Robust all-electrical topological valley filtering using monolayer 2D-Xenes

Koustav Jana\textsuperscript{1} and Bhaskaran Muralidharan\textsuperscript{1,\ast}

We propose a realizable device design for an all-electrical robust valley filter that utilizes spin protected topological interface states hosted on monolayer 2D-Xene materials with large intrinsic spin–orbit coupling. In contrast with conventional quantum spin-Hall edge states localized around the X-points, the interface states appearing at the domain wall between topologically distinct phases are either from the K or K' points, making them suitable prospects for serving as valley-polarized channels. We show that the presence of a large band-gap quantum spin-Hall effect enables the spatial separation of the spin–valley locked helical interface states with the valley states being protected by spin conservation, leading to robustness against short-range nonmagnetic disorder. By adopting the scattering matrix formalism on a suitably designed device structure, valley-resolved transport in the presence of nonmagnetic short-range disorder for different 2D-Xene materials is also analyzed in detail. Our numerical simulations confirm the role of spin–orbit coupling in achieving an improved valley filter performance with a perfect quantum of conductance attributed to the topologically protected interface states. Our analysis further elaborates clearly the right choice of material, device geometry and other factors that need to be considered while designing an optimized valleytronic filter device.

INTRODUCTION

Two-dimensional (2D) materials beyond graphene\textsuperscript{1} featuring honeycomb lattices, such as MoS\textsubscript{2} and other transition metal dichalcogenides (TMDCs)\textsuperscript{2,3}, group-IV and V 2D-Xenes\textsuperscript{4–13}, have enjoyed significant research activity targeting a wide range of applications. The uniqueness of these materials lies in their band structure having energy minima far apart in the momentum space, endowing the low-energy carriers a valley degree of freedom that can be exploited for information manipulation. This has paved the way for the field of valleytronics\textsuperscript{14–26}, in which the valley filter\textsuperscript{24} is a primary device paradigm that facilitates the generation of valley-polarized carriers.

There have been several proposals for valley filtering that include utilizing nanoconstrictions\textsuperscript{24}, optical pumping\textsuperscript{20,22,23,25,27}, the valley Hall effect\textsuperscript{18,19,21,25,26}, strain engineering\textsuperscript{28,29}, the valley-polarized quantum anomalous Hall phase\textsuperscript{30}, and domain walls with broken inversion symmetry\textsuperscript{33–41}. Two indices critical for a valley filter performance are the valley polarization and the total transmission, which should be immune against back-scattering\textsuperscript{30}.

Interface states at domain walls in monolayer 2D materials created using line junctions or defects which have been considered in previous works have different levels of topological robustness\textsuperscript{34,35,37–50}. Interface states formed along the zero mass lines, where the effective mass reverses sign, are valley–momentum locked and hence serve as perfectly valley-polarized channels. In 2D-Xenes with buckled honeycomb lattices\textsuperscript{51,52}, monolayer TMDCs in 1T'-configuration\textsuperscript{2} and bilayer materials such as bilayer graphene\textsuperscript{21,34,37–39,53} and bilayer MoS\textsubscript{2}\textsuperscript{54}, it is possible to break the inversion symmetry and control the band gap by the application of a perpendicular electric field using electrical gating, in order to possibly facilitate an all-electrical valley filter. Previous proposals and experimental realizations of domain wall-based valley filters in monolayer\textsuperscript{47,48} and bilayer structures\textsuperscript{34,37,38} suffer from a serious deterioration in the transmission and valley polarization due to back-scattering and bulk-assisted intervalley scattering from strong short-range disorder\textsuperscript{38,39,46}.

In this paper, we utilize the spin protection to the valley states through spin–valley locking\textsuperscript{41}, to demonstrate a realizable device design for robust valley filtering via the spatial separation of spin–valley locked interface states. This is possible in materials with strong spin–orbit (SO) coupling featuring a broken inversion symmetry, typical examples being monolayer MoS\textsubscript{2} and related materials\textsuperscript{55}, as well as group-IV and V 2D-Xenes under a perpendicular electric field\textsuperscript{52,56,57}. In our case, we center the proposal on monolayer group-IV 2D-Xenes with buckled lattice structures\textsuperscript{51,58–64} to design and realize topologically robust valley filtering.

Our device design is inspired by the following ideas. Buckled 2D-Xene materials, in the absence of an electric field possess a topologically nontrivial band structure with quantum spin-Hall (QSH) edge states and continue to do so until a critical field beyond which they transit to a topologically trivial band insulator phase also known as quantum valley Hall (QVH) phase\textsuperscript{57}. Adopting the existing so-called dual split-gate structure\textsuperscript{37,38} as depicted in Fig. 1a, with the side and top views as shown in Fig. 1b, we demonstrate that it is also possible to achieve QVH–QSH–QVH domain walls in contrast with the QVH–QVH domain walls of the earlier proposals. The QVH–QVH domain wall as illustrated in Fig. 1c hosts valley-momentum locked states, for both the spins, operating as valley-polarized channels. On the other hand, with the QVH–QSH–QVH domain walls illustrated in Fig. 1d, we can obtain spatially separated valley-polarized channels protected by spin conservation through spin–valley locking, provided time reversal symmetry (TRS) is preserved. This introduces the desired spin protection to the valley states via spin–valley locking in each of the two domain walls. Given the two domain walls are spatially well separated, we expect our valley filter to be robust, even against short-range disorder that can cause large momentum transfer, given the disorder is...
nonmagnetic and does not break TRS. This demands a QSH region that has a large gap, i.e., a large intrinsic SO coupling.

