Purely interfacial and highly tunable by gate or disorder spin-orbit torque in graphene doubly proximititized by two-dimensional ferromagnet Cr$_2$Ge$_2$Te$_6$ and monolayer WS$_2$

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Graphene sandwiched between semiconducting monolayers of ferromagnet Cr$_2$Ge$_2$Te$_6$ and transition-metal dichalcogenide WS$_2$ acquires both spin-orbit (SO), of valley-Zeeman and Rashba types, and exchange couplings. Using first-principles combined with quantum transport calculations, we predict that such doubly proximitized graphene within van der Waals heterostructure will exhibit SO torque driven by unpolarized charge current. Unlike SO torque on conventional metallic ferromagnets in contact with three dimensional SO-coupled materials, the predicted torque can be tuned by up to two orders of magnitude via combined top and back gates, and it can be further enhanced via introduction of impurities. Thus, even in the absence of spin Hall current, putatively considered to be necessary for efficient damping-like (DL) SO torque that plays a key role in magnetization switching, DL torque component can be generated by skew-scattering off spin-independent potential barrier or impurities in purely two-dimensional electronic transport due to the presence of proximity SO coupling and its spin texture tilted out-of-plane. This leads to current-driven nonequilibrium spin density in all spatial directions, whose cross product with proximity magnetization yields DL SO torque, unlike the ballistic regime in which only field-like SO torque appears.

**Introduction.**—The spin-orbit (SO) torque [1] is a phenomenon in which unpolarized charge current injected parallel to the interface of a bilayer of ferromagnetic metal (FM) and SO-coupled material induces magnetization dynamics of the FM layer. For many possible applications of torque [2], such as nonvolatile magnetic random access memories [3] or artificial neural networks [4], it is crucial to switch magnetization from up to down along the direction perpendicular to the interface. This has led to intense search for optimal SO-coupled materials and their interfaces with FM layers which yield large SO torque while using as small as possible injected current. Thus far, minimal current density $j$ for magnetization switching has been achieved using topological insulators ($j \sim 6 \times 10^5$ A/cm$^2$ [5]) and Weyl semimetals ($j \sim 3 \times 10^6$ A/cm$^2$ [6]), which is two orders of magnitude smaller than $j$ required in early devices employing heavy metals [1, 7].

Further optimization could be achieved by using van der Waals (vdW) heterostructures [8] of very recently discovered two-dimensional (2D) ferromagnets [9, 10] and 2D SO-coupled materials where current flows only through few monolayers and no Joule heat is wasted by its flow through the bulk. Furthermore, vdW heterostructures offer atomically flat and highly transparent interfaces, as well as possibility to use external manipulations—such as gating, straining and controlling coupling between 2D materials—in order to tune [11] the magnitude and ratio of field-like (FL) and damping-like (DL) components of SO torque. The traditional labeling of torque components stems from how they affect dynamics of magnetization $\mathbf{m}_C$ viewed as a classical vector—FL torque changes precession around an effective magnetic field (such as along the $y$-axis in the case of vdW heterostructure in Fig. 1), while DL torque competes with damping and plays a key role [12] in magnetization switching (such by directing magnetization $\mathbf{m}_C$ towards the $y$-axis in Fig. 1). Controlling their ratio and relative sign is of great interest for applications since it makes it possible to tailor switching probability [13].

The critical problem in the field of SO torques—understanding of competing microscopic mechanisms behind these components, especially the DL one, and control of their magnitude and ratio—remains unresolved.

![FIG. 1. Schematic view of Cr$_2$Ge$_2$Te$_6$/graphene/WS$_2$ vdW heterostructure attached to macroscopic left and right reservoirs with a small bias voltage $V_b$ between them injecting unpolarized charge current into graphene layer. A back gate voltage $U_{bg}$ and a top gate voltage $U_{tg}$ applied over a smaller “active region” are assumed to control the Fermi energy and the local on-site potential in graphene, respectively. The unit vectors of magnetic moments on Cr, Te and C atoms are denoted as $\mathbf{m}_{Cr}$, $\mathbf{m}_{Te}$ and $\mathbf{m}_{C}$, respectively, where only $\mathbf{m}_C$ experiences SO torque-driven dynamics.](https://example.com/figure1.png)
For example, experiments on FM/heavy-metal bilayers suggest [7] that DL SO torque is primarily generated by the spin Hall current [14] from the bulk of a heavy metal, while interfacial SO coupling (SOC) is detrimental because it generates spin memory loss [15–17] and, therefore, reduction of spin Hall current. Conversely, first-principles quantum transport calculations [18, 19] on FM/heavy-metal bilayers find that interfacial SOC and spin Hall current can equally contribute to total DL SO torque. The interfacial contribution is identified in experiments or in computational studies as being independent on the thickness of heavy-metal layer [18, 19], but its microscopic mechanisms remain poorly understood. For example, reflection and transmission of electron spins traversing SO-coupled interface can lead to interface-generated spin currents inducing DL SO torque [20, 21]. However, this mechanism or spin Hall current are inoperative in 2D transport within vdW heterostructures or in FM/topological-insulator bilayers [5, 22].

In this Letter, we design a realistic (i.e., built atom-by-atom) vdW heterostructure monolayer-Cr$_2$Ge$_2$Te$_6$/graphene/monolayer-WS$_2$, as depicted in Fig. 1. Here Cr$_2$Ge$_2$Te$_6$ [23, 24] is an example of the recently discovered 2D ferromagnets [9, 10], and WS$_2$ is a transition-metal dichalcogenide (TMD) with strong SOC in monolayer form [25]. Unlike isolated graphene which is nonmagnetic and it hosts minuscule intrinsic SOC [26], doubly proximitized graphene within Cr$_2$Ge$_2$Te$_6$/graphene/WS$_2$ trilayer offers a versatile “theoretical laboratory” to differentiate between competing mechanisms of SO torque and thereby learn how to control them. This can be accomplished by switching on and off different terms in the first-principles-derived Hamiltonian [Eq. (1)] of the heterostructure and then by performing quantum transport calculations.

