Towards a strong spin-orbit coupling magneto-electric transistor

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Abstract— Here we outline magneto-electric (ME) device concepts based on the voltage control of the interface magnetism of a magneto-electric antiferromagnet gate dielectric formed on a very thin semiconductor channel with large spin orbit coupling. The emphasis of the magneto-electric spin field-effect transistors (ME spin-FETs) is on an anti-ferromagnet spin-orbit read (AFSOR) logic device and a ME spin-FET multiplexer. Both spin-FET schemes exploit the strong spin-orbit coupling in the semiconducting channel materials but remain dependent on the voltage-induced switching of a magneto-electric, so that the switching time is limited only by the switching dynamics of the magneto-electric. The induced exchange field spin-polarizes the channel material, breaking time-reversal symmetry and resulting in the preferential charge transport direction, due to the spin-orbit-driven spin-momentum locking. These devices could provide reliable room-temperature operation with large on/off ratios, well beyond what can be achieved using magnetic tunnel junctions. All of the proposed devices spintronic functionality without the need to switch a ferromagnet, yielding a faster writing speed (~10 ps) at a lower cost in energy (~10 aJ), excellent temperature stability (operational up to 400 K or above), and requiring far fewer device elements (transistor equivalents) than CMOS.

Index Terms—magneto-electric transistor, spin-orbit coupling, nonvolatile logic and memory

I. INTRODUCTION

MODERN dynamic random access memory (DRAM) elements are volatile and require frequent refresh power. On the other hand, a solid-state device with a magnetically-ordered state, could be engineered into a memory or logic element whose information is non-volatile. For example, magnetic random access memories (MRAMs) are advanced in terms of access time and endurance and do not require continued power to store information. MRAMs have significant deficiencies, however, in terms of power consumption due to their high writing energy. Although major advances have been achieved in recent years by progressing from switching via Oersted fields to spin transfer or spin-orbit torques, these devices still require large current densities [1-5]. Current densities in excess of 1 MA/m^2 are required for writing of the magnetic state in spin-transfer-torque (STT) memory elements [6] and, consequently, are not energy efficient. Conventional schemes of non-volatile magnetic memories and logic largely rely on the functionality of magnetic tunnel junctions (MTJs) – key devices of modern spintronic technologies. MTJ operation is based on the switching of a free ferromagnetic layer, resulting in a change of its tunneling resistance. The speed of this operation is determined by the time required to rotate the magnetization of the nanomagnet, which is typically a few nanoseconds. This is nearly three orders in magnitude slower than the time required to charge a capacitor, as implemented in complementary metal-oxide-semiconductor (CMOS) field-effect transistors (FETs).

Based on the discussion above, it would be desirable, on one hand, to provide non-volatility of the state variable of the device, and on the other hand, be able to switch this state with low power and high speed. By adopting a transistor geometry, based solely on the switching of a magneto-electric, switching speed can be limited only by the switching dynamics of that material, thereby avoiding the long delay times plaguing other spintronic devices that rely on the slower switching delay (as long as 5 ns) of a ferromagnetic layer. Moreover, the devices discussed here promise to provide a unique FET-based interface for input/output of other novel computational devices that depend on magnetics (e.g., magnetic cellular logic [7]). This is spintronics without a ferromagnet, with faster write speeds (<20 ps/full adder), at a lower cost in energy (<200 aJ/full adder), greater temperature stability (operational to 400 K or more), and scalability, requiring far fewer device elements (transistor equivalents) than CMOS.

Magneto-electric materials also provide a unique way to read out and transmit information – through roughness insensitive boundary magnetization, which is intrinsically coupled to the antiferromagnetic order. As has been demonstrated in previous studies [8, 10-15], electrical switching of the AFM order

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parameter is accompanied by reversal of boundary magnetization, which allows for a plethora of functionalities and novel device concepts.