We also demonstrate this high degree of robustness by subjecting our channel to short-range nonmagnetic disorder of varying strength and examining the effect of SO coupling and line junction width on the valley filter performance. Based on our findings, we conclude the superiority of our QVH–QSH–QVH structure compared to other existing proposals. This implies the preservation of unity transmission and a mild degradation of the valley polarization with increase in disorder, guaranteeing a large enough valley-polarized current. To support our claims, we also present the local density of states (LDOS) calculations over the entire channel region. Apart from demonstrating the role of SO coupling and line junction width in achieving improved valley filtering, we also present a strategy to optimize the performance of the valley filter to tap into the full potential of our design.

RESULTS AND DISCUSSIONS

Device setup

In our proposed valley filter device sketched in Fig. 1a, b, we consider the channel as well as the leads to be made of monolayer 2D-Xene. The monolayer 2D-Xene is sandwiched between a top and a bottom dielectric layer. The top and bottom split-gates are used for the application of electric displacement field \( D_z \). Neglecting any possible screening in the direction perpendicular to the channel, we can assume that the actual perpendicular electric field \( E_z \) in the 2D-Xene channel can be approximated as \( E_z = D_z/C_0 \).

The tight binding Hamiltonian, based on the Kane-Mele model\(^6\), for a typical monolayer 2D-Xene having a honeycomb lattice structure reads\(^5,57\),

\[
H = -t \sum_{\langle ij \rangle} c_{i\alpha}^\dagger c_{j\alpha} + \frac{\lambda_{SO}}{\sqrt{3}} \sum_{\langle ij \rangle/\alpha} \alpha \lambda_{SO} c_{i\alpha}^\dagger c_{j\alpha} + \sum_{\alpha} \mu_i \Delta_{\alpha} c_{i\alpha}^\dagger c_{i\alpha}. \tag{1}
\]

where \( c_{i\alpha}^\dagger \) represents the annihilation (creation) operator of an electron on-site \( i \) with a spin \( \alpha \), and \( \langle ij \rangle \) and \( \langle \langle ij \rangle \rangle \) run over all the nearest and next-nearest neighbor hopping sites respectively. The spin index \( \alpha \) can be \( \uparrow, \downarrow \) represented with corresponding values \(+1/-1\) respectively. The first term in (1) corresponds to the usual nearest neighbor hopping term with a hopping strength \( t \). The second term represents the intrinsic SO coupling with strength \( \lambda_{SO} \), which is the hopping parameter, \( a \) is the lattice constant, \( \lambda_{SO} \) is the intrinsic SO coupling, \( I \) is half the buckling height\(^5\).

| Material      | \( E_z \) (eV) | \( a \) (Å) | \( \lambda_{SO} \) (eV) | \( I \) (Å) |
|---------------|----------------|--------------|--------------------------|-------------|
| Graphene      | 2.8            | 2.46         | 10^-6                    | 0           |
| Silicene      | 1.6            | 3.86         | 3.9 \times 10^{-3}       | 0.23        |
| Germanene     | 1.3            | 4.02         | 0.04                     | 0.33        |
| Stanene       | 1.3            | 4.7          | 0.1                      | 0.4         |

\( t \) is the hopping parameter, \( a \) is the lattice constant, \( \lambda_{SO} \) is the intrinsic SO coupling, \( I \) is half the buckling height\(^5\).

Choice of the material. Typical values of the parameters involved in (1) for the candidate materials\(^5\) have been summarized in Table 1. Graphene does not have a buckled structure \( (I = 0) \) and hence electrical gating cannot be an option to introduce the \( \Delta_z \) term in it. Also both graphene and silicene have very small \( \lambda_{SO} \) values of \( 10^{-3} \) meV and 3.9 meV respectively, thus not making them suitable candidates to exploit the topological robustness of the QSH phase that we intend to do in order to design an efficient valley filter. It is worth mentioning that theoretical possibilities of engineering QSH and QVH states in strained graphene exist\(^5\), even in the absence of SO coupling, but such proposals rely on complex quantum pumping processes.

Stanene with an intrinsic SO coupling of \( \approx 0.1 \) eV, seems to be a promising candidate for our valley filter\(^5\) proposal. In addition, functionalized germanene\(^8\) and stanene\(^9\) have shown sizable band gaps of around 0.3 eV along with a record band gap of around 1.34 eV in chemically decorated monolayer plumbene\(^10\).