Using density functional theory (DFT), we first compute the band structure [Figs. 2 and 3] of the trilayer. Since the Dirac cones of graphene are largely preserved within the band gap of Cr$_2$Ge$_2$Te$_6$, an effective Hamiltonian for graphene only can be extracted in Eq. (1) below. Such a Hamiltonian can be used as an input for diagrammatic perturbative analytic calculations [27] based on the Kubo formula [28] for nonequilibrium spin density $\langle \hat{s}(r) \rangle_{CD}$ within graphene, which exerts torque $\alpha \langle \hat{s}(r) \rangle_{CD} \times \mathbf{m}_C(r)$ on the local magnetization $\mathbf{m}_C(r)$ in graphene. Note that $\mathbf{m}_C(r)$ is induced by magnetic proximity effect originating from Te atoms of Cr$_2$Ge$_2$Te$_6$, so that $\mathbf{m}_C \parallel \mathbf{m}_{Te}$ but these two magnetic moments are antiparallel to $\mathbf{m}_{Cr}$ on Cr atoms, as illustrated in Fig. 1. Alternatively, one can discretize continuous Hamiltonian in Eq. (1) to obtain its tight-binding (TB) version, as provided in the Supplemental Material (SM) [31], and combine it with computational quantum transport. We feed such first-principles TB Hamiltonian into the calculations [29, 30] of current-driven (CD) part of nonequilibrium density matrix $\hat{\rho}_{CD}$, which yields $\langle \hat{s}(r) \rangle_{CD} = \operatorname{Tr}_{\text{spin}} [\hat{\rho}_{CD} \hat{s}]$ on site $i$ of TB lattice for $\hat{s} = (\hat{s}_x, \hat{s}_y, \hat{s}_z)$ as the vector of the Pauli matrices. The matrix $\hat{\rho}_{CD}$ is computed via the nonequilibrium Green function (NEGF) formalism [39] for the Landauer setup where vdW heterostructure in Fig. 1 is divided into the left (L) semi-infinite-lead connected to “active region” which is con-
TABLE I. The fitting parameters in the continuous Hamiltonian [Eq. (1)] of doubly proximitized graphene within Cr$_2$Ge$_2$Te$_6$/graphene/WS$_2$ vdW heterostructure. The values of parameters fit the DFT bands both with and without SOC.

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<th>calc.</th>
<th>X</th>
<th>$v_F$ [10$^3$ m/μs]</th>
<th>Δ [meV]</th>
<th>$\lambda^A_\text{ex}$ [meV]</th>
<th>$\lambda^B_\text{ex}$ [meV]</th>
<th>$\lambda_R$ [meV]</th>
<th>$\lambda^A_R$ [meV]</th>
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<td>1.326</td>
<td>-3.644</td>
<td>-3.534</td>
<td>-</td>
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<td>-0.054</td>
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<tr>
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<td>0.244</td>
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The fitting parameters for Cr$_2$Ge$_2$Te$_6$/graphene/WS$_2$ trilayer are summarized in Table I. They are in agreement with previous calculations for individual graphene/TMD [25, 51] and graphene/Cr$_2$Ge$_2$Te$_6$ slabs [33]. As seen from Fig. 3, Hamiltonian in Eq. (1) with parameters from Tab. I perfectly reproduces first-principles results, including the spin expectation values in both valleys. The valley degeneracy is broken, which is best manifested at the highest (lowest) spin↑ (spin↓) bands at K and K’. This is due to the interplay of the proximity exchange and SO couplings which splits the bands in the two valleys differently. Furthermore, the Rashba SOC mixes the spin states and opens a global band gap, different for the two valleys. The SM [31] also provides equilibrium spin textures, as well as the band structure and fitting parameters for other Cr$_2$X$_2$Te$_6$/graphene/WS$_2$ trilayers and Cr$_2$X$_2$Te$_6$/graphene bilayers with X = {Si,Ge,Sn}.

**Quantum transport calculations of SO torque.**—The NEGF is computed for the active region of vdW heterostructure in Fig. 1, which is chosen as graphene nanoribbon of width W with armchair edges (illustrated in Fig. S4 in the SM [31]) that is periodically repeated along the y-axis. The nanoribbon is described by the first-principles TB Hamiltonian [Eq. (1)] in the SM [31], and all transport quantities are $k_F$-points sampled to take into account an infinitely wide system [43].
The conventional spin-transfer torque [29] in spin valves and magnetic tunnel junctions is decomposed into the FL and DL components, \( \mathbf{T} = \mathbf{T}^{\text{DL}} + \mathbf{T}^{\text{FL}} \), each of which has relatively simple angular dependence. Conversely, the SO torque with its complex angular dependence [53] is naturally decomposed [18, 30], \( \mathbf{T} = \mathbf{T}^{\text{c}} + \mathbf{T}^{\text{o}} \), into the odd \( \mathbf{T}^{\text{o}} \) and even \( \mathbf{T}^{\text{c}} \) components in the magnetization \( \mathbf{m}_C \) receiving the torque. They are obtained by averaging over \( N_A \) atoms of the triangular sublattice A and \( N_B \) atoms of the triangular sublattice B of graphene

\[
\mathbf{T}^{\text{e,o}}(k_y) = \frac{1}{N_A} \sum_{i \in A} \left( -\frac{2\lambda_{\text{ex}}}{\hbar} \right) \langle \hat{s}_i \rangle^{\text{e,o}}(k_y) \times \mathbf{m}_C \\
+ \frac{1}{N_B} \sum_{j \in B} \frac{2\lambda_{\text{ex}}}{\hbar} \langle \hat{s}_j \rangle^{\text{e,o}}(k_y) \times \mathbf{m}_C. 
\tag{2}
\]

The total torque is the sum over the first Brillouin zone (BZ), \( \mathbf{T}^{\text{e,o}} = \frac{1}{2\pi} \int_{\text{BZ}} \mathbf{T}^{\text{e,o}}(k_y) dk_y \). The NEGF-based algorithm to split the density matrix, \( \hat{\rho}_{\text{CD}} = \hat{\rho}_{\text{CD}}^{\text{e}} + \hat{\rho}_{\text{CD}}^{\text{o}} \), is given in Refs. [29], so that tracing Pauli matrices with \( \hat{\rho}_{\text{CD}}^{\text{e}} \) and \( \hat{\rho}_{\text{CD}}^{\text{o}} \) yields directly \( \langle \hat{s}_i \rangle^{\text{e}}_\text{CD} \) and \( \langle \hat{s}_i \rangle^{\text{o}}_\text{CD} \) and the corresponding SO torque components in Eq. (2).