More conventional magneto-electric spin transistors have been proposed previously [16-19], but those studies have not emphasized the value of using a narrow channel conductor with strong spin-orbit coupling (SOC) to enhance the on/off ratio. Manipatruni et al. [20] proposed a device based on the combination of a magneto-electric dielectric layer and a spin-orbit coupling channel. However that scheme does not involve direct coupling between the ME and SOC materials. The latter is used as a transduction mechanism from the state of a ferromagnet to an electric signal. Another proposed device scheme involves the detection of the interface spin-current due to the anomalous Hall effect in a paramagnetic layer on top of the magneto-electric chromia [11, 12], which also did not explicitly exploit the spin Hall effect of a conduction channel with large spin orbit coupling.

There are several theoretical proposals to utilize voltage-controlled exchange bias in heterostructures, which use a ME antiferromagnet and an exchange coupled ferromagnetic layer as the fundamental building block of memory and logic devices [1, 21-37]. Exchange coupling between the boundary magnetization of the antiferromagnet and the ferromagnetic layer allows for the voltage control of the latter's magnetization, which then serves as a non-volatile state variable. This writing mechanism avoids dissipative currents and is thus energy-efficient and inert against detrimental effects from Joule heating. Symmetry constraints rigorously imply that reversal of magnetization, which is odd under time inversion, cannot be achieved by a quasi-static electric field which is even under time inversion. Pathways to overcome this fundamental problem include successive 90 degree magnetization rotation, timed voltage pulses exploiting voltage-controlled anisotropy and magnetization precession. In contrast, we employ small static applied magnetic fields breaking time inversion when utilizing voltage-controlled switching of boundary magnetization in magneto-electric antiferromagnets. The symmetry breaking magnetic field can be as low as Earth's magnetic field. Dipole field of a fixed ferromagnet can be utilized as a robust field source. For instance, the bottom metallic layer of the AFSOR shown in Fig. 1 can be designed to be ferromagnetic but exchange decoupled thus serving as electrode and magnetic field source.

The most commonly discussed readout mechanism relies on tunneling magnetoresistance (TMR), where the voltage-controlled ferromagnetic film constitutes the free layer of the TMR trilayer [1, 22-26, 31-38]. Problems arise with leakage currents, canted magnetization (as may occur with very high critical temperature magneto-electrics) and when scaling to very small dimensions. In the latter case, the AFM volume decreases. As a result, maintaining the required reversible ME energy for switching requires an increase of the electric field. However, dielectric breakdown prevents application of electric fields above a few MV/cm.

II. THE ANTI-FERROMAGNET SPIN-ORBIT READ (AFSOR) LOGIC DEVICE

Switching of any induced spin-polarization is a key element of the proposed magnetoelectric (ME) spinFET architectures that we discuss here. The idea is to exploit voltage-control of spin-polarization that has been induced via interface exchange in a thin semiconducting channel. The ME material can be ferroelectric (e.g. $BiFeO_3$), or a dielectric (e.g. Cr_2O_3). Switching of the induced spin-polarization is virtually instantaneous, which is the major advantage over the much slower precessional switching of remnant magnetization (typically a few ns, but no faster than 178 ps [29] to 500 ps [39]). Switching speed is, therefore, only limited by reversal of the AFM order parameter. The higher AFM resonance frequency indicates that switching of antiferromagnets is intrinsically much faster than switching of ferromagnets. The onset of the source-drain current with voltage, i.e. transistor operation, will be extremely sharp, because the ME switching has a very sharp non-linear response to applied voltage [9, 40]. The anti-ferromagnet spin-orbit read (AFSOR) logic device structure (Figure 1) has the following intriguing features: the potential for high and sharp voltage 'turn-on'; inherent non-volatility of magnetic state variables; absence of switching currents, which lowers power consumption; large on/off ratios; and multistate logic and memory applications. The design will provide reliable room-temperature operation with large on/off ratios well beyond what can be achieved using magnetic tunnel junctions. The core idea here is to use the boundary polarization of the magneto-electric to spin polarize or partly spin polarize a narrower (very thin) semiconductor.

Requirements for the material are:
1) Large spin-orbit coupling;
2) Topological protection of conducting states;
3) Spin polarization control by voltage;
4) Scalability, i.e. reasonable conduction even in narrow wires <10 nm.

