Tunable spin-polarized edge currents in proximitized transition metal dichalcogenides

Natalia Cortés,1,2,* O. Ávalos-Ovando,2 L. Rosales,1 P. A. Orellana,1 and S. E. Ulloa2

1Departamento de Física, Universidad Técnica Federico Santa Marí, Casilla 110V, Valparaíso, Chile
2Department of Physics and Astronomy, and Nanoscale and Quantum Phenomena Institute, Ohio University, Athens, Ohio 45701–2979, USA

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We explore proximity-induced ferromagnetism on transition metal dichalcogenide (TMD), focusing on molybdenum ditelluride (MoTe2) ribbons with zigzag edges, deposited on ferromagnetic europium oxide (EuO). A three-orbital tight-binding model incorporates the exchange and Rashba fields induced by proximity to the EuO substrate. For in-gap Fermi levels, electronic modes in the nanoribbon are strongly spin-polarized and localized along the edges, acting as one-dimensional (1D) conducting channels with tunable spin-polarized currents. Hybrid structures such as the MoTe2/EuO configuration can serve as building blocks for spintronic devices, and provide versatile platforms to further understand proximity effects in diverse materials systems.

Introduction. The successful combination of two-dimensional (2D) materials with magnetic insulator substrates [1,5] has opened interesting possibilities to exploit different material properties and create novel functionalities [6,7]. Recently, spintronics has been closely related with magnetic proximity [8], where the interactions between spins in a non-magnetic material arise from a ferromagnetic (FM) or antiferromagnetic crystal placed in close proximity. The magnetic behavior may be due to non-vanishing wave-function overlap of localized moments in the magnetic crystal with electrons in a 2D layer, for example [9,11]. A spin splitting of 5 meV was predicted for monolayer graphene deposited on FM europium oxide (EuO) [10], motivating the successful epitaxial growth of EuO on graphene [1]. Experiments with different FM substrates have obtained magnetic exchange fields (MEF) induced on graphene of ~14 T (on EuS) [2], and ~0.2 T (on YIG) [3]. Proximitized material interactions clearly allow for the effective control of the spin degree of freedom in 2D materials, a fundamental element in spintronic devices.

Transition metal dichalcogenide (TMD) monolayers are built as MX2 (M = Mo, W, and X = S, Se, Te) [12,13]. The direct bandgap is located at the K and K′ points in the Brillouin zone [14,15], and related by time reversal symmetry (TRS). Spin-orbit coupling (SOC) and intrinsic lack of inversion symmetry cause a sizable spin splitting at the valence band edges [16]. TMD valleytronics applications require the lifting of valley degeneracy, which has been achieved only by application of large magnetic fields [8]. Magnetic proximity effects may provide more practical alternatives [4,5]. When a TMD monolayer is set on a FM insulator substrate, proximity effects [11,17,20] are predicted to lead to valley degeneracy lifted by broken TRS, and effective exchange field splitting [17,19,21]. Experiments [4] found a few meV valley splitting in a WSe2 monolayer on a EuS FM substrate. WSe2 on another ferromagnetic substrate, CrI3, [5] was found to exhibit a slightly larger valley splitting (~3.5 meV). A giant valley splitting (300 meV) due to the induced MEF was predicted for a MoTe2 monolayer on EuO [17,21], together with a sizable Rashba field (~100 meV). As we will see, the competition between Rashba and exchange fields provides an important figure of merit that determines the behavior of the system.

In this paper we provide the missing piece on how TMD edges are affected by proximitized magnetism. As in graphene, the hexagonal lattice in TMDs allows clean edges to be labeled as zigzag or armchair-terminated, with the first being much more common in the lab [22–24]. Zigzag-terminated TMD structures reveal rich behavior, such as metallic 1D edge modes [25,27], and helical states (when in proximity to a superconductor) that host Majorana bound states at the ends of a ribbon [27]. We analyze a zigzag MoTe2 ribbon deposited on a FM substrate such as EuO [17,21]. The proximity-induced ferromagnetism is incorporated through a real space three-orbital tight-binding (3OTB) Hamiltonian [28], that allows us to explore the electronic eigenstates and associated spin-polarized currents in the proximitized MoTe2 ribbon. We find edge modes that are spatially confined to the zigzag edges, are strongly spin-polarized, and act as effective 1D conducting channels that carry spin-polarized currents while the bulk is insulating. We also construct an analytical 1D effective Hamiltonian that describes well the 1D spin-polarized currents in the proximitized MoTe2 zigzag edges. The generic existence of TMD edge states that can be accessed by gating suggests that these hybrid systems could be used as robust tunable spin filters for use in diverse applications, apart from providing exciting systems to explore proximity magnetism.