The magnitudes of odd and even SO torque components are plotted in Fig. 4(a),(b) in the units of eVb/A, where A is the area of a single hexagon of the honeycomb lattice. We assume that back gate and top gate can change the carrier density globally or locally, respectively, thereby making it possible to tune the Fermi energy \( E_F \) of the whole device while concurrently creating a potential barrier within its smaller region, as demonstrated experimentally [42]. Without a potential barrier, \( U_{tg} = 0 \), and in the ballistic regime with no impurities, the only nonzero component in Fig. 4(a) is \( \mathbf{T}^{\text{o}} \neq 0 \). Upon introducing \( U_{tg} \neq 0 \) in still clean graphene, Fig. 4(b) reveals emergence of \( \mathbf{T}^{\text{e}} \neq 0 \). Furthermore, combined tuning of \( E_F \) and potential barrier height in Fig. 4(b) modulates the ratio \( |\mathbf{T}^{\text{o}}|/|\mathbf{T}^{\text{e}}| \) by an order of magnitude, which is of great importance for applications [13]. We fix the height of the homogeneous barrier, within the gray rectangle of the active region region in Fig. 4(d),(e), at \( U_{tg} = 0.1 \text{ eV} \) which brings clean graphene into the “pseudo-diffusive” [54, 55] transport regime (characterized by the same shot noise [56] as truly diffusive regime due to impurities).

To clarify how \( \mathbf{T}^{\text{c}} \) emerges from zero in graphene without any scattering to nonzero value, Figs. 4(c) and 4(d),(e) plot spatial profiles of nonequilibrium spin densities \( \langle \hat{s}_i \rangle^{\text{e,o}}_\text{CD} \) [Eq. (2)] in the absence or presence of potential barrier, respectively. In Fig. 4(c), only \( \langle \hat{s}_i \rangle^{\text{o}}_\text{CD} \neq 0 \) is nonzero along the \( y \)-axis and slightly out of the plan in Fig. S5(a) in the SM [31] for current injected along the \( x \)-axis. This is the well-known inverse spin-galvanic (or Edelstein) effect [57–59] in which current through 2D electron system with SOC, and thereby generated spin texture with spin-momentum locking, induces \( \langle \hat{s}_i \rangle^{\text{o}}_\text{CD} \neq 0 \). But here this effect is operative in the ballistic transport regime [40, 41], instead of originally considered diffusive regime [57, 58]. Upon introducing impurities [leading to dashed red line in Fig. 4(c)], as random on-site potential to establish the diffusive regime, or the barrier [leading to solid red line in Fig. 4(e)], \( \langle \hat{s}_i \rangle^{\text{o}}_\text{CD} \) acquires additional components in the other two spatial directions. This means that components of \( \langle \hat{s}_i \rangle^{\text{e}}_\text{CD} \) emerge along the \( x \) [Fig. 4(c),(e)] and the \( z \)-axis [Fig. S5 in the SM [31]] to comprise \( \langle \hat{s}_i \rangle^{\text{e}}_\text{CD} \) vector. Thus, scat-

\[ \text{FIG. 4. The magnitude of odd \( |\mathbf{T}^{\text{o}}| \) and even \( |\mathbf{T}^{\text{c}}| \) SO torque components as a function of \( E_F \) for proximity magnetization of graphene \( \mathbf{m}_C \parallel \hat{z} \) [Fig. 1]: (a) without the on-site energy \( U_{tg} = 0 \); and (b) with a constant on-site energy \( U_{tg} = 0.1 \text{ eV} \) in the active region which creates a homogeneous potential barrier. The corresponding odd and even energy\( E \) for proximity magnetization of graphene \( \mathbf{m}_C \parallel \hat{z} \) [Fig. 1]: (a) without the on-site energy \( U_{tg} = 0 \); and (b) with a constant on-site energy \( U_{tg} = 0.1 \text{ eV} \) in the active region which creates a homogeneous potential barrier, respectively. In Fig. 4(c), only \( \langle \hat{s}_i \rangle^{\text{o}}_\text{CD} \neq 0 \) is nonzero along the \( y \)-axis and slightly out of the plan in Fig. S5(a) in the SM [31] for current injected along the \( x \)-axis. This is the well-known inverse spin-galvanic (or Edelstein) effect [57–59] in which current through 2D electron system with SOC, and thereby generated spin texture with spin-momentum locking, induces \( \langle \hat{s}_i \rangle^{\text{o}}_\text{CD} \neq 0 \). But here this effect is operative in the ballistic transport regime [40, 41], instead of originally considered diffusive regime [57, 58]. Upon introducing impurities [leading to dashed red line in Fig. 4(c)], as random on-site potential to establish the diffusive regime, or the barrier [leading to solid red line in Fig. 4(e)], \( \langle \hat{s}_i \rangle^{\text{o}}_\text{CD} \) acquires additional components in the other two spatial directions. This means that components of \( \langle \hat{s}_i \rangle^{\text{e}}_\text{CD} \) emerge along the \( x \) [Fig. 4(c),(e)] and the \( z \)-axis [Fig. S5 in the SM [31]] to comprise \( \langle \hat{s}_i \rangle^{\text{e}}_\text{CD} \) vector. Thus, scat-}
tering off either the barrier or impurities is required to produce $\langle \hat{s}_i \rangle_{CD}$ and $T^o \neq 0$. Previously discussed mechanisms [27, 60] for purely interfacial $T^o \neq 0$ require spin-active impurities that scatter spin-$\uparrow$ and spin-$\downarrow$ electrons differently. However, the potential barrier and/or short-ranged impurities we employ in Fig. 4 are spin-independent. Nonetheless, impurities can generate skew-scattering [44] due to proximity SOC in the band structure and sublattice-staggered potentials in Eq. (1) which conspire to tilt (Fig. S1 in the SM [31]) the equilibrium spin textures out of the plane, even when $m_C = 0$ [51], while the barrier also requires $m_C \neq 0$ to generate $\langle \hat{s}_i \rangle_{CD}$ components in all spatial directions.

