Atomistic modeling of spin and electron dynamics in two-dimensional magnets switched by two-dimensional topological insulators

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To design fast memory devices, we need material combinations which can facilitate fast read and write operation. We present a heterostructure comprising a two-dimensional (2D) magnet and a 2D topological insulator (TI) as a viable option for designing fast memory devices. We theoretically model spin-charge dynamics between the 2D magnets and 2D TIs. Using the adiabatic approximation, we combine the non-equilibrium Green’s function method for spin-dependent electron transport, and time-quantified Monte-Carlo for simulating magnetization dynamics. We show that it is possible to switch the magnetic domain of a ferromagnet using spin-torque from spin-polarized edge states of 2D TI. We further show that the switching between TIs and 2D magnets is strongly dependent on the interface exchange ($J_{int}$), and an optimal interface exchange depending on the exchange interaction within the magnet is required for efficient switching. Finally, we compare the experimentally grown Cr-compounds and show that Cr-compounds with higher anisotropy (such as CrI$_3$) results in lower switching speed but more stable magnetic order.

I. INTRODUCTION

Thanks to the recent discovery of two-dimensional (2D) magnets e.g., CrI$_3$ [1], CrBr$_3$ [2], and CrGeTe$_3$ [3], research into 2D magnetics has garnered unprecedented attention. 2D magnetic materials open a plethora of opportunities in their use in future application in devices including spintronics [4] [5], valleytronics [6], and skyrmion [7]-based magnetic memories [8]. However, many of the devices require low-dimensional magnets interfaced with semiconductors to function as memory devices [9][11].

An interesting avenue of designing electronic devices using low-dimensional magnets lies in interfacing low-dimensional ferromagnets (FM) with topological insulators (TI) [9][10]. The surface states of topological insulators can act as spin-channels with high spin-polarizability. Moreover, depending on the direction of applied bias, the spin of the edge states can be switched thanks to spin-momentum locking [12].

Although there have been some experimental works on realizing magnetic devices using TI-FM interfaces [9][12], a solid theoretical understanding of the interfacial physics is missing. Most of theoretical works have either investigated equilibrium TI-FM interfaces with a FM having a fixed magnetic orientation [13][14] or investigated the impact of magnetic materials on the topological order of the TIs [15].

For the technological application of TI-FM material systems, it is necessary to understand how the motion of spin-polarized charge carriers in TIs impact the spin dynamics of the FM and vice-versa. To understand such a coupled spin-charge effect, it is necessary to model the coupled spin-charge dynamics of TIs and FMs. There have been recent theoretical works on modelling FM-semiconductor interfaces [16][18], however a major issue lies with the description of the 2D magnets.

Most of the current methods use Landau–Lifshitz–Gilbert (LLG) [19] equation to describe magnetization dynamics, coupled with quantum transport methodologies, e.g., non-equilibrium Green’s function (NEGF) [20]. The largest limitation lies in the magnetization dynamics of the magnetic material because the LLG equation assumes a continuous description of the magnetic structure [16] and the atomistic description is lost. Moreover, interactions such as exchange anisotropy, which play a major role in determining the magnetic order of low-dimensional magnets [21][23] are hard to include in the LLG equation, and most frequently a scalar approximation to the exchange interactions is assumed [23].

On the other hand, Monte-Carlo (MC) simulations are shown to be very accurate in predicting temperature dependent observables for 2D magnets taking into account full anisotropy [21][22][27]. Unfortunately, MC simulations do not have a standard method of quantifying time to obtain time dependent observables such as magnetic switching. There have been previous works on quantifying time within MC simulations for systems with in-plane rotational invariance [28][29], called time-quantified Monte-Carlo (TQMC) simulations. Thankfully, most of the 2D magnetic materials yet discovered experimentally have an in-plane rotational invariance, and TQMC can be applied for such materials for magnetization dynamics.