Apart from the above, a QSH phase with a sizeable band gap has

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**Table 1.** The parameters corresponding to various monolayer 2D-Xenes.

| Material      | \( E_z \) (eV) | \( a \) (Å) | \( \lambda_{SO} \) (eV) | \( I \) (Å) |
|---------------|----------------|--------------|--------------------------|-------------|
| Graphene      | 2.8            | 2.46         | 10^-6                    | 0           |
| Silicene      | 1.6            | 3.86         | 3.9 \times 10^{-3}       | 0.23        |
| Germanene     | 1.3            | 4.02         | 0.04                     | 0.33        |
| Stanene       | 1.3            | 4.7          | 0.1                      | 0.4         |

\( t \) is the hopping parameter, \( a \) is the lattice constant, \( \lambda_{SO} \) is the intrinsic SO coupling, \( I \) is half the buckling height\(^5\).
also been proposed in monolayer TMDCs in 1T’ structure and group-V Xenes like arsenene, antimonene and bismuthene. In our analysis, we narrow down our focus on group-V Xenes like germanene and stanene. However, it is worth noting that there are other materials as listed above which can have QSH phase with a larger gap, and the use of such materials will only improve the valley filter performance. Also the above materials show a large enough buckling height, with \( \eta \) ranging from 0.4 to 0.7 Å and hence the possibility of achieving a large gap QVH phase as well. Thus the possibility of large band gap QSH and QVH phases in germanene and stanene makes them the ideal choice of materials to serve our purpose.

Having \( f = 0.4 \) Å would require an electrical field (\( E_f \)) of 5 V nm\(^{-1}\) to achieve \( \Delta_v = 0.2 \) eV. That would mean a displacement field corresponding to \( D_x/E_f = 5 \) V nm\(^{-1}\) which is practically quite achievable. In this case, the electric field inside the dielectric layers would be given by \( D_x/E_f \). Now using a high-k dielectric such as HfO\(_2\) (\( \varepsilon = 23.5\) eV\(^0\)) would lower the electric field inside the dielectric (\( \approx 2\) MV/cm for \( \varepsilon = 23.5\) eV\(^0\)), thus ruling out the possibility of dielectric breakdown at a high displacement field corresponding to \( D_x/E_f = 5 \) V nm\(^{-1}\).

Based on this discussion, we choose the parameters involved in our model to be the following: \( t = 1.3 \) eV, \( l = 0.4 \) Å and \( a = 4 \) Å. We then vary \( \lambda_{SO} \) and \( \Delta_v \) within the practically realizable limits, in order to optimize the valley filter performance.

### Table 2. Chern numbers (\( C_i \)) corresponding to the spin (\( s \)) and valley (\( \eta \)) degrees of freedom, along with the spin (\( C_i^s \)) and valley (\( C_i^\eta \)) Chern numbers, for the QSH, QVH-I, and QVH-II phases (\( 1,2,5,45,46,57 \)).

|        | \( C_i^s \) | \( C_i^\eta \) | \( C_i^\eta \) | \( C_i^\eta \) | \( 2C_i \) | \( C_v \) |
|--------|-------------|-------------|-------------|-------------|----------|----------|
| QVH-I  | 1/2         | 1/2         | -1/2        | -1/2        | 0        | 2        |
| QSH    | 1/2         | -1/2        | 1/2         | -1/2        | 2        | 0        |
| QVH-II | -1/2        | -1/2        | 1/2         | 1/2         | 0        | -2       |

### Topological phases.

Based on the low-energy Dirac Hamiltonian, the gap of the energy spectrum corresponding to a spin \( s \) and valley \( \eta \) is given by \( 2\Delta_{vi}^s \), where \( \Delta_{vi}^s = \Delta_s - \eta\lambda_{SO} \) is the Dirac mass term. We define the point \( (4m/3a, 0) \) as the \( K \) valley and \( (2m/3a, 0) \) as the \( K' \) valley. On varying \( \Delta_s \), \( \Delta_{vi}^s \) reverses its sign when \( \Delta_s = \eta\lambda_{SO} \) signifying a topological phase transition.

The above phase transitions can be better understood by an analysis of the Berry curvature and the Chern number. It is well known that the Berry curvature of the given Hamiltonian (1) is strictly localized around the \( K \) and \( K' \) points, allowing us to associate each valley with a Chern number \( C_i^\eta \), where spin index \( s = \uparrow, \downarrow \) and valley index \( \eta = \pm \). The Chern number \( C_i^\eta \) can be obtained using the Dirac Hamiltonian and is given by

\[
C_i^\eta = -\frac{2}{\pi} \text{sgn}(\Delta_i^s) \quad (1,2,45,46,57)
\]

Figure 2a shows the variation of \( \Delta_{vi}^s \) with \( \Delta_v \) for all four pairs of \( (s, \eta) \) values and the corresponding Chern numbers have been listed in Table 2.

Here it is important to further introduce the spin Chern number \( C_s \) and the valley Chern number \( C_v \) as:

\[
C_s = \frac{1}{2} \left( C_{i_{2}}^{s_{2}} + C_{i_{2}}^{s_{2}} - C_{i_{2}}^{s_{1}} - C_{i_{2}}^{s_{1}} \right)
\]

\[
C_v = C_{i_{2}}^{s_{2}} - C_{i_{2}}^{s_{1}} + C_{i_{2}}^{s_{1}} - C_{i_{2}}^{s_{2}}
\]

Based on \( C_s \) and \( C_v \), we can now label the various topological phases, namely the QSH phase and the QVH phases by varying \( \Delta_v \).