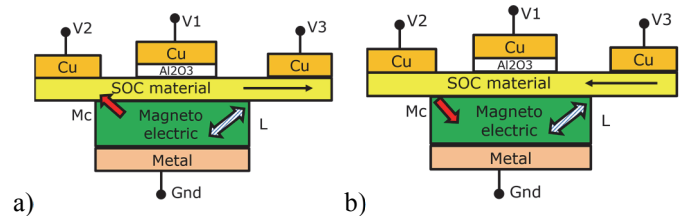*Figure 1: Scheme of anti-ferromagnet spin orbit read (AFSOR) logic. a) The state with positive V1 applied and the surface or interface magnetization of the magnetoelectric gate M_{surf} pointing up. b) The state with negative V1 applied and surface magnetization M_{surf} pointing down.*

The roughness-insensitive boundary magnetization at the interface between the ME film and the narrow channel semiconductor or paramagnetic overlayer is strongly coupled to the bulk AFM order parameter and follows the latter during voltage-controlled switching [8, 11, 12]. If the narrow channel conductor is sufficiently thin, the transport channel will be spin polarized by a proximity effect [16, 24, 41, 42]. Quantum-mechanical exchange coupling between the boundary magnetization and the carrier spins in the narrow channel of the FET can give rise to a damped precession of the spins injected

from the source of the FET. When utilizing channel materials with weak spin-orbit coupling, such as graphene or Si, the effective exchange field of the voltage-controlled boundary magnetization is the sole source for spin precession. If the semiconductor channel retains large spin orbit coupling, then the spin current, mediated by the gate boundary polarization, may be enhanced and, to some extent, topologically protected. The latter implies that each spin current has a preferred direction. Modulated spin precession, and added functionality is possible if spin-orbit coupling is exploited, such as in BiSeTe and the transition metal dichalcogenides (TMDs), as would be the case in the magneto-electric multiplexer that is discussed later.

Both the *AFSOR logic* device and the *ME spinFET multiplexer (spin-MUX)* exploit the modulation of the spin-orbit splitting of the electronic bands of the semiconductor channel materials through a "proximity" magnetic field derived from a voltage-controlled ME material. We utilize the electrically switchable and nonvolatile boundary magnetization of a ME antiferromagnet, such as chromia [8], to generate a voltage-controlled exchange field, which determines the carrier spin in the conducting channel (Figure 2). For a given remanent boundary magnetization, the exchange field will determine the spin state of the carriers at the analyzer (drain) in concert with the length of the channel (Figure 1), while spin-orbit coupling could be exploited to determine the direction of current flow (Figure 3). The combination provides a class of nonvolatile digital circuits that resemble multiple collector bipolar junction transistors (BJT) [43] or might be considered as nonvolatile, low power merged transistor logic, but with the advantage of being a planar technology. With variants of the device of Figure 3, where inversion symmetry is not so strictly broken, one can imagine a modern version of multiplexer logic (Mux), with the added bonus of nonvolatility.
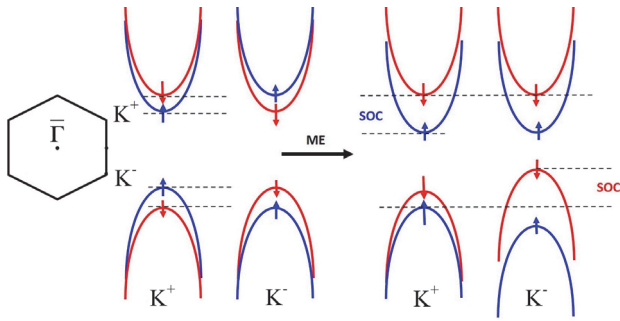

Figure 2. *The schematic of exchange splitting induced by the boundary magnetization of a magneto-electric such as chromia, in a 2D channel system with large spin orbit coupling. The induced polarization is altered at K+ and K- points of the Brillouin zone by a Zeeman like effect, so the channel, in a material like WSe2, is nearly 100% polarized at the top of the valence band.*

The operational procedure of the AFSOR logic device is outlined as follows. To write the state, a positive or negative voltage V_1 is applied to the cell of Fig. 1. In response to the electric field associated with this voltage, paraelectric polarization as well as the AFM order (L) in the ME insulator (such as chromia, Cr_2O_3) are switched. Surface magnetization

