

Giant Spin-Orbit Torque in Cr-based Janus Transition Metal Dichalcogenides

Libor Vojáček,^{1,*} Joaquín Medina Dueñas,^{2,3,*} Jing Li,⁴ Fatima Ibrahim,¹
Aurélien Manchon,⁵ Stephan Roche,^{2,6} Mairbek Chshiev,^{1,7} and José H. García²

¹Université Grenoble Alpes, CEA, CNRS, IRIG-Spintec, 38000 Grenoble, France

²ICN2 — Catalan Institute of Nanoscience and Nanotechnology,
CSIC and BIST, Campus UAB, Bellaterra, 08193 Barcelona, Spain

³Department of Physics, Universitat Autònoma de Barcelona (UAB),
Campus UAB, Bellaterra, 08193 Barcelona, Spain

⁴Université Grenoble Alpes, CEA, Leti, F-38054, Grenoble, France

⁵Aix-Marseille Université, CNRS, CINAM, Marseille 13288, France

⁶ICREA — Institució Catalana de Recerca i Estudis Avançats, 08010 Barcelona, Spain

⁷Institut Universitaire de France, 75231 Paris, France

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We report a very large spin-orbit torque (SOT) capability of chromium-based transition metal dichalcogenides (TMD) in their Janus forms CrXTe, with X=S,Se. The structural inversion symmetry breaking, inherent to Janus structures is responsible for a large SOT response generated by giant Rashba splitting, equivalent to that obtained by applying a transverse electric field of $\sim 100 \text{ V nm}^{-1}$ in non-Janus CrTe₂, completely out of experimental reach. By performing transport simulations on custom-made Wannier tight-binding models, Janus systems are found to exhibit a SOT performance comparable to the most efficient two-dimensional materials, while allowing for field-free perpendicular magnetization switching owing to their reduced in-plane symmetry. Altogether, our findings evidence that magnetic Janus TMDs stand as suitable candidates for ultimate SOT-MRAM devices.

Introduction.— The spin-orbit torque (SOT) mechanism represents an innovative method to electrically manipulate the magnetization of a magnetic material [1, 2], providing remarkable energy-efficiency, writing speed and scalability prospects which have earned their insertion in magnetic random access memory (MRAM) applications [3, 4], among other developing technologies [5–7]. SOT-MRAM prototype cells have been shown to operate on the sub-nanosecond timescale [8–11], with a power consumption of merely one percent of their (already in commercial use) spin-transfer torque counterpart [12, 13]. Although next-generation SOT-based technologies advance at a steady pace, they still face issues regarding massive density and integration. The development of SOT-MRAMs remains limited to multi-layered devices, where SOT figures of merit are strongly sensitive to interface quality; while additionally, a densely packed SOT-MRAM requires electrical switching of a perpendicular magnetic anisotropy (PMA) [14], which is only achieved in conventional devices with the assistance of an external magnetic field.

Two-dimensional materials offer alternative paths to overcome these issues. Atomically clean interfaces have been shown to enhance both charge-to-spin conversion [15–17] and tunneling magnetoresistance [18, 19] while reducing the cell dimensions. Furthermore, precise control of crystal symmetries enables novel SOT mechanisms that allow for *field-free* PMA switching [20, 21]. Materials such as CrTe₂ [22–25] and Fe_nGeTe₂ ($n = 3, 4, 5$) [26–30] offer the most promising alternatives to overcome the usually low Curie temperature (T_C) of van der Waals ferromagnets (FM); where additional gating, strain and chemical composition engineering allow to

tune their magnetic properties [27, 31–33]. New avenues for SOT devices are opened when exploiting the metallic nature of these materials along with their strong spin-orbit coupling (SOC), overcoming multi-layer designs in favor of an all-in-one platform where the FM acts as both the SOC material and the free magnetization in a self-induced SOT scheme [34–38]. In this context, Janus transition metal dichalcogenide (TMD) monolayers stand out as the material of choice [39–41]. Indeed, the CrXTe ultrathin layers, similar to their non-Janus counterpart CrTe₂ [42], are expected to be magnetic with PMA under the adequate experimental conditions, high T_C even exceeding room temperature, and are most stable in their metallic 1T-phase [43, 44]. Inversion symmetry forbids a SOT response in CrTe₂; however, this stepback is overcome by breaking the symmetry between both chalcogen atoms, for instance, by applying an electric field transversal to the crystal plane. Another symmetry-breaking mechanism is obtained by substituting one Te atom with S or Se, thus forming the Janus CrXTe structures, where the symmetry breaking is manifested in the crystal field.