### Topological domain walls.

We now move on to investigate the interface states at the topological domain walls between different phases (1,39-40). At the QVH-I/QSH interface, \( \Delta_{vi}^s \) is non-zero only for the \( (\uparrow, K') \) and \( (\downarrow, K) \) states and has opposite signs, thus yielding a pair of counter-propagating helical interface states. Hence at the domain wall between the QVH-I and QSH phases, we have spin-valley-momentum locked interface states, \( (\uparrow, K') \) and \( (\downarrow, K) \) propagating in opposite directions. A similar analysis of the domain wall between the QVH-II and QSH phases yields counter-propagating \( (\uparrow, K) \) and \( (\downarrow, K') \) interface states. There is a third possible scenario that arises when \( \Delta_{vi}^s = 0 \), that is, no QSH phase exists and we will have a domain wall between the QVH-I and QVH-II phases. In this case \( \Delta_{vi}^s \) is non-zero for all the four possible states with opposite signs for the \( K \) and \( K' \) valley states. Thus we expect four interface states with the \( K \)-valley states propagating in one direction and the \( K' \) states in the opposite direction. One special feature of these interface states which makes them an attractive option for valley filtering is that the counter-propagating states are localized at the \( K \) and \( K' \) points and are immune to any back-scattering due to long range disorder (16,39,46).

### Device structure.

The domain walls discussed above can be easily realized by creating a line junction between oppositely gated regions using a dual split-gate structure shown in Fig. 1a. The given configuration of voltage sources ensures that a voltage of \( U \pm V \) is applied to the gates, where \( V \) is responsible for modulating \( E_f \) and \( U \) allows us to control the channel electrochemical potential. Thus the channel has an additional on-site potential \( U \) on every site realized via the addition of the Hamiltonian term \( H_U = \sum_{\mu} \xi_\mu c_\mu^\dagger c_\mu \). For the leads, we consider both \( \lambda_{SO} \) and \( \Delta_v \) to be zero.

Given the width of the nanoribbon is \( W_{\text{nr}} \), we consider its \( y \)-coordinates to be in the range \( \left[ -\frac{W_{\text{nr}}}{2}, \frac{W_{\text{nr}}}{2} \right] \). The dual split-gates
Fig. 3 Gate voltage configuration, corresponding band structure and valley polarization of our proposed valley filter. a "+" configuration gives a $K$-valley-polarized filter for transmission from the left ($L$) to the right ($R$) lead, given the channel electrochemical potential lies within the band gap, because of the right-going electrons being locked to the $K$-valley. b "−" configuration gives a $K'$-valley-polarized filter as the right-going electrons of the interface states are locked to the $K'$-valley.

have a spacing of $W_j$ with the adjacent edges located at $y = \pm \frac{W_j}{2}$. We have modeled the spatial dependence of $E_z$ using the following analytical expression:

$$E_z(y) = \frac{E_{zo}}{2} \left( \tanh \left( \frac{y - \frac{W_j}{2}}{\frac{W_j}{2}} \right) + \tanh \left( \frac{y + \frac{W_j}{2}}{\frac{W_j}{2}} \right) \right),$$

where $E_{zo}$ is the maximum magnitude of the perpendicular electric field applied and $W_j$ is the fringing width of the electric field at the gate edges. In an actual setup $W_j$ has a direct dependence on the perpendicular spacing between the gates, which we assume to be 3.125 nm. Figure 2b, c illustrate the potential variation ($\mu_{A}$) along sublattices $A$ and $B$ for the two cases: $W_j = 6.25$ nm (small $W_j$) and $W_j = 20.8$ nm (large $W_j$) respectively. The above two cases differ in the fact that in the former case, the width of the region having $\Delta_0 = 0$ is negligible, whereas in the latter this width is large enough. Interestingly, exploiting the above potential variations, it is possible to have different cases of domain walls as depicted in Fig. 1c, d, a deeper discussion of which will follow in the upcoming section. 

In all our calculations, we consider a zig-zag nanoribbon which is 180 atoms wide, corresponding to a width $W_o = 62.5$ nm. The channel region $C$ as well as the leads $L$ and $R$ have the same width $W_o$, with the length $L_o$ of the channel region being 40 nm i.e., 100 atoms long, which is long enough such that the out-going carriers are completely valley-polarized in the clean limit. The electrochemical potential of the leads ($E$) is fixed at $E = t/\sqrt{3}$, corresponding to precisely seventy eight propagating modes, and that of the channel ($E - U$) is controlled by varying $U$. For all the numerical results that follow, unless explicitly mentioned, the width of the nanoribbon, length of the channel region $C$ and the electrochemical potential of the leads are fixed.