(M_{surf}), tied to the value of L, polarizes the spins of carriers in the SOC material and induces preferred conduction, i.e. much lower resistance, in only one direction along the SOC channel. In other words, the influence of M_{surf} on the channel produces directionality of conduction, which is not possible through conventional gate dielectrics, as indicated in Figure 3. The current *versus* voltage dependent on the direction of magnetoelectric polarization is obtained by NEGF transport simulation [27] in a 2D ribbon width 20 nm, band mass $0.1m_e$, for illustration we assume a conservative value of exchange splitting of 0.1 eV, V3-V2=0.1 V, at 300 K. To read the state, a positive or negative voltage V_2-V_3 is applied between the source and drain of the devices. The charge current mainly flows in the low-resistance direction. The current conducted in the channel is used to charge the next stage of capacitors, and in turn switch the AFM in these elements. Thus, the AFSOR elements are easily cascaded. The use of a 2D material as the channel gives much better control of conductivity by boundary polarization M_{surf}. Unidirectional conductance has been demonstrated in a ferromagnet/topological insulator heterostructure [44]; and a similar effect in ferromagnet/spin Hall metal heterostructure [45]. As noted above, to break symmetry, the dipole field of a fixed ferromagnet can be utilized. For the AFSOR, shown in Fig. 1, the bottom metallic layer of the can be designed to be ferromagnetic but exchange decoupled thus serving as electrode and magnetic field source. Quantum mechanical exchange and the corresponding exchange field depend on orbital overlap giving rise to an exponentially fast decay with separation of the exchange coupled atoms. The magnetic dipole field, in contrast, decays algebraically and is long range in comparison with the exchange field. It is therefore straightforward to achieve decoupling between a ferromagnetic electrode and an adjacent antiferromagnet. An interlayer of just one unit cell of Al_2O_3 can effectively disrupt exchange interaction between the ferromagnet and the antiferromagnet and at the same time serve as lattice matching seed layer for the epitaxial growth of chromia.
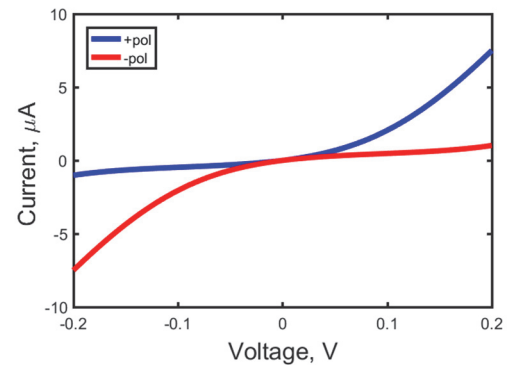

Figure 3. *Source to drain current vs. voltage V1 in the AFSOR device of Figure 1. The SOC channel polarized in opposite directions (+ or -) by the magnetoelectric gate.*

This device exploits the spin of the electron (or hole) by utilizing the non-volatile switching of magnetoelectric gates to influence the exchange splitting in a large atomic number, Z, narrow channel conductor with spin-orbit coupling. Those

include materials such as WSe_2, HfS_3, $(Bi_{1-x}Sb_x)_2Te_3$, In_4Se_3, In_4Te_3 or the electron gas that forms at the surface/interface of InP and InAs, ideally systems where there is strong spin-orbit coupling. Non-volatility in such possible devices comes from the magnetoelectric gate, while the magnetoelectric sensing effect comes from the voltage control of the large spin orbit coupling. Spin Hall effect as a means of translating spin orbit coupling into spintronic devices has been discussed for decades [46-48], but only realized fairly recently [49-51] for 3D materials and hetero-interfaces, not narrow channel 2D materials where the effect might be expected to be much larger.

