $c_x = M_{10}/M_{00}$ and $c_y =$

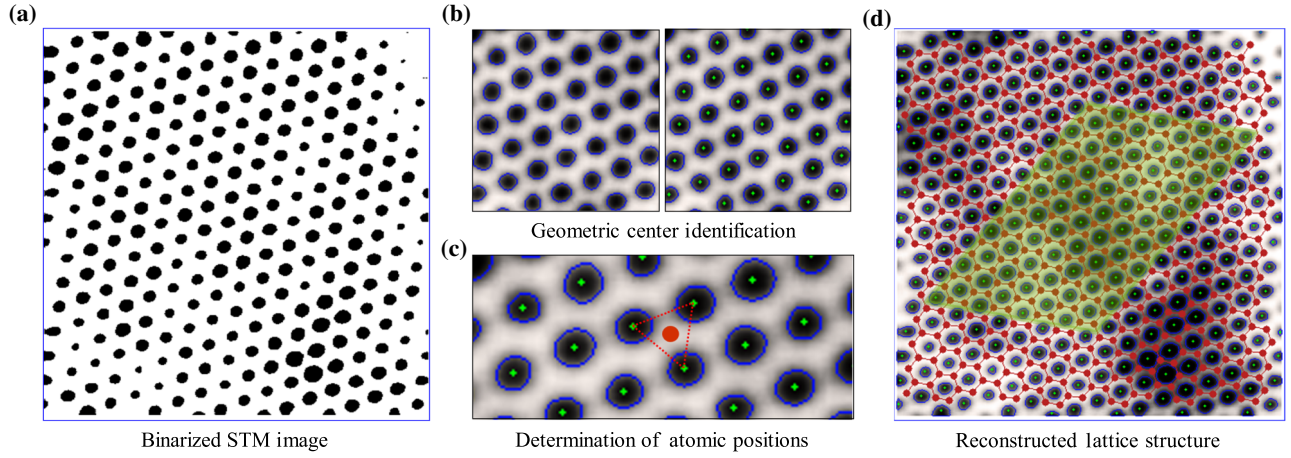


FIG. 7. (a) Binarized STM image of Xene (10 nm $\times$ 10 nm), where black regions denote background areas. (b) Geometric center contours (blue circles) and centroids (green dots) identified through computer vision recognition. (c) Atomic positions (red dots) determined from centroids adjacent to each other. (d) Honeycomb lattice structure of Xene reconstructed from STM data, with green regions indicating all-armchair-edged Xene.

M_{01}/M_{00} , where $M_{00} = \sum_x \sum_y f(x, y)$ is the zero-order moment representing the contour area, and M_{10} and M_{01} are first-order moments representing the weighted sums of the x and y coordinates. The calculated centroid positions are marked with green dots in Fig. 7(b).

(3) **Lattice model reconstruction:** Establish a threshold for centroid spacing by randomly selecting several pairs of nearest centroids, calculating their average distance, and applying a scaling factor. Ensure that distances between nearest centroids do not exceed this threshold. Traverse all centroids to identify nearest and next-nearest neighbors within the threshold, forming approximate triangles. Label the centers of these triangles, representing atomic positions, as red dots in Fig. 7(c). Connect the triangle centers within the threshold range to reconstruct the complete lattice structure, as shown in Fig. 7(d).

Finally, we briefly outline a potential experimental approach for realizing optically controlled transistors based on all-armchair-edged Xenes:

(1) **Epitaxial synthesis of Xenes:** Xenes can be synthesized via molecular beam epitaxy in an ultrahigh vacuum chamber and deposited onto thin metal substrates [17–27].

(2) **Encapsulation and protection:** After synthesis, the Xenes can be encapsulated *in situ* with a nonreactive protective layer to prevent oxidation and degradation under ambient conditions.