We present a theoretical study of spin-dynamics...
FIG. 1: The interface between a 2D TI and a layered magnet. The electrons are injected from the contacts (illustrated by the blue arrow below right contact) at time $t + \Delta t$. The flowing electrons carry a small magnetic moment (illustrated by the small blue arrows) exerting a torque due to electronic magnetic configuration: $m(t + \Delta t)$ on the interfacing magnet with magnetic configuration: $M(t + \Delta t)$ (illustrated by the red arrows).

and spin-induced switching in a TI-FM heterostructure. We combine the non-equilibrium Green’s function method for spin-dependent electron transport with time-quantified Monte-Carlo for simulating magnetic systems. We use our method to study spin-induced switching in a heterostructure of a two-dimensional topological insulator and a two-dimensional ferromagnet. We show that it is possible to change the magnetic-domain structure in the ferromagnet using spin-injection from TIs, which can be used to design high-speed memory devices. We then show that the switching can only be achieved efficiently for an optimal interfacial exchange interaction between TI and FM. Finally, we compare the switching time for four experimentally grown Cr-compounds: CrI$_3$, CrBr$_3$, CrCl$_3$, and CrGeTe$_3$. We show that the higher anisotropy of CrI$_3$ results in a much larger switching time compared to CrBr$_3$ and CrCl$_3$, which have lower anisotropy.

II. METHODOLOGY

II.1. The Heisenberg Hamiltonian

We model the 2D magnetic structure using the Heisenberg Hamiltonian

$$H_m = \frac{1}{2} \sum_{i \neq j} \mathbf{S}_i \cdot \mathbf{J}_{ij} \cdot \mathbf{S}_j + D \sum_i (S^z_i)^2$$  \hfill (1)

where, $\mathbf{S} = S^x \mathbf{x} + S^y \mathbf{y} + S^z \mathbf{z}$ is the spin-vector with magnitude $|\mathbf{S}| = \sqrt{(S^x)^2 + (S^y)^2 + (S^z)^2}$. The exchange interaction strength $\mathbf{J}_{ij}$ between spins at site $i$ and $j$ is a $3 \times 3$ tensor [21] whose parameters are obtained by fitting to DFT calculations [21,22]. The second term in Eq. (1) is the single-ion anisotropy with strength $D$. We assume in-plane rotational invariance for the 2D magnetic materials which leads to the Hamiltonian reducing to,

$$H_m = \sum_{i,j} \frac{J_{ij}}{2} \left[ \mathbf{S}_i \cdot \mathbf{S}_j + \Delta_{ij}(S^z_i S^z_j - S^x_i S^x_j - S^y_i S^y_j) \right] + D \sum_i (S^z_i)^2, \hfill (2)$$

where the exchange anisotropy ($\Delta_{ij}$) accounts for the distinct values for the in-plane and out-of-plane anisotropic exchange strength, $J^x_{ij} = J^y_{ij} = J_{ij}(1 - \Delta_{ij})$ and $J^z_{ij} = J_{ij}(1 + \Delta_{ij})$ [21], respectively.

Moreover, we define the total magnetization per atom in the x, y, and z direction as,

$$S^x/y/z = \frac{1}{N_{\text{atom}}} \sum_i S^x_i/y_i/z_i.$$  \hfill (3)

Here, $N_{\text{atom}}$ is the total number of atoms.

II.2. Electronic Hamiltonian

We model the electronic structure of the topological insulators using a tight-binding Hamiltonian,

$$H_{\text{elec}} = -t \sum_{\langle r,r' \rangle, \alpha} c^\dagger_{r,\alpha} c_{r',\alpha} + i \Lambda_{so} \sum_{\langle r,r' \rangle} v_{r,r'} c^\dagger_{r,\alpha} \sigma^z_{\alpha, \beta} c_{r', \beta}. \hfill (4)$$