Model. To describe the low-energy spectrum of a commensurate FM/TMD heterostructure over the entire Brillouin zone [17,29], we generalize a successful 3OTB model to include magnetic exchange field effects [28]. The 3OTB model has the relevant lattice symmetries and has been proven to reliably describe TMD ribbons [27] and flakes in diverse situations [30,33]. The nearly commensuration of the MoTe2/EuO structure [17,21],
as the EuO (111) surface and this TMD lattice constants have only a 2.7% mismatch, incorporates the substrate effects into the pristine MoTe$_2$ 30TB as effective on-site magnetic exchange and Rashba fields for every transition metal atom, as $\mathcal{H}_{\text{MoTe}_2/\text{EuO}} = \mathcal{H}_{\text{MoTe}_2} + \mathcal{H}_{\text{ex}} + \mathcal{H}_R$. Here, $\mathcal{H}_{\text{MoTe}_2}$ is the pristine TMD Hamiltonian \cite{28,34}. It is written in a basis of relevant transition metal d-orbitals, $\{|d_{z^2},s\}, |d_{xy},s\}, |d_{x^2+y^2},s\rangle$, with spin index $s = \uparrow, \downarrow$ \cite{28}. The induced MEF is spin diagonal, with blocks $\mathcal{H}_{\text{ex},\uparrow\uparrow} = -\mathcal{H}_{\text{ex},\downarrow\downarrow} = \text{diag}\{-B_e,-B_v,-B_e\}$, where $B_e = 206$ meV and $B_v = 170$ meV correspond to conduction and valence exchange fields respectively \cite{17}. A Rashba field also arises from the broken inversion symmetry provided by the polar EuO (111) surface. This field mixes the spin components in the MoTe$_2$ monolayer, which provides overall canting of spins, especially for the edge states, as we will see later. The Rashba Hamiltonian reads

$$\mathcal{H}_{R,\uparrow\downarrow} = \mathcal{H}_{R,\downarrow\uparrow} = \sqrt{2}\lambda_R \begin{bmatrix} 0 & -1 & i \\ 1 & 0 & 0 \\ -i & 0 & 0 \end{bmatrix},$$

where $\lambda_R = 72$ meV. All parameters are obtained from DFT calculations \cite{17}. Notice this 30TB exchange field Hamiltonian, with the right choice of TMD/substrate parameters and appropriate boundaries, could be used to study other heterostructures of interest, such as WSe$_2$/CrI$_3$ and WS$_2$/MnO \cite{5,20}. This provides an efficient and reliable approach to study different properties and behavior of the magnetic proximity-induced magnetism \cite{8}.

Results. We consider a zigzag MoTe$_2$ ribbon with 1600 Mo-sites, equivalent to a ribbon width of $\sim 125$ Å (40 Mo sites), and length of $\sim 144$ Å (40 Mo sites) along the zigzag edge, although different sizes do not qualitatively change results or main conclusions here. Figure 1(a) shows the zigzag MoTe$_2$ ribbon on a EuO substrate. The intrinsic lack of inversion symmetry in the 2D MoTe$_2$ monolayer results in two different terminations of the zigzag edges, with outer Mo or Te atoms \cite{27}, as shown in Fig. 1(b). This asymmetry produces different edge state dispersions along the ribbon. The large intrinsic SOC in MoTe$_2$ competes with the proximity exchange field from the FM substrate, and leads to giant valley polarization in the 2D bulk \cite{17}, as well as to strongly spin polarized edge-modes in the finite ribbon, as will be discussed below.

Figure 2 shows the energy spectrum for the MoTe$_2$/EuO zigzag ribbon near the bulk bandgap, projected along the ribbon edge. In general, the spectrum shows broken TRS due to exchange fields seen in the bulk bands, as well as on the edge states dispersing through the midgap and hybridizing with bulk bands. Panels (a) and (b) show the spin component content along $S_Y$ and $S_Z$, respectively, for EuO exchange fields. For comparison, panel (c) shows the $S_Z$ projection of the spectrum for weaker exchange fields (here set to 25% of the EuO values). Different exchange fields could be achieved by different substrate surfaces, biaxial strains, and/or van der Waals engineering of FM heterostructures \cite{31}.