In this Letter, using first principles approach and quantum transport simulations performed on Wannier tight-binding models carefully designed to represent the reciprocal spin textures, together with critical field-free PMA switching current calculations, we report an exceptional SOT performance of chromium-based Janus TMD monolayers CrXTe, with X=S,Se. We compare both the Janus and non-Janus materials under electric field, demonstrating that Cr-based Janus monolayers constitute an optimal SOT platform for low-energy magnetization reversal.

Electronic structure and spin textures.— We perform first-principles calculations of the selected TMDs using

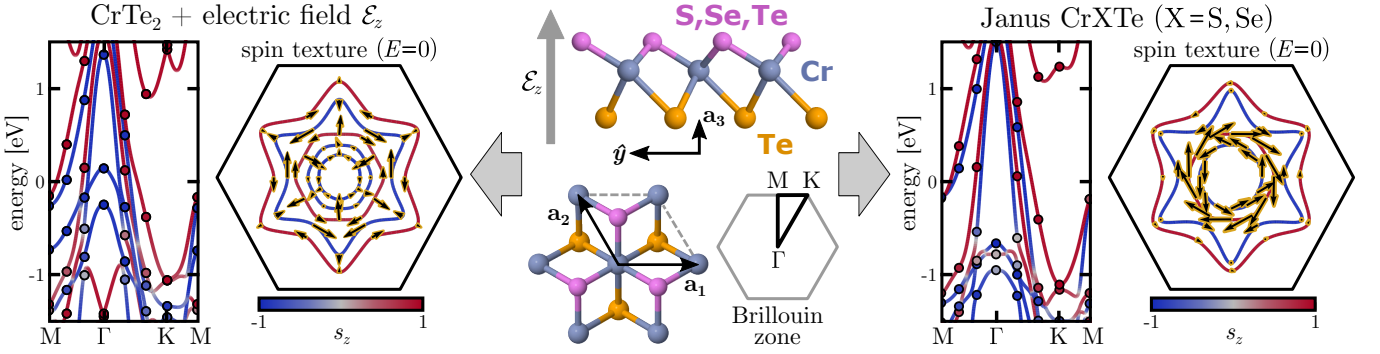


FIG. 1. Middle Panel: CrXTe Janus structure, lattice vectors and Brillouin zone. Left panel: Band structure and spin-textures of symmetric CrTe₂ under the effect of an applied electric field [$\mathcal{E} = 2 \text{ V nm}^{-1}$]. The continuous band structure curves and black spin texture arrows are obtained from the Wannier model, while the discrete band structure dots and yellow highlighted spin texture arrows are obtained from DFT calculations. Right panel: Band structure and spin textures of CrXTe [X=S, Se].

density functional theory (DFT) [45, 46] with GGA-PBE pseudopotentials [47] and an effective Hubbard U correction of 3.0 eV to localize the Cr-d orbitals. The usual metallic 1T phase displayed at the center of Fig. 1 proves to be more stable than the semiconducting 1H phase. Based on the maximally-localized Wannier functions [48, 49], we then derive tight-binding models of the DFT ground state. Accurate representations require a 22-orbital basis comprising the Cr-d and the chalcogen-p bands, with the interactions expanded into a 25×25 supercell. The *ab initio* band structure is thereby represented with an impressive $\sim 1 \text{ meV}$ accuracy in a large window of ≈ -5 to $+4 \text{ eV}$ around the Fermi level. We also carefully derive the real-space spin operator in the Wannier basis, resulting in a non-local spin that replicates the *ab initio* spin texture with $\sim 1\%$ error [50].

Overall, the comparison between DFT results and those of the Wannier model yields an excellent agreement, as shown in Fig. 1. This demonstrates the capability of our methodology, allowing to reach a DFT-level accuracy via tight-binding models for general systems.

Note that the remarkable SOT capability of the low-symmetry Janus systems is already apparent from its Fermi-level spin textures, showing a prominent helical winding in CrXTe, displayed in the right panel of Fig. 1. This large Rashba term comes from a strong inversion-symmetry breaking due to a huge *internal* out-of-plane electric field $\sim 1\text{--}2 \text{ V nm}^{-1}$ caused by a charge imbalance at the two inequivalent chalcogen atoms S/Se and Te [50]. On the contrary, an *external* electric field $\mathcal{E}_z$ applied on CrTe₂ to break its innate inversion symmetry is heavily screened due to its large dielectric constant ϵ_{CrTe_2} , reducing any applied field by a factor of $\epsilon_{\text{CrTe}_2}^{-1} \sim 0.02$ inside the layer [50]. This is apparent in the left panel of Fig. 1 where the odd-in-momentum Rashba helical winding induced by the (heavily screened) external field is very small compared to the visibly prominent even-in-momentum spin texture stemming from the CrTe₂ centrosymmetric crystal field. Achieving a Rashba term in

CrTe₂ similar to that of the Janus CrXTe would require an immense applied field $\mathcal{E}_z \sim \epsilon_{\text{CrTe}_2} \cdot 1\text{--}2 \text{ V nm}^{-1} \approx 50\text{--}100 \text{ V nm}^{-1}$ [50]. This illustrates the remarkable SOT potential of Janus CrXTe already at this ground-state level.