Depicted in Fig. 3 is the operation of our valley filter in the absence of any form of disorder, i.e., the clean limit. The electrochemical potential of both the leads is fixed at $E$. For this case: $W_j = 6.25$ nm, $E = t/\sqrt{3}$, $\lambda_{so} = 0.1$ eV and $\Delta_{zo} = 0.2$ eV (max. value of $\Delta_o$), thus creating a gap of $2(\Delta_{zo} - \lambda_{so}) = 0.2$ eV. The gap defined above corresponds to the gap of the QVH regions, given that the QSH region gap is independent of $\Delta_o$ and depends only on $\lambda_{so}$. Both Fig. 3a, b corresponding to opposite gate configurations, show close to perfect valley polarization in the gap range $[-0.1 \text{eV}, 0.1 \text{eV}]$. Since the valley polarization plotted is for transmission from $L$ to $R$, whenever the $K$-valley electrons are right going, our filter is $K$-valley polarized as in Fig. 3a and similarly $K'$-valley polarization in Fig. 3b. The fact that the valley polarization of the filter can be reversed by just reversing the signs of the gate voltages, makes this valley filter design quite convenient for practical purposes.

Valley filtering performance

To ensure a fair comparison across all the cases, we assume the band gap of the bulk states in the QVH regions to be 0.2 eV, i.e., a gap range of $[-0.1 \text{eV}, 0.1 \text{eV}]$, demanding $\Delta_{zo} = 0.1 + \lambda_{so}$, which implies that as $\lambda_{so}$ is varied, the applied gate voltage $V$ also needs to be varied accordingly. Figure 4a-f shows the spatial variation of local band gap along the nanoribbon width for six different combinations of $\lambda_{so}$ and $W_j$ along with the corresponding band structures in Fig. 4g-i. As indicated by the blue bands in Fig. 4a-f, localized interface states appear at the locations where the band gap closes. The total transmission $T$ and valley polarization $P_v$ (see Methods) are plotted in Fig. 5, in two different ways: (a) Disorder strength $W$ (see Methods) varied, for $E - U = 0$, with $E = t/3$, as shown in Fig. 5a-d, (b) $E - U$ varied over the gap range $[-0.1 \text{eV}, 0.1 \text{eV}]$ for $W = 2$ eV, as in Fig. 5e-i. In the clean limit, within the gap range, we expect $P_v$ to be close to unity, and $T = 2$, corresponding to two interface states, one for each spin. However for disorder strength $W = 2$ eV, $P_v$ deteriorates significantly, suggesting an increased intervalley scattering between the helical interface states and hence a suppressed transmission due to increased back-scattering. This does hold true for $E - U$ around zero, but when $E - U$ approaches the band edge, an enhancement in $T$ is observed indicating the bulk state assistance in intervalley scattering, similar to what has been reported in39. Thus the intervalley mixing that is detrimental to the efficiency of our valley filter can happen either directly via back-scattering between the helical interface states or indirectly assisted by the bulk states. The former is dominant when the electrochemical potential lies in the middle of the band gap and the latter takes over as the electrochemical potential approaches the band edge.
Although there is no clear way to get rid of the bulk-assisted intervalley scattering other than having a larger band gap, the direct one can be evaded by introducing a spatial separation between interface states of the same spin. The results in Fig. 5c, g indeed confirm this. Unlike the other cases, as suggested by Fig. 5c, T remains unchanged when \( \lambda_{SO} = 0.1 \text{ eV} \) and \( W_j = 20.8 \text{ nm} \), even in the presence of very strong disorder (\( W = 2.4 \text{ eV} \)) and does not degrade with \( W \) as seen in other cases. Figure 5g shows that \( T \) remains perfectly quantized when the electrochemical potential lies around the mid-gap before getting affected by the bulk states as we move closer to the band edge. Despite showing a mild degradation in \( P_v \) with \( W \) like the others, it still has the best valley polarization in the presence of strong disorder.

The obtained results make more sense once the local band gap profiles in Fig. 4 are analyzed. Since the interface states appear at the locations where the gap closes, for the \( W_j = 6.25 \text{ nm} \) case, the four interface states co-exist and overlap with one another (Fig. 4a–c). On the other hand when \( W_j = 20.8 \text{ nm} \), the interface states can now be hosted with spatial separation. However that alone is not enough to ensure spatial separation without any overlap. For example, in the case of \( \lambda_{SO} = 0 \text{ eV} \), the central line junction region is semimetallic and gapless thus leading to the interface states spreading out uniformly over the entire central region instead of being localized as depicted in Fig. 4d.

A wide semimetallic region also leads to bulk states, thus decreasing the available band gap as suggested by Fig. 4j. This has a detrimental effect on the valley filter performance, with the device now not only having a diminished operational energy range, but also a degrading valley polarization within this range, as confirmed by Fig. 5h, thus highlighting the role of bulk-assisted intervalley scattering in deteriorating the filtering efficiency. Similarly when \( \lambda_{SO} = 0.04 \text{ eV} \) there exists a low band gap QSH region in the line junction. Although the interface states are hosted at different locations as depicted in Fig. 4e, they can still interact with one another via tunneling through the low band gap central region, thus leading to inevitable back-scattering. Even in this case, some bulk states enter the band gap as shown in Fig. 4k and further deteriorate the valley filter performance.