For both exchange fields shown, there are clear edge modes with dispersion in the bulk bandgap, and residing on either the Te-edge (labeled $\text{Te}_\pm$) or the Mo-edge (labeled $\text{Mo}_\pm$), where the subindex sign indicates the two spin projections appearing with significant $S_Y$, canting away from $S_Z$, due to the Rashba coupling. These edge modes have clear metallic behavior for Fermi levels in the bulk midgap \cite{26,35}, propagating along the zigzag edges with momentum $k$ and characteristic spin \cite{27,36}. For EuO full exchange fields, Fig. 2(a)-(b) show that the $\text{Mo}_+$ mode is non-degenerate and hybridized with the bulk valence band states for small $k$, an effect not present for weaker exchange fields [Fig. 2(c)] when the Mo-edge modes are fully decoupled from the bulk and located midgap. In contrast, Te-modes are always hybridized to the bulk conduction bands for larger $|k|$ values, regardless of the exchange field strength. We should also notice the opposite group velocity of the different Mo- or Te-termination edge states at given $k$ values.

The proximity of the EuO substrate breaks inversion symmetry perpendicular to the plane of the MoTe$_2$ ribbon, allowing a Rashba field that generates spin mixing and canting spin for the edge states \cite{37}. In this case, the Rashba field is along the $y$-axis, confining the spin dynamics to the YZ plane \cite{38,39}. It is also clear that weaker exchange fields result in reduced $S_Z$ polarization, as evident from Fig. 2(b) and (c), with larger $S_Y$ projection as the ratio of $\lambda_R/B_v$ increases \cite{34}. Notice that as $\lambda_R$ is in principle tunable via gate fields for a given substrate-specific exchange field $B_v$, it is reasonable to anticipate that the overall spin projection (or canting) could be tunable in a given structure at specific Fermi energy.

Essential elements to achieve a spintronic device include being able to inject, manipulate or detect spin polarization \cite{6,40}. The Te- and Mo-edge modes are strongly spin-polarized along $S_Z$, as shown in Fig. 2.
Notice Te± and Mo± modes with opposite momentum ($k \rightarrow -k$) propagate in opposite directions with the same $S_Z$ projection, while the $S_Y$ component reverses for opposite momentum, as seen in Fig. 2(a). This behavior is unchanged for larger $\lambda_R/B_c$ ratios, although with larger $S_Y$ projection (see [34]), as the Rashba field is effectively stronger.

To characterize the propagation along the 1D Te- and Mo-edges, we select different in-gap Fermi levels (which could be achieved by electrostatic gating fields) [41, 42], to calculate the spin currents $j_{\text{spin}}$. The Fermi level can be shifted by an overall gate field perpendicular to the TMD layer, allowing for tunable spin current values and polarizations. Each spin current component at a given Fermi level is proportional to the momentum and to the spin projection, and calculated as $j_{l}^{\text{spin}} = k S_l \hbar/m$ [36, 38, 39], with $l = Y, Z$, given the corresponding spin projection, and $m(k)$ the carrier mass. Figure 3 shows spin currents for the MoTe$_2$ ribbon in Fig. 2(c). Given that the bulk current vanishes for in-gap Fermi levels, the non-vanishing spin currents for such levels are contributed by only the Mo- and Te-edge states and propagate along the edges of the ribbon. A 1D spin current along the edge is shown for right-movers ($k > 0$) at $E_{F1}$ in Fig. 3(a). At this Fermi level, both spin-split Mo-modes contribute to the spin current with $j_{Y}^{\text{spin}}$ and $j_{Z}^{\text{spin}}$ pointing to negative and positive directions, respectively—notice no Te-modes contribute yet at this level. As higher Fermi levels are reached, as in the case of $E_{F2}$ and $E_{F3}$, the spin-polarized Te-modes are turned on, and contribute to the spin currents, as shown in Fig. 3(b)-(c).

The spin currents along the Mo-edge are small in magnitude, and have nearly the same spin polarization for all chosen Fermi levels, as shown by the green arrows in Fig. 3, as the spin projections for both spin-split Mo modes nearly cancel each other. The spin currents along the Te-edge vary drastically with Fermi level, orange arrows in Fig. 3. The spin current for $E_{F2}$ has a large $j_{Y}^{\text{spin}}$ component and non-vanishing $j_{Y}^{\text{spin}}$, as only the Te± mode contributes. However, the Te-edge spin current becomes small and with reverse polarization for $E_{F3}$ (or $E_{F4}$), as both Te± modes contribute with nearly the same magnitude and opposite spin polarization. Accordingly, one could modulate the spin-polarized currents along the Mo-edge, or simultaneously along the Te-edge of the zigzag ribbon, by tuning the Fermi level across the structure [11, 12]. Similar spin-polarization in graphene nanoribbons has been proposed as spin injector device [3], with perhaps some practical advantages in the current TMD-based structure. Although both Te- and Mo-edges are found in experiments, the latter suffers from chalcogen-passivation [22, 24, 43], which may shift its midgap position and overall dispersion. However, the chalcogen-edge has an unambiguous single midgap state [27], unlike the multiple metal-edge states [27, 28]. We should mention that while the assumed pristine edges have been recently obtained in experiments [22, 23], we anticipate that low defect densities will not qualitatively affect the spin-polarized edge currents, while perhaps shifting their dispersions across the midgap. In fact, weak random bulk and edge disorder have been proved to not affect the edge modes significantly, producing only slight deviations of the pristine-edge structure [27].