Non-equilibrium response.— CrXTe generally exhibits C_{3v} (also denoted $3m$) point group symmetry. In the case of CrTe₂, the degeneracy between both chalcogens raises the symmetry group to D_{3d} , which includes inversion symmetry and thus forbids any SOT response. However, C_{3v} symmetry is recovered by applying an out-of-plane electric field. The magnetization dynamics, described by the Landau-Lifshitz-Gilbert equation, is driven by the torque surface density $\mathbf{T}$, which is determined by the non-equilibrium spin surface density $\mathbf{S}$ as

$$\mathbf{T} = \hbar^{-1} J_{\text{ex}} \hat{\mathbf{m}} \times \mathbf{S}, \quad (1)$$

where $\hat{\mathbf{m}}$ is the magnetization direction unit vector, and J_{ex} is the exchange energy which couples the localized magnetic moments with those of the itinerant electrons [1]. The exact form of the non-equilibrium response is dictated by the subjacent crystal symmetries via invariant theory [51]. The non-equilibrium spin density, expanded up to first order with respect to both the driving electric field $\mathcal{E}$ and the magnetization direction $\hat{\mathbf{m}}$, reads

$$\mathbf{S} = \chi_{\text{FL}} \hat{\mathbf{z}} \times \mathcal{E} - \chi_{\text{DL}} \hat{\mathbf{m}} \times (\hat{\mathbf{z}} \times \mathcal{E}) - \chi_{\text{DL}}^z (\hat{\mathbf{m}} \cdot \mathcal{E}) \hat{\mathbf{z}} + \chi_{3m} [(\mathcal{E}_x m_y + \mathcal{E}_y m_x) \hat{\mathbf{x}} + (\mathcal{E}_x m_x - \mathcal{E}_y m_y) \hat{\mathbf{y}}], \quad (2)$$

with χ_α the spin linear response coefficients, and $\tau_\alpha = \hbar^{-1} J_{\text{ex}} \chi_\alpha$ the associated spin-torque conductivity. The terms proportional to χ_{FL} and χ_{DL} represent the conventional field-like and damping-like torques respectively, while χ_{DL}^z corresponds to an out-of-plane anisotropy of the damping-like torque. These torques are general to arbitrary non-centrosymmetric systems and drive the magnetization to an *in-plane* stationary state along the $\hat{\mathbf{z}} \times \mathcal{E}$ direction. Thus, additional fields are required in order to switch a system with *perpendicular* magnetic anisotropy.

The term proportional to χ_{3m} represents the so-called 3m torque, which is particular to systems with 3m symmetry. This contribution is related to a current-induced in-plane magnetic anisotropy [52] which modifies the stationary state of the magnetization inducing an out-of-plane instability, thus enabling field-free switching of a perpendicular magnetization [21]. We remit the reader to the supplementary material for a more complete calculation of the non-equilibrium spin density [50].

Within the Kubo quantum transport framework, we calculate the non-equilibrium spin density at Fermi level ε_F using the Kubo-Bastin formula

$$\mathcal{S}(\varepsilon_F) = -2\hbar \int d\varepsilon f(\varepsilon) \text{Im Tr} \left[\delta(\varepsilon - \hat{H}) \hat{s} \partial_\varepsilon G^+ (\hat{j} \cdot \boldsymbol{\varepsilon}) \right], \quad (3)$$

where $\hat{s}$, $\hat{H}$ and $\hat{j}$ are the spin, Hamiltonian and current density operators respectively, f is the Fermi-Dirac distribution, and $G^+ = \lim_{\eta \rightarrow 0} [\hat{H} - \varepsilon + i\eta]^{-1}$ represents the retarded Green's function. We numerically compute the Kubo-Bastin formula employing a kernel polynomial method expansion which includes the choice of a finite broadening $\eta = 25 \text{ meV}$ [53]. To discern the symmetry-allowed torque contributions, we compute the non-equilibrium spin density in a set of 18 magnetization directions, for each material [50]. Note that each of these systems requires its own *ab initio* and Wannier calculations as well; thus, we highlight the computational capability of the developed workflow. The exchange coupling J_{ex} is calculated as the average spectral difference between the spin majority and spin minority density of states.