Finally, to connect $T^o$ and $T^o$ to traditionally discussed DL and FL torque components, we need to take into account typically complex angular dependence of SO torque observed experimentally [53] or in first-principles quantum transport studies [8, 18, 30]. For this purpose, we fit computational data (dots in Fig. S6 in the SM [31]) with an infinite series [8, 30, 53] for $T^o$ and $T^o$ vector fields on the unit sphere of orientations of $m_C$. The non-negligible terms, compatible with the lattice symmetry, are given by

\[
T^o = [\tau^o_0 + \tau^o_2 |\hat{z} \times m_C|^2 + \tau^o_4 |\hat{z} \times m_C|^4] (\hat{y} \times m_C),
\]

(3a)

\[
T^o = [\tau^o_0 + \tau^o_2 |\hat{z} \times m_C|^2 + \tau^o_4 |\hat{z} \times m_C|^4] m_C \times (\hat{y} \times m_C),
\]

(3b)

with parameter values listed in Table SIII in the SM [31]. Here we recognize the lowest-order term $\tau^o_0 \hat{y} \times m_C$ as the FL SO torque, which is the only term (Table SIII in the SM [31]) generated in the ballistic transport regime of Fig. 4(a),(c). The usual DL SO torque [1] is $\tau^o_0 m_C \times (\hat{y} \times m_C)$. Higher order terms in Eq. (3) can have properties of both FL and DL torques [18]. Fitted functions in Eq. (3) are also required for coupling [8] computed SO torque to micromagnetic simulations [12] of classical dynamics of $m_C(t)$.

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[31] See Supplemental Material at https://wiki.physics.udel.edu/qttg/Publications (which includes Refs. [32–38]) for details of DFT calculations; equilibrium spin textures; band structure and fitting parameters for Cr$_2$X$_2$Te$_6$/graphene trilayers with and without additional monolayer WS$_2$, where X = {Si, Ge, Te}; TB Hamiltonian counterpart of Eq. (1); and fitting parameters in Eq. (3).


M. Chshiev, Tailoring magnetic insulator proximity effects in graphene: First-principles calculations, 2D Mater. 4, 025074 (2017).


Purely interfacial and highly tunable by gate or disorder spin-orbit torque in graphene doubly proximitized by two-dimensional ferromagnet Cr$_2$Ge$_2$Te$_6$ and monolayer WS$_2$

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$^2$Department of Mathematical Sciences, University of Delaware, Newark, DE 19716, USA
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I. ADDITIONAL INFORMATION FOR FIGURES 2 AND 3 IN THE MAIN TEXT

A. Computational details of DFT calculations

The electronic structure calculations and structural relaxation for graphene on Cr$_2$Ge$_2$Te$_6$, as well as for graphene sandwiched between WS$_2$ and Cr$_2$X$_2$Te$_6$ with X = {Si, Ge, Te}, are performed by density functional theory (DFT) implemented in Quantum ESPRESSO package [1]. The heterostructure supercell consists of 5 × 5 supercell of graphene whose bottom surface is covered by a $\sqrt{3} \times \sqrt{3}$ supercell of Cr$_2$Ge$_2$Te$_6$, while its top surface is covered by a 4 × 4 supercell of WS$_2$. We stretch the lattice constant of graphene by roughly 2%—from 2.46 Å to 2.5 Å—and stretch the lattice constant of Cr$_2$Ge$_2$Te$_6$ by roughly 6%—from 6.8275 Å [2] to 7.2169 Å. The WS$_2$ lattice constant is compressed by roughly 1%—from 3.153 Å [3] to 3.125 Å. The heterostructure supercell has a lattice constant of 12.5 Å and it contains 128 atoms. The distance between WS$_2$ and graphene is $\approx$ 3.28 Å, in agreement with previous calculations [4]. The distance between Cr$_2$Ge$_2$Te$_6$ and graphene is about 3.52 Å, also in agreement with previous calculations [5].

Bulk vdW crystal Cr$_2$Ge$_2$Te$_6$, which is composed of weakly bound monolayers, has Curie temperature $T_C \approx 60$ K and PMA. Each monolayer is formed by edge-sharing CrTe$_6$ octahedra where Ge pairs are located in the hollow sites formed by the octahedra honeycomb. The layers are ABC-stacked, resulting in a rhombohedral $R\bar{3}$ symmetry.

We use 24 × 24 × 1 (18 × 18 × 1 for the sandwich structure) $k$-point grid in self-consistent calculations to ensure converged results for the proximity exchange interaction and proximity spin-orbit coupling (SOC). We also perform open shell calculations that provide the spin-polarized ground state of Cr$_2$Ge$_2$Te$_6$. The Hubbard $U = 1$ eV is used for Cr $d$-orbitals, being in the range of proposed $U$ values for this compound [6]. The Perdew-Burke-Ernzerhof parametrization [7] of the generalized gradient approximation for the exchange-correlation functional is employed. We use an energy cutoff for charge density of 500 Ry, and the kinetic energy cutoff for wavefunctions is 60 Ry for the scalar relativistic pseudopotential within the projector augmented wave method [8] describing electron-core interactions. When SOC is included, we use the relativistic versions of the pseudopotentials.