Compared to prior spin-logic devices, the advantages of AFOSR are that the AFM order is not sensitive to external magnetic fields and its switching is not affected by sidewall roughness. By avoiding a ferromagnet channel and ferromagnetic switching, the write operation is much faster, ~3 to 20 ps [29, 52]. Switching of the induced spin-polarization therefore has the major advantage to be virtually instantaneous when compared with the precessional switching of remnant magnetization (typically ns but no faster than 178 ps [29] to 500 ps [39]),

In the proposed device scheme, even a single gated device would enable high on/off ratios, as described [53, 54]. Since the spin current undergoes a lateral force, spin up and down are separated and could be "read" by "split drains, although the use of spin polarized drain electrodes will clearly enhance the on/off ratio of the drain current and the spin Hall voltage (voltage at one drain minus the voltage at the other drain). This spin Hall voltage will be very material dependent. In a material like WSe_2, the spins would be defined perpendicular to the plane, so that the magnetized drain electrode should, in the simplest implementation, have magnetization perpendicular to the plane as well. This would align with the induced spin polarization from a magnetoelectric like chromia, which is also perpendicular to the plane. Note that if a ferromagnetic contact is used, there would be no "switching" of this contact, in normal device operation.

The AFSOR (Figure 1) device uses a Zeeman like perturbation of the spin-orbit coupling in the channel (schematically illustrated in Figure 3, for a transition metal dichalcogenide) to modulate spin polarization in the device. The output is a voltage difference when spin-orbit coupling is "turned on" between the two FM drain contacts due to the spin-Hall effect. This output voltage can be modulated by the gate or gates (when top and bottom gated), which influences the spin-orbit interaction in the channel. Such control will be especially effective when involving both top and bottom gates. The spin-Hall voltage in the device can be increased by using different FMs in the source and drain. By adopting a scheme based solely on magnetoelectric switching, its speed will be limited only by the switching dynamics of the magnetoelectric (somewhere in the region of 10 ps to 100 ps [20]).

Magnetization in the conduction channel with spin-orbit coupling is switched by precessional switching [55]. The effective spin polarization in inverse Rashba-Edelstein effect is

$$P_{eff} \sim w * \lambda / d \sim 60nm * 0.5nm/3nm \sim 10 \qquad (1)$$

Where w is the width of the magnet, d is the thickness of the spin-orbit channel, $\lambda \sim 0.5$ nm is the spin orbit coefficient for Bi_2Se_3. Then the charge required for switching is

$$Q_{fm} = eN_s/P_{eff} \sim 1.6x10^{-19} * 1x10^4/10 \sim 160 \ aC \qquad (2)$$

for a magnet with $N_s = 10^4$ spins (Bohr magnetons). Current delivered by a present day transistor at a drain voltage of 0.1 V can be as large as 6 μA. Then, the pulse needed to conduct this charge can be shorter than 20 ps, but depends critically on the leakage through the magnetoelectric gate dielectric - the greater the resistance of the magnetoelectric, the faster the switching speed and the smaller the energy cost.

Transistors typically have better on/off ratios than a tunnel junction device. As such, they have greater potential for use in logic devices, than a spintronic device based on a tunnel junction. On/off current ratio in 2D FETs is experimentally shown to extend up to 10^8 for MoS_2 [56] and 10^6 for WSe_2 [57], while magneto-resistance effect in magnetic tunnel junctions does not exceed 10^2. As the exchange splitting in the 2D channel of the transistor approaches the value of the surface potential change in a FET, one expects similar on/off ratio.

The induced spin polarization of the channel can be altered by changing the boundary polarization of the gates, and manipulated by using the magnetoelectric properties of the gates. The spin-orbit coupling can be changed by the electric field across the channel, and the current channel can be turned off by the net bias applied to the channel. This multistate memory or logic is especially robust if the source is spin polarized as well, although the magnetization of the source is by no means essential as for the overall device to work, as spin injection is *not* essential. The advantage of this device over conventional spin-FET devices is that the output voltage can be directly used to drive the next stage in a circuit, without the need for additional devices. This will help in reducing the device count in logic circuits. Another advantage of using channel materials with large SOC is that the SOC can lead to enhanced carrier mobility, as the spin flip scattering is then much suppressed at room temperature.