SOT enhancement in Janus systems.— The equilibrium electronic structure analysis of the systems foresees an enhanced SOT response in Janus systems compared to those of the electric-field-assisted CrTe_2 . This is further confirmed and quantified by employing quantum transport simulations.

A SOT response is activated in CrTe_2 by applying a transversal electric field $\mathcal{E}_z$, which breaks inversion symmetry. Indeed, our results show that while the SOT response is negligible in the centrosymmetric system, all SOT components are enhanced with an increasing applied field, as showcased for the field-like torque in Fig. 2-(a). The enhancement is more prominent on the hole side of the spectrum, which can be associated with larger Fermi contours close to the K-point of the Brillouin zone.

The field-like spin-torque conductivity at the Fermi level compares moderately to that of other two-dimensional systems, with values of the order of $10^3 \frac{\hbar}{2e} (\Omega\text{m})^{-1}$ [17]. At a fixed energy, the spin-torque conductivity exhibits a linear dependence with respect to the applied symmetry-breaking field $\mathcal{E}_z$, as shown in the inset of Fig. 2-(a). We note that the signal for the centrosymmetric system at $\mathcal{E}_z = 0$ is non-zero, which derives from numerical approximations performed in the Wan-

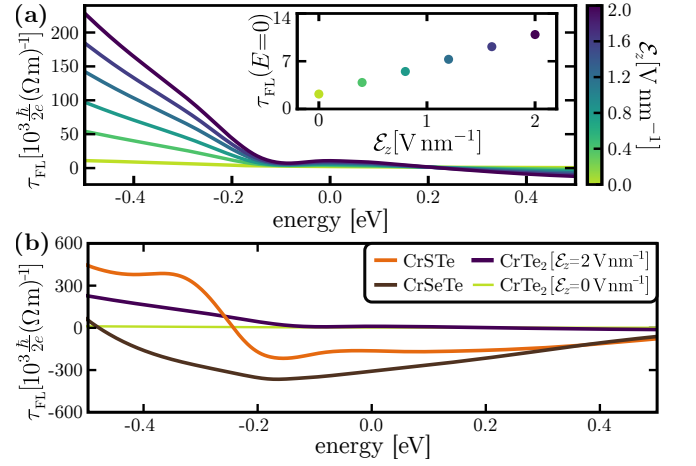


FIG. 2. (a) Field-like spin-torque conductivity τ_{FL} in CrTe_2 computed as a function of the transversal electric field $\mathcal{E}_z$. Inset: τ_{FL} at the Fermi level, exhibiting a linear dependence with $\mathcal{E}_z$. (b) τ_{FL} in Janus CrXTe systems, showing much larger SOT than non-Janus CrTe_2 .

nierization procedure, yet it is negligible compared to the $\mathcal{E}_z \neq 0$ signals. The linear dependence persists through the entire $\mathcal{E}_z$ range explored, showing that even large symmetry-breaking applied fields up to 2 V nm^{-1} remain perturbative with respect to the internal centrosymmetric crystal field.

Janus CrXTe systems allow us to fully achieve the potential of chromium-based TMDs for SOT. The strong internal electric field generated by the asymmetric crystal structure enables a field-like torque at the Fermi level of $\sim 10^5 \frac{\hbar}{2e} (\Omega\text{m})^{-1}$ in Janus systems, 10–100 times larger than the electric-field-assisted CrTe_2 , as shown in Fig. 2-(b). This huge SOT enhancement is present throughout a wide energy window about the Fermi level. The obtained values are comparable with the highest torques reported in two-dimensional systems, which however rely on spin transfer from a SOC material to a ferromagnet, thus being highly susceptible to the interface quality [15, 54–56].

The SOT enhancement due to structural inversion symmetry breaking comes at the expense of a modification of the ferromagnetic properties. Our *ab initio* calculations show that the ferromagnetic phase shifts to an in-plane magnetic anisotropy for the Janus CrXTe systems. A PMA is recovered by applying tensile strain, as shown in Fig. 3-(a). Additionally, a prominent enhancement of the SOTs is observed due to strain. Indeed, the strain-induced magnetic anisotropy shift in CrXTe is driven by the Te atom, which presents larger SOC than its S/Se counterpart [43, 44], thus enhancing the SOT response.