For the relaxation of the heterostructures, we add vdW corrections [9, 10] and use quasi-Newton algorithm based on trust radius procedure. In order to simulate quasi-two-dimensional systems, we add a vacuum of 20 Å which avoids interactions between periodic images in the slab geometry. To determine the interlayer distances, the atoms of graphene and WS$_2$ are allowed to relax only along the $z$-axis (perpendicular to the layers), while the atoms of Cr$_2$Ge$_2$Te$_6$ are allowed to move in all directions, until all components of all forces are reduced below $10^{-3}$ Ry/Å$_0$ ($a_0$ is the Bohr radius).

Table S1 summarizes fitting parameters in the continuous Hamiltonian [Eq. (1) in the main text] for graphene within Cr$_2$X$_2$Te$_6$/graphene/WS$_2$ trilayers with X = {Si, Ge, Sn}. The same parameters are also used in the tight-binding (TB) version [Eq. (1)] of the continuous Hamiltonian.

B. Equilibrium spin textures in Cr$_2$Ge$_2$Te$_6$/graphene/WS$_2$ trilayer

Figure S1 shows DFT-calculated equilibrium spin textures (i.e., expectation values of the Pauli matrices in the eigenstates of the DFT Hamiltonian) for Cr$_2$Ge$_2$Te$_6$/graphene/WS$_2$ trilayer, with proximity magnetization of graphene pointing out of the plane [Fig. S1(a)–(d)] or in the plane [Fig. S1(e)–(h)]. The textures are plotted in the $k_x k_y$-plane in the vicinity of the K and K’ points at energies belonging to the conduction and valence bands, respectively. Thus, they complement the low-energy band structure shown in Fig. 3 in the main text. The bands are strongly $s_z$-polarized with some small in-plane contribution. The pattern of the in-plane contribution and the corresponding spin-momentum locking is characteristic of the Rashba SOC-induced spin texture [12].

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FIG. S1. The DFT-calculated equilibrium spin texture of: (a) conduction; and (b) valence band of Cr$_2$Ge$_2$Te$_6$/graphene/WS$_2$ trilayer around the K point. Color corresponds to $\langle \hat{s}_z \rangle$ expectation value, while arrows represent $\langle \hat{s}_x \rangle$ and $\langle \hat{s}_y \rangle$ expectation values. The dashed white lines mark the edges of the Brillouin zone. Panels (c) and (d) plot the same information as panels (a) and (b), respectively, but around the K$'$ point. Panels (e)–(h) plot the same information as panels (a)–(d), where the proximity magnetization of graphene $m_C \parallel \hat{z}$ is orthogonal to the plane in (a)–(d) and parallel to the plane $m_C \parallel \hat{x}$ (i.e., along the x-axis in Fig. 1 in the main text) in (e)–(h).

TABLE SI. The fitting parameters of continuous Hamiltonian in Eq. (1) in the main text for Cr$_2$X$_2$Te$_6$/graphene/WS$_2$ trilayers with $X = \{\text{Si, Ge, Te}\}$. Here $v_F$ is the Fermi velocity; $\Delta$ is the staggered potential gap; $\lambda_R$ is the Rashba SOC strength; $\lambda^A_{ex}$ and $\lambda^B_{ex}$ are sublattice-resolved intrinsic SOC parameters; $\lambda^A_{I}$ and $\lambda^B_{I}$ are sublattice-resolved exchange interaction parameters; $\xi$ is the valley exchange parameter; and $E_D$ is the Dirac point energy. The values of parameters fit the DFT-computed bands both with and without SOC.

<table>
<thead>
<tr>
<th>calc.</th>
<th>$X$</th>
<th>$v_F$ [10$^5$ m/s]</th>
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<td>-</td>
<td>-0.053</td>
</tr>
<tr>
<td>SOC</td>
<td>Si</td>
<td>7.921</td>
<td>0.809</td>
<td>-1.964</td>
<td>-1.875</td>
<td>-0.397</td>
<td>1.127</td>
<td>-1.152</td>
<td>0.268</td>
<td>0.008</td>
</tr>
<tr>
<td>SOC</td>
<td>Ge</td>
<td>7.903</td>
<td>1.252</td>
<td>-3.481</td>
<td>-3.650</td>
<td>-0.489</td>
<td>1.083</td>
<td>-1.118</td>
<td>0.244</td>
<td>-0.247</td>
</tr>
<tr>
<td>SOC</td>
<td>Sn</td>
<td>7.746</td>
<td>2.055</td>
<td>-6.281</td>
<td>-6.310</td>
<td>-0.696</td>
<td>1.009</td>
<td>-1.057</td>
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<tr>
<td>no SOC</td>
<td>Ge</td>
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<td>1.602</td>
<td>-4.591</td>
<td>-4.422</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
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<tr>
<td>SOC</td>
<td>Ge</td>
<td>8.026</td>
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<td>-4.566</td>
<td>-4.559</td>
<td>-0.467</td>
<td>1.148</td>
<td>-1.184</td>
<td>0.158</td>
<td>0.004</td>
</tr>
</tbody>
</table>

*a* Calculated with WIEN2k package [11], using the relaxed geometry from Quantum ESPRESSO package [1], and a k-point sampling of 12 $\times$ 12 $\times$ 1. The cutoff is $R_{\text{Kmax}} = 4.0$ and the muffin-tin radii are $R_{\text{TP}} = 2.5$, $R_{\text{Ge}} = 2.25$, $R_{\text{Cr}} = 2.5$, $R_{\text{C}} = 1.36$, $R_{\text{W}} = 2.48$, and $R_{\text{S}} = 2.03$. The vdW corrections and a Hubbard $U = 1.0$ eV are also included.

C. Band structure of Cr$_2$Ge$_2$Te$_6$/graphene bilayers

The supercell of Cr$_2$Ge$_2$Te$_6$/graphene bilayer is depicted in Fig. S2(d), where a 5 $\times$ 5 supercell of graphene is placed on a $\sqrt{3} \times \sqrt{3}$ supercell of Cr$_2$Ge$_2$Te$_6$. We keep the lattice constant of graphene unchanged at $a = 2.46$ Å and stretch the lattice constant of Cr$_2$Ge$_2$Te$_6$ by roughly 4% from 6.8275 Å [2] to 7.1014 Å. The resulting supercell has a lattice constant of 12.3 Å and contains 80 atoms in the unit cell. The average distance between graphene and Cr$_2$Ge$_2$Te$_6$ is relaxed to 3.516 Å, consistent with previous calculations [5]. In the case of Cr$_2$Si$_2$Te$_6$/graphene and Cr$_2$Sn$_2$Te$_6$/graphene we get interlayer distances of 3.568 Å and 3.541 Å, respectively.