Here the first term, with coupling strength $t$, accounts for the nearest neighbor hopping, $\langle r,r' \rangle$, between adjacent lattice sites $r$ and $r'$, with respective electron creation and annihilation operators $c^\dagger_{r,\alpha}$, $c_{r,\alpha}$. $\alpha$ and $\beta$ represent spin degrees of freedom, i.e., $\alpha \in \{\uparrow, \downarrow\}$ and $\beta \in \{\uparrow, \downarrow\}$. The second term is the next nearest neighbor spin-orbit coupling term with strength $\Lambda_{so}$. $\sigma^z$ is the $z^{th}$ component of the Pauli matrices. The parameter $v_{r,r'}$ is +1 when the shortest next nearest neighbor path from $r$ to $r'$ with respect to atom $r$ is clockwise, and -1 if it is counterclockwise.
II.3. Combined Hamiltonian

We combine the model for the Heisenberg Hamiltonian and the electronic Hamiltonian using the interaction Hamiltonians

\[ H'_{\text{m}} = J_{\text{int}} \sum_{r,i} \mathbf{m}_r \cdot \mathbf{S}_i, \]  
\[ H'_{\text{elec}} = J'_{\text{int}} \sum_{i,\alpha,\beta} c_{r,\alpha}^\dagger \mathbf{S}_i \cdot \sigma_{\alpha,\beta} c_{r,\beta}. \]  

Here, the \( J_{\text{int}} \) and \( J'_{\text{int}} \) are the interface interactions at the semiconductor-FM interface. The electron magnetization, \( \mathbf{m} = m^x \mathbf{x} + m^y \mathbf{y} + m^z \mathbf{z} \) is the expectation value of the Pauli spin matrix: \( \mathbf{\sigma} = \sigma^x \mathbf{x} + \sigma^y \mathbf{y} + \sigma^z \mathbf{z} \). Explicitly, we calculate the electron magnetization \( \mathbf{m} \) by taking the trace of the density matrix over the spin degrees of freedom,

\[ \mathbf{m}(r) = \frac{\hbar \gamma}{4\pi} \text{Tr}[\mathbf{\sigma} \cdot \rho(r, r')]_{\text{spin}}, \]  

with the electronic density matrix,

\[ \rho(r, r') = \int G^<(r, r', E)dE, \]  

where, \( G^<(E) \) is the lesser Green’s function. As is standard in ballistic NEGF, the lesser Green’s function is obtained from, \( G^<(r, r', E) = A_L(r, r', E)f(E - \mu_L) + A_R(r, r', E)f(E - \mu_R). \) Here, \( A_{L/R}(r, r', E) \) are the spectral functions for the left (L) and the right (R) contacts, and \( \mu_{L/R} \) are the respective chemical potentials with \( f(E) \) being the Fermi-Dirac distribution function. The spectral functions are obtained using, \( A_{L/R} = G^0 \Gamma_{L/R} G^a, \) with \( \Gamma_{L/R} = i(\Sigma_{L/R} - \Sigma_{L/R}^r)^{-1} \). \( G^0(E) = (E - H'_{\text{elec}} - \Sigma_{L} - \Sigma_{R})^{-1} \) is the retarded Green’s function. The advanced Green’s function is \( G^a = (G^0)^\dagger \). The contact self-energies \( \Sigma_{L/R} \) are obtained using the quantum transmitting boundary method (QTBM) [30][31]. Similar to magnet, we define the magnetization per atom in TIs as,

\[ m_{x/y/z} = \frac{1}{N_{\text{atom}}} \sum_i m_i^{x/y/z}. \]  

Here, \( N_{\text{atom}} \) is the total number of atoms in TI.