Field-free PMA switching.— We finally showcase the enormous potential of chromium-based Janus TMDs for SOT applications by computing the critical PMA switching current. The critical switching current is estimated

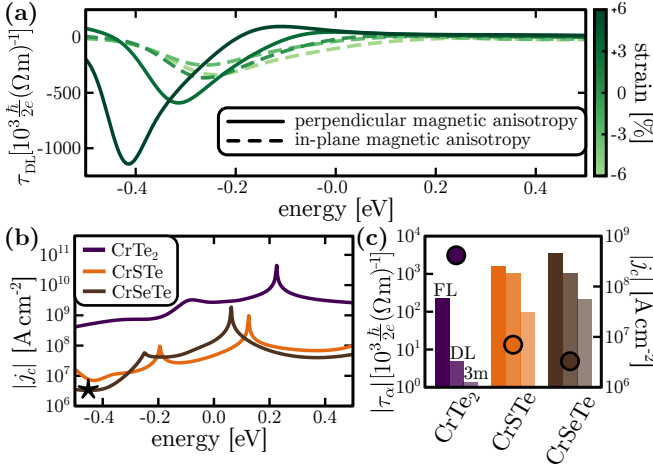


FIG. 3. (a) τ_{DL} in CrSTe for various strain values, exhibiting PMA for strain larger than 1% (solid curves), and in-plane anisotropy otherwise (dashed curves) [50]. (b) Critical switching current j_c in Janus CrXTe (+6% strain), and in non-Janus CrTe₂ (0% strain, and $\mathcal{E}_z = 2 \text{ V nm}^{-1}$). The star marks the overall optimal switching current $j_c^* = 3 \times 10^6 \text{ A cm}^{-2}$. (c) Maximal SOT efficiency (left y -axis; bars) and switching current (right y -axis; filled circles) in Janus and non-Janus systems.

as [57, 58]

$$j_c = \frac{M_s t_{FM} \sigma}{\tau_{DL}} \sqrt{\frac{\alpha}{\beta(2 + \alpha\beta)}} \sqrt{2B_{PMA}^2 - B_x^2}. \quad (4)$$

Here, M_s is the saturation magnetization, t_{FM} the system's thickness, σ the longitudinal conductivity and $\beta = \tau_{FL}/\tau_{DL}$; with all of these quantities obtained from our *ab initio* and quantum transport results. For the remaining parameters; namely, the Gilbert damping $\alpha = 0.01$, and the perpendicular anisotropy field $B_{PMA} = 0.1 \text{ T}$, we choose reasonable constant values, noting that they are fairly tunable by experimental conditions [59, 60]. Finally, B_x represents an in-plane effective magnetic field that drives the system out of the in-plane stationary state along $\hat{z} \times \mathcal{E}$ (promoted by the field-like and damping-like torques), allowing PMA switching. In conventional systems, an applied magnetic field B_x is required [61]; however, the 3m torque serves this purpose in CrXTe [21].

Because j_c gathers multiple magnetic and transport properties, it serves as an ultimate SOT figure of merit, providing a direct grasp of the power efficiency gain. The potential of Janus CrXTe systems is once again manifested, achieving critical switching currents 10–100 times smaller than those of non-Janus CrTe₂, as shown in Fig. 3-(b). The reduction of the switching current is indeed the result of enhanced SOTs in the Janus systems, evidenced in Fig. 3-(c), which shows τ_{FL} , τ_{DL} and τ_{3m} at the optimal j_c energy value for each system. Moreover, we note that the critical switching currents calculated by Eq. (4) correspond to an upper bound for the real values, as it is derived within a macrospin approximation,

whereas experimental evidence indicates that the switching occurs via domain wall nucleation and propagation [21, 62]. We find an overall optimal switching current of $j_c^* = 3 \times 10^6 \text{ A cm}^{-2}$, occurring for CrSeTe with +6% strain at 0.4 eV below the Fermi level. Experimentally, such strain can appear naturally by the substrate or the growth conditions [50]. This value is already highly competitive among 2D magnetic materials [63–66], while experimental conditions may result in further reduction of the critical current.

Conclusions.— We have found that magnetic chromium-based Janus TMDs offer a remarkable SOT performance. Concatenating *ab initio* and quantum transport methodologies we show that the large SOT response stems from huge internal electric fields due to their asymmetric structure, yielding a competitive switching current with the additional advantage of neither requiring assistance of external fields nor the transmission of spin current through an imperfect interface. Such results put forward magnetic Janus TMDs as efficient materials for designing ultimate SOT-MRAM technologies.

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* Authors contributed equally

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