It has been shown previously [5] that proximity in-
TABLE SII. The fitting parameters of continuous Hamiltonian in Eq. (1) in the main text for Cr$_2$X$_2$Te$_6$/graphene bilayers with X = Si, Ge, Te. These parameters have the same meaning as those in Table SI. The values of parameters fit the DFT-computed bands both with and without SOC.

<table>
<thead>
<tr>
<th>calc.</th>
<th>X</th>
<th>$\nu_F$ [10$^3$ m/s]</th>
<th>$\Delta$ [meV]</th>
<th>$\lambda_{\alpha}$ [meV]</th>
<th>$\lambda_{\beta}$ [meV]</th>
<th>$\lambda_{\gamma}$ [meV]</th>
<th>$\lambda_{\delta}$ [meV]</th>
<th>$\xi$ [meV]</th>
<th>$E_D$ [meV]</th>
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<tbody>
<tr>
<td>no SOC</td>
<td>Si</td>
<td>8.214</td>
<td>0.005</td>
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<td>-1.243</td>
<td>-</td>
<td>-</td>
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<td>-</td>
</tr>
<tr>
<td>no SOC</td>
<td>Ge</td>
<td>8.175</td>
<td>0.115</td>
<td>-4.705</td>
<td>-4.543</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
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<td>Sn</td>
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<td>0.119</td>
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<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>SOC</td>
<td>Si</td>
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<td>-1.195</td>
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<td>-0.185</td>
<td>0.122</td>
<td>-0.092</td>
<td>0.204</td>
</tr>
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<td>SOC</td>
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<td>0.133</td>
<td>-0.093</td>
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<td>SOC</td>
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<td>0.118</td>
<td>-0.124</td>
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<tr>
<td>no SOC</td>
<td>Ge</td>
<td>8.204</td>
<td>0.118</td>
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<td>-5.850</td>
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<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>SOC $^a$</td>
<td>Ge</td>
<td>8.213</td>
<td>0.114</td>
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<td>-5.216</td>
<td>-0.318</td>
<td>0.149</td>
<td>-0.121</td>
<td>0.037</td>
</tr>
</tbody>
</table>

$^a$ Calculated with WIEN2k package [11], using a k-point sampling of 12 × 12 × 1. The cutoff is RK$_{max}$ = 4.3 and the muffin-tin radii are R$_{Te}$ = 2.5, R$_{Ge}$ = 2.25, R$_{Cr}$ = 2.5, and R$_C$ = 1.33. The vdW corrections and a Hubbard U = 1 eV are also included.

FIG. S2. (a) The DFT-calculated electronic band structure of Cr$_2$Ge$_2$Te$_6$/graphene bilayer without SOC. Bands with spin $\uparrow$ ($\downarrow$) are shown in red (blue). (b) A zoom to DFT-calculated low energy bands (symbols) in panel (a) at the K point with a fit to the continuous Hamiltonian (solid lines) in Eq. (1) in the main text. (c) DFT-calculated electronic band structure of Cr$_2$Ge$_2$Te$_6$/graphene bilayer with SOC. The color corresponds to $\langle \hat{s}_z \rangle$ expectation value. (d) Side view of the geometry of monolayer graphene on monolayer Cr$_2$Ge$_2$Te$_6$.

FIG. S3. (a) Zoom to DFT-calculated low energy bands in Fig. S2(c) for Cr$_2$Ge$_2$Te$_6$/graphene bilayer around the K point with SOC. Color of the bands corresponds to $\langle \hat{s}_z \rangle$ expectation value. (b) The $\langle \hat{s}_z \rangle$ expectation value of the valence (conduction) band is shown in blue (red). Symbols are DFT-bands and solid lines are continuous Hamiltonian [Eq. (1) in the main text] bands. Panels (c) and (d) plot the same information as panels (a) and (b), respectively, but around the K$'$ point.

Reduced exchange interaction in graphene due to monolayer Cr$_2$Ge$_2$Te$_6$ is an order of magnitude larger than proximity induced SOC by the same monolayer. Therefore, we first perform calculations with SOC turned off. Figure S2(a) shows DFT-calculated band structure for Cr$_2$Ge$_2$Te$_6$/graphene bilayer without SOC. In general, the band structure resembles that of an isolated ferromagnetic semiconductor Cr$_2$Ge$_2$Te$_6$ [6], with the graphene Dirac cone located in the gap of monolayer Cr$_2$Ge$_2$Te$_6$. The linear dispersion of graphene is nicely preserved, however the bands are spin-split due to proximity induced exchange interaction.

Without SOC, the band structure around the two val-


FIG. S4. Schematic view of an armchair nanoribbon of doubly proximitized graphene from Fig. 1 in the main text, which is employed in quantum transport calculations of SO torque as the active region of the device in Fig. 1 in the main text. The nanoribbon is periodically repeated along the y-axis in order to model the whole trilayer being infinite in the x-y plane. Solid and dashed arrows denote the direction of positive next-nearest neighbor hopping in Eq. (1) and periodic (k_y-dependent) hopping connecting the carbon atoms along the armchair edges of the nanoribbon, respectively.

...les K and K' are the same. When SOC is turned off the global band gap at \( E - E_F = 0 \) is absent. Figure S2(c) shows how the band structure gets modified when SOC is turned on. As demonstrated in Fig. S2(b), the bands of the continuous Hamiltonian in Eq. (1) in the main text, with parameters provided in Table SII, fit perfectly the DFT-calculated low energy bands in a small energy window around the Fermi level.