However, when \( \lambda_{SO} = 0.1 \text{ eV} \), the gap is free from bulk states as the QSH region has a gap equal to that of the QVH regions and any possible tunneling between the interface states is suppressed owing to the larger band gap central region. Thus the back-scattering is strongly suppressed even in presence of strong disorder and we get a perfectly quantized transmission \( T = 2 \) around the mid-gap. However the bulk-assisted intervalley scattering still persists and hence the degradation of \( P_v \) with \( W \).

To further validate the arguments made above, the LDOS in the absence of disorder, for \( E - U = 0 \), has been plotted for all the cases in Fig. 6 (refer Supplementary Note 1 for LDOS plots corresponding to few more cases of \( W_j \)). The spatial variation of the interface states is illustrated for varied \( \lambda_{SO} \), when \( W_j \) is small, in Fig. 6a–c and similarly in Fig. 6d–f for large \( W_j \). The LDOS plots confirm our previous claims of the interface states being spatially separated only for the case with \( \lambda_{SO} = 0.1 \text{ eV} \) and \( W_j = 20.8 \text{ nm} \) (Fig. 6f). Thus our simulation results shed light on the possibility of achieving an improved valley filter performance, with a perfectly quantized \( T \), by spatially separating the interface states with the same spin through a suitable chosen gate configuration. We now look into the important aspect of optimizing the proposed valley filter device.

**Device optimization**

As mentioned before, a good electrical valley filter should have a large valley polarization along with a large enough total current in order to achieve a large valley current. In other words, perfect valley polarization with a very small amount of current is of no practical
utility to any of the valleytronic applications. Thus exploiting the topological robustness and dissipation-less nature of spatially separated interface states with the introduction of intrinsic SO coupling is the key to achieve improved valley filtering.

Our valley filter can be optimized by considering the following two crucial requirements: Firstly, the QSH region should be well-gapped and wide enough to ensure that the spatially separated interface states do not overlap with each other. This is necessary to ensure that back-scattering is negligible and $T$ is perfectly quantized even in the presence of strong nonmagnetic disorder. Secondly, the QVH regions also need to be well-gapped and wide enough to ensure that the interface states do not spread out to the nanoribbon edges. Ensuring this is critical to maintain the valley-polarized character of the interface states so that the valley filter produces significant valley polarization.

Optimal $\lambda_{SO}$. So far, the comparison between the different cases was made after considering the same bulk band gap of the QVH region and this requires different perpendicular fields $E_z$ for different values of $\lambda_{SO}$. In Fig. 5, we notice that when $\lambda_{SO} = 0$ eV, the valley filter performs the best when the adjacent gates are as close as possible, whereas for $\lambda_{SO} = 0.1$ eV the valley filter efficiency is enhanced when the adjacent gates are far apart to ensure spatial separation of interface states. Hence for $\lambda_{SO} = 0$ eV we consider $W_j = 6.25$ nm whereas when $\lambda_{SO} = 0.1$ eV we increase $W_j$ to $20.8$ nm to have the best possible valley filter. Similar to Fig. 4, we consider $\Delta = 0.1$ eV for $\lambda_{SO} = 0.1$ eV case and this requires $E_z = 5$ V nm$^{-1}$ given $l = 0.4$ Å, which is practically achievable. For the same $E_z$ and $l$, in the $\lambda_{SO} = 0$ eV case we can achieve $\Delta = 0.2$ eV.

The transmission plots in Fig. 7a, b clearly show the superiority of $\lambda_{SO} = 0.1$ eV case in its robustness to back-scattering. However, as
suggested by Fig. 7c, d, $P_v$ degrades a bit in this case compared to the $\lambda_{SO}=0$ eV case because of a smaller band gap leading to increased bulk-assisted intervalley scattering. Thus when the same gate voltage is applied, addition of SO coupling to host spatially separated interface states helps us achieve a perfectly quantized $T$ but at the cost of a reduced $P_v$. In the above comparison, we considered $E_{so} = 5 \text{ V nm}^{-1}$ where for the $\lambda_{SO}=0.1$ eV case we had $\Delta = 0.1$ eV and hence we achieved reasonably good valley filtering whereas for a lower $E_{so}$ say, $3 \text{ V nm}^{-1}$, the performance degrades due to a very small $\Delta$ of $0.02$ eV. The bare minimum one needs to ensure is that $\lambda_{SO} < E_{so}/2$, in order to assure the existence of the QSH/QVH domain walls, and hence the interface states. Hence the best case would be when the QSH as well as the QVH regions have the same gap implying $\lambda_{SO} = E_{so}/2$ for a given $E_{so}$. Thus for $E_{so} = 5 \text{ V nm}^{-1}$ and $l = 0.4 \text{ Å}$, $\lambda_{SO} = E_{so}/2 = 0.1$ eV is the optimal one to get the best yields as valley filter given the interface states are well separated after choosing a suitable $W_j$.