II.4. Magnetization dynamics and time-quantification

To simulate the magnetization dynamics as a function of time, we use the time-quantified Monte-Carlo (MC) approach [28][29]. Within TQMC, one step of a MC simulation is assigned a time step \( \Delta t \) of,

\[ R^2 = \frac{20 k_B T \alpha \gamma}{(1 + \alpha^2) M \Delta t}. \]  

Here, \( R \) is a cone radius up to which a trial spin-rotation is allowed in each MC step. \( k_B \) is the Boltzmann constant, \( \alpha \) is the Gilbert damping parameter, \( M = \sqrt{S_x^2 + S_y^2 + S_z^2} \) is the magnetic moment, and \( \gamma \) is the gyromagnetic ratio.

Figure 2 shows a single magnetic atom with spins chosen for three successive time steps using TQMC (\( S_1 \), \( S_2 \), \( S_3 \)). Within TQMC for each time step, we make a cone of radius of \( R \) around the spin-vector of the present spin configuration (\( S_1 \), green). The next spin-configuration (\( S_2 \), black) is chosen within the cone using the Metropolis algorithm [22][32]. Once, the spin-configuration is updated to \( S_2 \), we choose the next spin configuration (\( S_3 \), blue) by using the same method of making a cone of radius \( R \) around \( S_2 \).

The expression in Eq. (9) for time-discretization has been obtained by assuming only single-spin interactions and Langevin dynamics [28][29]. Therefore, this time discretization is valid only under the condition that the magnetization dynamics can be approximated using Langevin dynamics, and is more accurate for materials with in-plane rotational invariance and Gilbert damping:\( \alpha \leq 1 \) [28][29]. The approximation of magnetization dynamics to Langevin dynamics is only valid under high out-of-plane anisotropy or very low temperatures (\( T < 10 \) K) where the spins start behaving collectively as a single unit. Due to the above reason, we perform all our calculations below \( T < 10 \) K.

II.5. Algorithm for spin-charge dynamics

The energy of the magnetic interaction is of the order of meV, while the electronic interaction energy is of the order of eV. Therefore, the time scales of magnetization dynamics are in ps, whereas that of electrons is in
FIG. 3: (a) The device configuration studied for TI-FM switching. The 2D TI is contacted with a drain and a source contact and a voltage ($V_{ds}$) is applied between the contacts. (b) The magnetization of the 2D FM as a function of time. (b.1) The bias is applied at $t = 0$ ns and switched to 100 meV from -100 meV at 0.25 ns. (b.2) The magnetization of the 2D FM in the z-direction ($S_z$) switches its direction (from $3\mu_B$ to $-3\mu_B$). (b.3) The induced magnetization in the 2D TI.

FIG. 4: The magnetic configuration ($M(t)$) of the FM (upper three panels), and the electronic spin configurations ($m(t)$) of the TI (lower three panels) at $t = 0.23$ ns, $0.27$ ns, and $0.41$ ns while the voltage pulse is switched at $t = 0.25$ ns. The atomic structure of the FM is shown as an imprint within the magnetic configuration of the TI.

Within the adiabatic approximation, we assume that due to the large differences in the time scale, the electrons are considered to only see an adiabatic change in magnetic moment and are thus always found to occupy instantaneous eigenstates. Hence, as shown in Fig. 1, we start with a magnetic orientation of the magnetic material, and at each time-step ($t + \Delta t$), we rotate the spin of the top magnetic layer using MC sampling. After the MC step, we calculate the magnetic moment of the magnet $M(t + \Delta t)$. For the same time-step, we obtain the lesser Green’s function using the NEGF method and calculate the electronic magnetization $m(t + \Delta t)$. For the next time step, the magnetization of the electronic system is an input to the magnetic system, and the loop continues.

II.6. Computational Details

For all calculations unless mentioned specifically, we have used values $\alpha = 0.05$, $k_B T = 0.5$ meV, $J_{int} = J_e^{\text{int}} = 25$ meV. We have used the parameters of a CrI$_3$ monolayer to parameterize the interface 2D ferromagnet, which we obtained from DFT calculations using the procedure in Ref. 21. The saturation magnetization used for the Cr-atoms is $3\mu_B$. To model the TIs we have used the parameters of the tight-binding Hamiltonian for stanene [31].