In addition, Fig. S3 shows a zoom to the fine structure around the K and K' points, including a fit with bands of the continuous Hamiltonian in Eq. (1) in the main text, when SOC is turned on. The fit can perfectly reproduce the DFT-computed band structure around both valleys.

The fitting parameters are summarized in Table SII for the calculations with and without SOC. We find that a tiny gap opens due to SOC, which is responsible for mixing the two spin components. The proximity exchange parameters are on the order of 5 meV, and proximity SOC is an order of magnitude smaller. As shown in Table SII, DFT calculations with and without SOC show no significant change of the proximity exchange parameters \( \lambda_{ex}^A \) and \( \lambda_{ex}^B \), the staggered potential induced gap \( \Delta \) and the Fermi velocity \( v_F \).

In addition to matching the bands, Fig. S3(b),d demonstrates that \( \langle s_z \rangle \) expectation values of the valence and conduction band agree perfectly with those from the model Hamiltonian. The bands are fully \( s_z \)-polarized due to the strong proximity exchange coupling induced by monolayer Cr_2Ge_2Te_6. Where SOC mixes the spin-up and spin-down bands, a gap is opened and \( \langle s_z \rangle \) expectation values change in sign. The \( \langle s_x \rangle \) and \( \langle s_y \rangle \) expectation values (not shown) are very small and show a signature of Rashba SOC in agreement with the small \( \lambda_R \) parameter in Table SII.

As a further consistency check, we recalculated the band structure with Quantum ESPRESSO package [1], which we can attribute to the different basis sets, number of k-points, and cutoffs used.

II. ADDITIONAL INFORMATION FOR FIGURE 4 IN THE MAIN TEXT

A. Tight-binding version of continuous Hamiltonian in Eq. (1) in the main text

The first-principles TB Hamiltonian employed in quantum transport calculations in Fig. 4 in the main text, as well as in Figs. S5 and Fig. S6 below, is discretized version of the continuous Hamiltonian in Eq. (1) in the main text. Its terms are given by

\[
\hat{H} = \hat{H}_0 + \hat{H}_\Delta + \hat{H}_1 + \hat{H}_R + \hat{H}_{ex},
\]

\[
\hat{H}_0 = -t \sum_{\langle i,j \rangle} \sum_{\sigma} c_{i\sigma}^\dagger c_{j\sigma} + U_{tg} \sum_i c_{i\uparrow} c_{i\downarrow} c_{i\downarrow}^\dagger c_{i\uparrow}^\dagger
\]

\[
\hat{H}_\Delta = \sum_{S=A,B} \sum_i \sum_{\sigma} \Delta \xi_{S} c_{i\sigma}^\dagger c_{i\sigma},
\]

\[
\hat{H}_1 = \sum_{S=A,B} \sum_{\langle i,j \rangle} \sum_{\sigma} \nu_{ij} \xi_{\sigma} \xi_{\sigma}^\dagger c_{i\sigma}^\dagger c_{j\sigma},
\]

\[
\hat{H}_R = \frac{2i\lambda_R}{\sqrt{3}} \sum_{\langle i,j \rangle} \sum_{\sigma \neq \sigma'} \mathbf{d}_{ij} \cdot \mathbf{d}_{ij}^\dagger c_{i\sigma}^\dagger c_{j\sigma'},
\]

\[
\hat{H}_{ex} = \sum_{S=A,B} \sum_{i} \sum_{\sigma} \xi_{ex}^{S} \mathbf{m}_{C} \cdot \mathbf{\hat{r}}_{i\sigma} \mathbf{c}_{i\sigma}^\dagger \mathbf{c}_{i\sigma}.
\]

Here \( c_{i\sigma}^\dagger (\mathbf{c}_{i\sigma}) \) creates (annihilates) electron on site \( i \) with spin \( \sigma = \uparrow, \downarrow; t = 2.7 \text{ eV} \) is the nearest-neighbor hopping; \( \xi_{A} = 1 \) for triangular sublattice A and \( \xi_{B} = -1 \) for triangular sublattice B; sum \( \langle i,j \rangle \) goes over all pairs of nearest-neighbor sites, while sum \( \langle i,j \rangle \) goes over all pairs of next-nearest-neighbor sites on sublattices A and B; and \( \mathbf{d}_{ij} \) is the vector connecting nearest neighbor sites \( i \) and \( j \). The parameter \( \nu_{ij} \) is either \(+1\) or \(-1\) depending on the hopping direction, where positive direction for the next-nearest-neighbor hoppings on sublattices A and B is shown in Fig. S4. Other symbols have the same meaning as in Eq. (1) in the main text, and the values of the fitting parameters are the same as in Table I in the main text or Table SII.

The only difference between the continuous Hamiltonian in Eq. (1) in the main text and the TB Hamiltonian in Eq. (1) is neglect of \( \hat{H}_\xi \) term in Eq. (1) due to small value of \( \xi \) parameter in Table SII. Another difference is in that \( \mathbf{m}_{C} \) as the unit vector along the proximity induced magnetization of graphene in \( \hat{H}_{ex} \) can point in any direction to make it possible to study the angular dependence of the SO torque in Fig. S6. In contrast, this term is fixed only along the z-axis in Eq. (1) in the main text.

To remove the effect of the edges and mimic wide junctions along the y-axis often employed experimentally [13], sites on the lower and upper edge of armchair graphene...
TABLE SIII. The fitting parameters in Eq. (2).