Optimal $W_j$. One might expect that a larger $W_j$ should ensure a greater degree of robustness for the interface states. However, since we have considered a fixed width for the nanoribbon ($W_o = 62.5 \text{ nm}$), invariably increasing $W_j$ implies that the widths of the QVH regions keep decreasing and the interface states move closer to the nanoribbon edges. As a consequence, the interface states start resembling the conventional QSH edge states as shown in Fig. 7e, in which $W_j = 60 \text{ nm}$, which then results in diminishing $P_v$ as they move towards the X-point of the Brillouin zone. On the other hand, decreasing $W_j$ also brings the interface states closer from which they interact with each other via tunneling, thus further degrading $T$ via back-scattering. Thus $W_j$ needs to be chosen such that the interface states are neither too close to each other nor too far apart that they come in the vicinity of the nanoribbon edges.

To quantify the above arguments, we consider the spatial extent of the interface states on either side of the domain wall given by the damping length, $\zeta = h\nu r/2\Delta = (3/\pi)^{1/4}\Delta^{1/4}l$. One thing to note is that this expression is valid for an abrupt topological phase transition. However, in our case, it is rather smooth over a fringing width of $W_f = 3.125 \text{ nm}$. Hence the actual $\zeta$ would be slightly larger than what we estimate. It is clear that $\zeta$ is inversely proportional to $\Delta$, thus maintaining our earlier conclusion that $\Delta$ needs to be large enough for all the QSH as well as QVH regions, so that the interface states are well confined. For the electric field we consider ($E_{so} = 5 \text{ V nm}^{-1}$) the corresponding optimal $\lambda_{SO}$ was $0.1$ eV, thus $\Delta = 0.1$ eV for the QSH as well as QVH regions. The $\zeta$ calculated for our case comes out to be $2.25 \text{ nm}$ which is in fact smaller than $W_o = 3.125 \text{ nm}$ and hence we choose $\zeta = 3.125 \text{ nm}$. Considering exponential variation of the wavefunction along the $y$-direction on either sides of the domain wall, $96\%$ of the wavefunction remains confined within a distance i.e., three times the damping length $\zeta$, for our case $3\zeta = 9.5 \text{ nm}$.

Based on the above calculations, we can conclude for the spatially separated interface states to be decoupled from each other, we require $W_j > 2 \times 9.5 = 19 \text{ nm}$ and to ensure that they do not spread out all the way into the nanoribbon edges $W_j < W_o − 2 \times 9.5 = 43.5 \text{ nm}$ is required. Hence choosing $19 \text{ nm} < W_j < 43.5 \text{ nm}$, ensures the desirable valley filtering performance both in terms of $T$ and $P_v$.

Our analytical calculations are also validated by the simulation results in Fig. 7f, where $T$ and $P_v$ are plotted against varying $W_j$ for $E − U = 0$ and $W = 2 \text{ eV}$. The total transmission $T$ remains constant at $2$, as we lower $W_j$ before declining rapidly as $W_j$ goes below $20 \text{ nm}$. On the other hand, the valley polarization $P_v$ decreases steadily as we increase $W_j$, before showing a sudden drop once $W_j$ goes past $40 \text{ nm}$. Thus our choice of $W_j = 20.8 \text{ nm}$ when $E_{so} = 5 \text{ V nm}^{-1}$ and $\lambda_{SO} = 0.1$ eV, as suggested by both our analytical calculations and simulation results, is optimal in terms of both $T$ and $P_v$. The variation of $T$ and $P_v$ over the entire band gap, for different values of $W_j$, is illustrated in Fig. 7g, h. One important thing to note is that in our above optimization strategy, we were constrained by the maximum electric field $E_{so}$ we can apply and the nanoribbon width $W_o$, unconstrained by which, we can further enhance the valley filter performance.

Effect of temperature and vertical electric field
At this stage, we must remark that the analysis done until now is completely based on intervalley and intravalley transmission coefficients at the Fermi level, which actually relates to the zero-bias conductance at absolute zero temperature. Thus, the aforementioned results capturing the transmission at a given energy level (Fermi level), do not take into account the smearing of the Fermi function to levels surrounding the Fermi level at non-zero temperatures. However, to gauge the utility of this proposal...
Fig. 8 Effect of temperature variation and $\Delta_{\text{SO}}$ variation on valley filter performance. a, b Effect of temperature variation on zero-bias conductance $G$ and valley polarization $P_V$ (c, d) Effect of $\Delta_{\text{SO}}$ variation on zero-bias conductance $G$ and valley polarization $P_V$. The different cases of $\Delta_{\text{SO}}$ chosen are 0.2, 0.12, and 0.08 eV, corresponding to $E_{\text{SO}} = 5$, 3, and 2 V nm$^{-1}$. for commercial applications one needs to analyze this proposal at non-cryogenic temperatures. In the results given in Fig. 8a, b, we demonstrate the effect of temperature on zero-bias conductance of each valley component (refer Supplementary Note 2 for more details) for the case of $W_l = 20.8$ nm and $\lambda_{\text{SO}} = 0.1$ eV. It can be observed that as temperature rises, the zero-bias conductance $G$ increases slightly because of the Fermi function smearing into the bulk states. For the same reason, it can also be verified that the valley polarization at high disorder strength degrades with increasing temperature.