III. RESULTS AND DISCUSSION

III.1. TI-FM interface operation

Figure 3 (a) shows the TI-FM configuration we are investigating. For the TI we use a 5 nm wide stanene ribbon, for the 2D FM we use CrI$_3$ with size: $3 \text{nm} \times 3.5 \text{nm}$. The 2D FM is positioned near one of the edges of the 2D TI as shown in the top view in Fig. 3 panel (a.2). A potential ($V_{ds}$) is applied across the TI ribbon to inject charge carriers in the TI ribbon. For $V_{ds} > 0$, the edge states on the top edge of the TI have up-spin, whereas the bottom edge exhibit down-spin. For $V_{ds} < 0$, spin polarization of the edge states is flipped. Therefore, the interfaced FM experiences positive or negative spin-torque from the underlying charge carriers of the TI, depending on the applied $V_{ds}$.

Figure 3 (b) panel (b.1) shows the applied $V_{ds}$ as a function of time. We apply a step $V_{ds}$ pulse of 100 mV at
FIG. 5: (a) The applied $V_{ds}$ (panel a.1) and the magnetization of the top 2D FM for $\alpha = 0.02, 0.03, 0.04, 0.05$ (panel a.2). (b) The applied $V_{ds}$ and the magnetization of the top 2D FM for interface interaction strengths $J_{\text{int}} = 5, 25, 50, 100, 150$ meV (panel b.2). (c) The transition time for the applied pulse in panel (b.1) as a function of $J_{\text{int}}$. (d) The magnetization at $t = 0.45$ ns for $J_{\text{int}} = 25$ meV and $J_{\text{int}} = 150$ meV. The upper two panels show the magnetization of the 2D FM in the $z$-direction ($S_z/|M|$), and the lower two panels show the induced magnetization in the 2D TI ($m_z$).

At $t = 1.75$ ns. Figure 3 (b) panel (b.2) shows the average magnetization in the $x$, $y$, and $z$-direction as a function of time. We observe that due to the change in the applied $V_{ds}$ from -100 mV to 100 mV at $t = 0.5$ ns, the magnetization in the $z$-direction ($S_z$) switches from $3 \mu_B$ to $-3 \mu_B$. When the applied voltage switches from 100 mV to -100 mV, we observe that the magnetization switches again from $-3 \mu_B$ to $3 \mu_B$.

Figure 3 (b) panel (b.3) shows the induced magnetization of the TI ribbon in the $x$, $y$, and $z$ direction as a function of time. We observe that due to the magnetization of the top FM, there is a finite induced magnetization in the TI ribbons when the applied bias is non-zero. Interestingly, we find that whenever the bias switches and the magnetization of the top FM transitions, the total induced magnetization of the TI ribbon also shows a peak.

To further analyze the magnetization dynamics of the TI-FM interface, we plot the out-of-plane projection of the magnetization of the entire TI and FM sample at various time steps in Fig. 4. Figure 4 shows the magnetization in the $z$-direction for the 2D magnet (top panels, $S_{\text{m}}/|M|$) and the TI (bottom panels, $m_z/|M|$), respectively. We observe that at $t = 0.23$ ns, the TI has a positive bias $V_{ds} > 0$ and both the TI and the FM have positive magnetization at the interface. Note that we have taken the interface parameter to be positive, meaning the interaction is ferromagnetic.

At $t = 0.27$ ns, the bias of the TI has opposite polarization $V_{ds} < 0$. We observe that the magnetization of the TI reverses. The reversal of the magnetization in TI induces a spin-torque on the interfacing FM, which results in the formation of a small region of magnetization, with opposite orientation as that of the entire FM ($S_z < 0$).
At $t = 0.41$ ns, we observe that the domain with $\hat{S}_z <$ 0 grows and changes completely to a FM configuration with a magnetization of the 2D magnet equal to $-3\mu_B$. Interestingly, we find that the top magnetization of the FM does not have a significant impact on the magnetization of the TI. The reason for such behavior is because we have assumed in our calculations that the interface interaction strength $J_{\text{int}} = J_{\text{int}}^* = 25$ meV. The interaction strength felt by the TI is of the order of meV, whereas the topological energy gap of TIs is of the order of eV. Hence, the weak interaction strength will always lead to a negligible response of the TI magnetization due to magnetization at the interface with the FM.