<table>
<thead>
<tr>
<th>$U_{tg}$ (eV)</th>
<th>$\tau_0^0$ (eV_b/A)</th>
<th>$\tau_2^0$ (eV_b/A)</th>
<th>$\tau_4^0$ (eV_b/A)</th>
<th>$\tau_0^T$ (eV_b/A)</th>
<th>$\tau_2^T$ (eV_b/A)</th>
<th>$\tau_4^T$ (eV_b/A)</th>
</tr>
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<td>0.0</td>
<td>$1.112 \times 10^{-8}$</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>0.100</td>
<td>$1.770 \times 10^{-8}$</td>
<td>$2.416 \times 10^{-9}$</td>
<td>$-2.967 \times 10^{-9}$</td>
<td>$1.560 \times 10^{-9}$</td>
<td>$1.234 \times 10^{-11}$</td>
<td>$2.262 \times 10^{-9}$</td>
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</table>

FIG. S5. Out-of-plane (i.e., along the $z$-axis in the coordinate system of Fig. 1 in the main text) component of CD nonequilibrium spin density $\langle \hat{s}_i \rangle_{CD}$ in doubly proximitized graphene with: (a) no potential barrier $U_{tg} = 0$ eV; or (b) with potential barrier due to homogeneous on-site energy $U_{tg} = 0.1$ eV within the region marked by gray rectangle. Solid lines are for clean graphene, while dashed line include spin-independent impurities modeled by random on-site energies $\in [-W/2, W/2]$ drawn from a uniform distribution with $W = 3$ eV to ensure diffusive transport. Each dashed line is geometric average over 20 disorder realizations. The magnetization $\mathbf{m}_C$ is oriented along the $z$-axis and the Fermi energy is $E_F = -0.02$ eV. The corresponding in-plane components of $\langle \hat{s}_i \rangle_{CD}$ are shown in Fig. 4(c)–(e) in the main text. The arrows denote how different $\langle \hat{s}_i \rangle_{CD}$ curves contribute to $\langle \hat{s}_i \rangle_{CD}^c$ or $\langle \hat{s}_i \rangle_{CD}^o$ vectors.

FIG. S6. (a)–(c) The angular dependence of SO torque components $|\mathbf{T}^c|$ (blue dots) and $|\mathbf{T}^o|$ (red dots) for different orientations of magnetization $\mathbf{m}_C$ of proximitized clean graphene at $E_F = -0.02$ eV and with potential barrier in the active region due to on-site potential $U_{tg} = 0.1$ eV. Gray lines in the background fit, using Eq. (2), numerically calculated SO torque values (dots). The vector $\mathbf{m}_C = (\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta)$ rotates within the $xz$-plane in (a); within the $xy$-plane in (b); and within the $yz$-plane in (c).

nanoribbon illustrated in Fig. S4 are connected [14] by a hopping with $e^{ik_y W}$ phase, where $k_y \in [-\pi/W, \pi/W]$ and $W$ is the width of the nanoribbon. Solid and dashed arrows within the nanoribbon in Fig. S4 denote the direction of positive next-nearest neighbor hopping in $\hat{H}_I$ and periodic ($k_y$-dependent) hopping connecting the carbon atoms along the edges of the nanoribbon, respectively.

We note that quantum transport calculations using TB Hamiltonian in Eq. (1) are equivalent to computationally much more expensive calculations using DFT Hamiltonian [15], as long as one remains in the linear-response transport regime driven by small applied bias voltage. The small bias voltage $V_b \ll E_F$ is indeed utilized in the calculations in Figs. 4 in the main text and Figs. S5 and S6. This is due to the fact that self-consistent re-calculation of particle densities and the Hamiltonian due to current flow is nonlinear effect in the bias voltage. Trivially, one should also keep the Fermi energy $E_F$ in Fig. 4 in the main text and in Fig. S6 within the energy window around the Dirac point where the continuous Hamiltonians [Eq. (1) in the main text] or TB Hamiltonian [Eq. (1)] with parameters in Table S1 are applicable.

Figures S5(a) and S5(b) complement Figs. 4(c) and 4(d),(e) in the main text, respectively, where the latter plot only the in-plane component of current-driven (CD) nonequilibrium spin density $\langle \hat{s}_i \rangle_{CD}$. Even though the impurities we employ generate spin-independent potential, scattering off them in the presence of proximity induced band SOC terms in Eq. (1) and spin texture tilted out of the plane [Fig. S1] leads to spin-dependent skew-
scattering [16]. This then generates large out-of-plane component \((\hat{s}_1)_{CD}\) (dashed lines) in Fig. S5 which contributes to \((\hat{s}_i)_{CD}\) and the corresponding even component of SO torque, \(T_e\), via Eq. (2) in the main text.

**B. Fitting of angular dependence of SO torque**

The computed angular dependence of even, \(T_e\), and odd, \(T_o\), SO torque components—as the magnetization vector \(\mathbf{m}_C = (\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta)\) rotates within the \(xz\) and \(yz\) planes in the setup of Fig. 1 in the main text with nonzero potential barrier—is shown by dots in Fig. S6. Note that for \(\theta = 0\)°, the results in Fig. S6 correspond to the results in Fig. 4(b) in the main text at \(E_F = -0.02\) eV. As discussed in the main text, we fit these dots with the following expansions

\[
T_e = \left[\tau_0^e + \tau_2^e |\hat{z} \times \mathbf{m}_C|^2 + \tau_4^e |\hat{z} \times \mathbf{m}_C|^4\right] (\hat{y} \times \mathbf{m}_C),
\]

\[
T_o = \left[\tau_0^o + \tau_2^o |\hat{z} \times \mathbf{m}_C|^2 + \tau_4^o |\hat{z} \times \mathbf{m}_C|^4\right] \mathbf{m}_C \times (\hat{y} \times \mathbf{m}_C),
\]

These functions, with fitting parameters listed in Table SIII, are then plotted as solid lines in Fig. S6. Here \(\hat{y}\) and \(\hat{z}\) are the unit vectors along the \(y\)- and \(z\)-axis, respectively, for the coordinate system in Fig. 1 in the main text. Note that prior to fitting, data sets in all three planes \((xz, xy, yz)\) are joined in a single continuous line for each case (with and without the on-site potential \(U_{1g}\)), so that they could all be fitted with a single set of fitting parameters.

---


[6] G. Menichetti, M. Calandra, and M. Polini, Electronic structure and magnetic properties of few-layer \(\text{Cr}_2\text{Ge}_2\text{Te}_6\): The key role of nonlocal electron-electron interaction effects, 2D Mater. 6, 045042 (2019).