A critical limiting factor of our design, as discussed earlier, is the strength of the vertical electric field that can be applied. In Fig. 8c, d we study the effect of varying electric fields on the valley filter performance. Building on our previous findings for each different case of perpendicular field $E_{\text{SO}}$ and hence $\Delta_{\text{SO}}$, the intrinsic SOI strength $\lambda_{\text{SO}}$ which would maximize the performance would be $\lambda_{\text{SO}} = \Delta_{\text{SO}}/2$. The different cases of $\Delta_{\text{SO}}$ chosen are 0.2, 0.12, and 0.08 eV, corresponding to $E_{\text{SO}} = 5$, 3, and 2 V nm$^{-1}$, for $I = 0.4$ A. As expected, as the value of $\Delta_{\text{SO}}$ goes down, PV degrades drastically. However, the total transmission $T$ remains unchanged. The given results on varying $\Delta_{\text{SO}}$ also provide useful insights on the effect of varying buckling height that may happen as a result of any mechanical strain on the sample.

In conclusion, we proposed a design for an all-electrical robust valley filter that utilizes topological interface states hosted on monolayer group-IV 2D-Xene materials with large intrinsic SO coupling. In contrast with conventional QSH edge states localized around the X-points, the interface states appearing at the domain wall between topologically distinct phases are either from the K or K$'$ points, making them suitable prospects for serving as valley-polarized channels. We showed that the presence of a large bandgap quantum spin-Hall effect facilitates the spatial separation of the spin-valley locked helical interface states with the valley states being protected by spin conservation, leading to robustness against short-range nonmagnetic disorder. By adopting the scattering matrix formalism on a suitably designed device structure, valley-resolved transport in the presence of nonmagnetic short-range disorder for different 2D-Xene materials was analyzed in detail. Our numerical simulations confirm the role of SO coupling in achieving an improved valley filter performance with a perfect quantum of conductance attributed to the topologically protected interface states. Our analysis further elaborated clearly the right choice of material, device geometry and other factors that need to be considered while designing an optimized valley filter device. We believe that our work opens the door for researching the utility of the 1D topological conducting channels hosted in the monolayer 2D-Xene bulk for possible applications in valleytronics and spintronics.

**METHODS**

**Valley-resolved transport calculations**

We use the software package "KWANT" for calculating the transfer matrix $T$, which gives us the transmission amplitude $t_{\text{K,K}}$ from the $k_1$ state of lead $l$ to the $k_2$ state of lead $R$. The inter- and intravalley ($T_{\text{K,K}}$ and $T_{\text{K,K}}$) transmission coefficients can be calculated using the following formula $^{12,13,14,15}$

$$T_{\text{K,K}} = \sum_{k_1, k_3, k_4} |t_{k_1, k_2}|^2$$

(5)

Now the transmission coefficient corresponding to scattering into the K-valley in lead $R$ is given by $T_{\text{K,K}} = T_{\text{K,K}} + T_{\text{K,K}}$ and similarly $T_{\text{K,K}} = T_{\text{K,K}} + T_{\text{K,K}}$. Once we have the valley-resolved transmission coefficients ($T_{\text{K}}$ and $T_{\text{K}}$), we can now calculate the valley polarization $P_V$ and the total transmission $T_{\text{K,K}}$, the two important metrics to evaluate the performance of a valley filter.

$$P_V = \frac{T_{\text{K}} - T_{\text{K}}}{T_{\text{K}} + T_{\text{K}}}$$

(6)

$$T = T_{\text{K}} + T_{\text{K}}$$

(7)

**Inclusion of Anderson disorder**

To evaluate the performance of our valley filter in actual experimental conditions, we subject it to short-range Anderson nonmagnetic disorder which does not break TRS and this can be done by introducing random on-site potential for each site. Despite the Anderson disorder not reflecting all the potential valley-mixing mechanisms in experimental samples, it does provide a computationally efficient means to model the intervalley scattering and allows us to examine the effect of varying parameters such as $\lambda_{\text{SO}}$ and $W_l$ on the valley filter performance. This is achieved by adding the term $H_{\text{SO}} = \sum_{\alpha} C_{\text{SO}} C_{\text{SO}}$ to the channel Hamiltonian, with $C_{\text{SO}}$ being randomly distributed in the interval $[-\Delta_{\text{SO}}, \Delta_{\text{SO}}]$.

**DATA AVAILABILITY**

The data that support the plots within this paper and other findings of this study are available from the corresponding author upon reasonable request.

**CODE AVAILABILITY**

The codes generated during the simulation study are available from the corresponding author upon reasonable request.

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AUTHOR CONTRIBUTIONS
B.M. and K.J. conceived the idea. K.J. performed all numerical simulations. All authors contributed in analyzing the results and writing the paper.

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Correspondence and requests for materials should be addressed to Bhaskaran Muralidharan.

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