III.2. Impact of $J_{\text{int}}$ and $\alpha$

Figure 5 (a) panel (a.1) shows the applied bias across the 2D TI. We apply a $V_{\text{ds}}$ pulse with a pulse width of 0.4 ns and an amplitude of 100 mV at $t = 0.8$ ns. Figure 5 (a) panel (a.2) shows the normalized magnetization in the z-direction ($S_z/|M|$) as a function of time of the interface 2D FM for Gilbert damping parameter $\alpha = 0.02, 0.03, 0.04, 0.05$ for a pulse bias. With the transition in applied $V_{\text{ds}}$, the normalized magnetization of the 2D magnet transitions from 1 to $-1$. We also observe that with increasing $\alpha$, the transition occurs faster, suggesting that the switching speed increases.

Figure 5 (b) panels (b.1) and (b.2) show a pulse bias applied across the 2D TI with a pulse width of 0.2 ns applied at 0.4 ns as a function of time, the normalized magnetization in the z-direction ($S_z/|M|$) as a function of time of the interface 2D FM for interface exchange parameter $J_{\text{int}} = 20, 25, 50, 75, 100,$ and 150 meV. We observe that with increasing $J_{\text{int}}$, the transition occurs faster up to $J_{\text{int}} = 50$ meV. For $J_{\text{int}} > 50$ meV, we see that the magnetization does not switch smoothly, and the magnetization stabilizes for the entire duration of the pulse. After the applied pulse returns to 0 mV, the magnetization still switches for all $J_{\text{int}} > 50$ meV, albeit with some delay.

Figure 6 (a) shows the transition time as a function of nearest-neighbor anisotropy $\Delta_{\text{NN}}$. For 10 different starting configurations. The solid line shows the median and the shaded region shows the 25th-75th percentile. (b) Comparison of switching in CrI$_3$, CrBr$_3$, CrCl$_3$, and CrGeTe$_3$. Panel (b.1) shows the applied $V_{\text{ds}}$ and panel (b.2) shows the magnetization ($S_z/|M|$) for CrI$_3$, CrBr$_3$, CrCl$_3$, and CrGeTe$_3$. We use an interface exchange $J_{\text{int}} = 25$ meV, and $\alpha = 0.005$.

To further understand the reason for the low transition rate at higher $J_{\text{int}}$, we compare the magnetization at $t = 0.45$ ns in Fig. 5 (d) for $J_{\text{int}} = 25$ meV and $J_{\text{int}} = 150$ meV. The upper two panels show the magnetization of the 2D FM in the z-direction ($S_z/|M|$), and the lower two panels show the induced magnetization in the 2D TI ($m_z$). We observe that for $J_{\text{int}}$ up to $J_{\text{int}} = 50$ meV and then increases for $J_{\text{int}} > 50$ meV. Therefore, we find that an optimal value of interface exchange ($J_{\text{int}}$) is required for obtaining a small transition time.
TABLE I: $J$-parameters and anisotropies of experimental Cr-compounds

| Parameters | $J_{NN}$ | $J_{NNNN}$ | $\Delta_{NN}$ | $\Delta_{NNNN}$ |
|------------|----------|------------|----------------|-----------------|
| CrI$_3$    | 2.21     | 0.75       | -0.020         | 0.045           |
| CrBr$_3$   | 1.38     | 0.44       | -0.010         | 0.012           |
| CrCl$_3$   | 1.31     | 0.24       | 0.001          | 0.008           |
| CrGeTe$_3$ | 5.87     | -0.28      | 0.345          | 0.020           | 0.028