Effective 1D model. We can write an effective 1D Hamiltonian for the hybrid MoTe$_2$/EuO edges, as

$$H_{\text{eff}}^\alpha(k) = \varepsilon^\alpha - \alpha [\hat{\sigma}_z + 1] \hat{t}_z^\alpha \cos k + \alpha [\hat{\sigma}_z - 1] \hat{t}_z^\alpha \cos k + \alpha \hat{\sigma}_z (\hat{t}_z^\alpha \sin k + b^\dagger) - \hat{\sigma}_y \hat{t}_y^\alpha \sin k,$$

where $\alpha$ indicates Mo ($\alpha = 1$) or Te ($\alpha = -1$) edges,
FIG. 3. Spin currents $j_{\text{spin}} = (j_Y, j_Z)$ for system in Fig. 2(c), for both Mo (green arrows) and Te (orange arrows) ribbon edges. Results for different Fermi levels, $E_{F1}$ (a), $E_{F2}$ (b) and $E_{F3}$ (c). The spin current is along the zigzag direction ($k > 0$). The arrow’s size indicates the magnitude of the spin current, and their directions indicates the spin current orientation. The magnetic substrate is not shown and the ribbon size is only schematic. $E_{F4}$ yields similar results to $E_{F3}$ (not shown).

in terms of onsite energies $\varepsilon^n$, effective bandwidths for the spin up/down $t^n_{1/2}$ bands, as well as Rashba $t^n_{SO}$, and diagonal SOC $t^n_{SO}$ and exchange fields $b^n$. The edge dispersion calculated from Eq. 2 is shown in Fig. 7(a). There is an excellent agreement between the numerical results (gray dots) and the fitted model \[ \text{for all Mo- and Te-} \]

The analytical and tight-binding spin currents are shown in Fig. 4(b) and (c) for Mo and Te modes. The spin currents are non-vanishing for Fermi levels in the bulk gap region. As the Fermi level changes from $p$- to $n$-doping, the Mo$_+$/mode is never singly-populated, as bulk states in the valence band will also be reached before Mo$_-$ is populated, as seen in Fig. 4(a) for $-0.05 \lesssim E_F \lesssim 0.1$ eV (measured with respect to the bottom of the Mo$_+$ mode). Then, for $E_F \sim 0.15$ to 0.3 eV, both Mo-edge modes are populated, and the spin current will remain nearly constant throughout that window and only present on that edge. As the Te$_-$ mode is reached, and for an energy window $E_F \sim 0.3$ to 0.45 eV, only one spin branch at the Te-edge is populated, with a correspondingly large spin current on that border. This is strongly suppressed as the Te$_-$ mode is reached for $E_F \gtrsim 0.5$ eV, and the spin current progressively decreases as the Fermi level reaches the conduction band.

These results suggest that indeed a finite size ribbon of a TMD such as MoTe$_2$ monolayer on a FM substrate such as EuO could be used to produce tunable spin currents along the edges of experimental samples. This proximity-induced functionality would contribute to the diverse behavior of different van der Waals systems.

**Conclusions.** A three-orbital tight-binding Hamiltonian and effective 1D description are able to incorporate the effects of magnetic proximity from a ferromagnetic substrate onto the spin-polarized states and currents at the zigzag edges of a transition metal dichalcogenide monolayer ribbon. The broken inversion and time-reversal symmetries in the proximitized ribbon split the electronic edge states residing in the bulk midgap and produce effective 1D conducting channels with spin-polarized currents. Competition between the effective exchange and Rashba fields produces canting of the spin orientation of the spin currents. The spin current polarization and onset could be experimentally modulated by tuning the Fermi level \[ 41, 42 \], tuning the effective exchange field by van der Waals engineering of heterostructures \[ 5 \], or through biaxial strain \[ 11 \]. The ready avail-
ability of samples and the flexibility of this effect suggests that such proximitized TMD ribbons could be effectively used as robust 1D spin injectors [8].

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* natalia.cortesm@usm.cl
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