(3) **Device fabrication:** High-resolution imaging of Xenes can be achieved using STM. The computer vision method detailed in Sec. III E and illustrated in Fig. 7 can directly analyze lattice structures from STM images and identify all-armchair-edged Xene channels with high precision. By directly patterning the channel and electrode shapes onto a photoresist using electron beam exposure, latent images can be formed. These patterns can then

be accurately transferred onto Xenes using electron beam etching [70], atomic layer etching (ALE) [71], or thermal ALE [72]. For the fabrication of source and drain electrodes, the encapsulated delamination with a native electrode process can be utilized to etch the underlying metal substrate, leaving only the electrode regions intact [51].

(4) **Optical field manipulation:** Metamaterials and metasurfaces can achieve effective control and integration of optical fields [73]. These technologies enable not only the manipulation of individual properties, such as amplitude, phase, polarization, and frequency, but also the simultaneous and independent control of multiple properties.

It is important to note that realizing the proposed switching effect requires specific conditions for both light intensity and frequency. Specifically, the light field must satisfy the off-resonance condition, $\hbar\Omega \gg t_0$ [60,61], to validate the high-frequency approximation. Under these conditions, the field alters the band structure through virtual photon processes without directly exciting electrons. The minimum frequency is dictated by the bandwidth, $\hbar\Omega = 3t_0 \approx 10^{15}$ Hz. Frequencies below this threshold suppress the second-order photocoupling effect, leading instead to optical absorption. Once the light frequency is fixed, the light parameter, $\lambda_\Omega = 9t_0^2\Lambda^2/4\hbar\Omega$, can be tuned by adjusting the dimensionless light intensity, $\Lambda = eaA/\hbar$, where A represents the light amplitude. Typically, in the off-resonance frequency regime of interest, the intensity parameter, Λ , for the available lasers and pulses remains less than 1 [61].

IV. CONCLUSIONS

This study presents a theoretical model of an all-armchair-edged Xene structure, which is characterized by

armchair configurations on all edges. Our analysis reveals that the band gap of these Xenes can be finely tuned in a nearly continuous manner, showing an inverse relationship with nanoribbon width and effective spin-orbit coupling strength. For narrower nanoribbons, the band gap can reach hundreds of meV, indicating semiconductor behavior, while wider ribbons transition to metallic behavior as the gap closes. The band gap formation in all-armchair Xenes is linked to the spatial distribution of electronic states: narrow ribbons have localized states that promote band gap formation, while wider ribbons exhibit delocalized states that lead to metallic conduction.

The uniaxial strain affects the hopping energy and effective spin-orbit coupling, leading to significant changes in electronic properties and transport characteristics. Significant enhancements in band gaps across various nanoribbon widths are achieved when the strain direction aligns with specific angles ($\theta = 0, \pi/2$, or π) under optimal conditions ($t_1 = t_2 > t_3$). Additionally, the low buckling structure of Xenes results in a reduction of bond angles under tensile strain. This change triggers structural transitions that reduce spin-orbit coupling, enhancing edge-state interactions and significantly widening the band gap, especially in wider nanoribbons.

Off-resonant circularly polarized light affects the overlap of edge-state wave functions differently, depending on the spin orientation: it enhances coupling for one spin direction while reducing it for the other, leading to distinct energy band splitting. A single optical field can achieve 100% spin polarization without external electric or magnetic fields. By adjusting the nanoribbon width or applying uniaxial strain, the energy window for complete spin polarization can be independently controlled. Additionally, applying uniaxial strain can double the range of this energy window.

We propose a novel enhancement-mode transistor controlled solely by a single circularly polarized light field—either left- or right-handed—using all-armchair-edged Xenes as the channel material. In the absence of light, the transistor blocks electron transport, while illumination reduces the band gap, activating a conductive channel. The channel's band gap can be tuned by adjusting the width of all-armchair Xenes, enabling tailored operating voltages and transfer characteristics for diverse applications. Narrow-channel transistors show higher breakdown voltages and improved thermal stability, while wide-channel transistors require lower optical thresholds. Moreover, this optically controlled transistor can generate and manipulate spin-polarized currents, producing either fully spin-polarized or nonpolarized output, depending solely on the light parameter.

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DATA AVAILABILITY

The data are not publicly available. The data are available from the authors upon reasonable request.

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