III.3. Impact of anisotropy and Cr-compounds

We compare the transition time for the device in Fig. 3 (a) as a function of nearest-neighbor anisotropy ($\Delta_{NN}$) of the FM as shown in Fig. 6. We perform the same sweep of $\Delta_{NN}$ for 10 different starting configurations. The solid line shows the median and the shaded region shows the 25th-75th percentile. We use $J_{int} = 0.025$ eV and $\alpha = 0.05$ and nearest neighbor exchange for the 2D magnet to be $J_{NN} = 2.5$ meV.

We find that with increasing $\Delta_{NN}$ the transition time increases. Therefore, for faster switching of the TI-FM device, it will be ideal to use materials with lower $\Delta_{NN}$. However, lower $\Delta_{NN}$ results in a lower Curie temperature [21]. Hence, the choice of the FM material should take into account the temperature of operation and the required switching time for the device.

For the device shown in Fig. 3 (a), we use CrI$_3$, CrBr$_3$, CrCl$_3$, and CrGeTe$_3$ as the 2D magnetic material. Although, many studies in previous works have used a parametric value of $\alpha$ [33] for Cr-compounds, recent reports on the measurement of intrinsic Gilbert damping of a sister compound CrCl$_3$ have found a value of $\alpha = 0.002$ [34]. Unfortunately, there is no similar report for other Cr-compounds, therefore we have used an $\alpha$ of similar order, $\alpha = 0.005$, for all the three Cr-compounds for a fair comparison. The parameters used for modeling their magnetic structure of the Cr-compounds is shown in Table I.

Figure 6 (b) panel (b.1) shows the applied $V_{bias}$ and panel (b.2) shows the out-of-plane magnetization $S_z$ for CrI$_3$, CrBr$_3$, CrCl$_3$, and CrGeTe$_3$. We find that the magnetization of CrI$_3$ is the most stable among the Cr-compounds followed by CrGeTe$_3$, CrBr$_3$, and CrCl$_3$, respectively. However, CrI$_3$ is also the slowest to respond to a change in the applied bias and has the highest transition time.

Comparing the parameters for the Cr-compounds in Table I we find that the transition time is inversely proportional to the nearest-neighbor anisotropy ($\Delta_{NN}$). The higher the anisotropy, the higher the transition time. On the other hand, the stability of magnetization is directly proportional to the anisotropy.

IV. CONCLUSION

We have presented a method to model spin-charge dynamics at a magnetic-topological insulator interface. Our model is general and not limited to only the TI-FM interface. Our method combines NEGF and TQMC to model the spin-charge dynamics. The benefit of TQMC+NEGF over conventional methods such as LLG+QTBM or LLG+NEGF lies in the atomistic description of the spins, which allows one to implement the full exchange tensor for modelling the magnetic exchange interactions.

Using our method, we have theoretically investigated the spin-charge dynamics in a 2D TI-FM heterostructure where the size of the 2D FM was smaller than the 2D TI and placed on one of the edges of the 2D TI. We have shown that by electrically biasing the 2D TI, it is possible to switch the magnetization of the 2D FM without destroying the edge state of the 2D TI. The most important result of our work is that the switching of the 2D FM using 2D TI spin-torque can only be achieved efficiently in TI-FM material combinations that have an optimal interface exchange interaction $J_{int}$. We have also compared experimentally grown 2D Cr-compounds. We have shown that the transition rate of magnetization significantly depends on the anisotropy, and low anisotropic Cr-compounds (CrBr$_3$ and CrCl$_3$) show faster switching in comparison to the higher anisotropic Cr-compounds (CrI$_3$ and CrGeTe$_3$). Finally, there are recent reports of experimentally growing 2D FM-semiconductor heterostructures for spintronic devices [35], and given the device design presented in our paper is feasible to make experimentally, and we believe it should be explored experimentally.

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