III. THE MAGNETOELECTRIC SPIN-FET MULTIPLEXER

In a variant of Figure 1, where inversion symmetry is not as strictly broken as in the case of Figure 4, one can imagine a modern version of multiplexer logic (MUX), with the added function of nonvolatility. The *magnetoelectric spin-FET multiplexer* (Figure 4) also exploits the modulation of the spin-orbit splitting of the electronic bands of the semiconductor channel through a "proximity" magnetic field derived from a voltage-controlled ME material. Here, by using semiconductor channels with large spin-orbit coupling, we expect to obtain a transverse spin Hall current, as well as a spin current overall. Depending on the magnitude of the effective magnetic field in the narrow channel, we anticipate two different operational regimes. Like the AFSOR ME spin FET, the magnetoelectric spin-FET multiplexer in Figure 4 uses spin-orbit coupling in the channel to modulate spin polarization and hence the conductance (by spin) of the device. There is a source-drain voltage and current difference, between the two FM source contacts, due to the spin-Hall effect when spin-orbit coupling is

present. This output voltage can be modulated by the gate or gates, which influences the spin-orbit interaction in the channel especially when it is both top and bottom gated especially. The spin-Hall voltage in the device can be increased by using different FMs in the source and drain.

In addition to being configured as a logic element, this device can also be used to provide multi-valued logic as the source can be turned on or off either by different combinations of gate
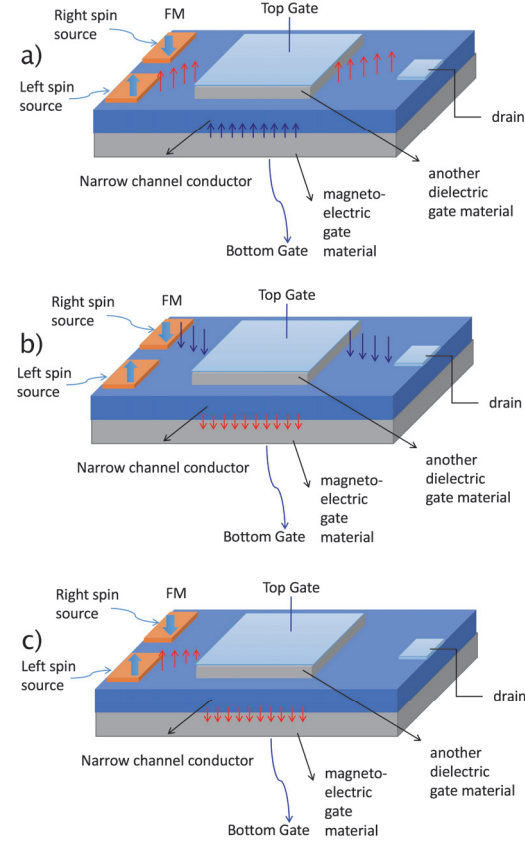

Figure 4: *The basic nonvolatile ME spinFET multiplexer (spin-MUX), with ferromagnetic source contacts. The thin channel conductor/semiconductor (blue) would be polarized (a) up or (b) down. A spin polarized current in the opposite sense from the polarization induced by the magnetoelectric gate is blocked, as schematically indicated in (c). Device considerations favor semiconductors with large spin-orbit coupling, where the boundary polarization alters the spin orbit coupling and polarizes the channel, as indicated in Figure 5 [24,52].*

electrode voltages, or by switching of the boundary polarization of the magnetoelectric gate. As a logical device, the magnetoelectric spinFET multiplexer has two inputs – the direction of magnetization in the channel as a result of the boundary polarization, and the voltage at the gate. Up and down directions of magnetization are designated as '0' and '1'. Also the two directions of the polarization (switched by voltage, e.g. 0 V and 0.1 V) producing opposite values of spin-orbit coupling in the channel are designated as '0' and '1'. Note that these states are non-volatile, i.e. the state condition remains even when the power is turned off. The advantage of this device over conventional spin FET devices is that the output voltage can be directly used to drive the next stage in a circuit, without the need

for additional devices. This will help in reducing the device count in logic circuits. A schematic view of the variations of these magnetoelectric devices is shown in Fig. 4, which utilize the atomic-scale thickness of 2-D crystals for spintronic applications. The on/off ratio of spin FETs is known to be degraded by low spin injection efficiencies, as noted above, caused by the spin-conductivity mismatch between their ferromagnetic (FM) contacts and the non-magnetic (NM) semiconductor channel [58]. This mismatch might be circumvented by inserting a thin tunnel barrier between the FM contact and the semiconductor, allowing the barrier-related resistance to dominate.

Several other types of devices in which a ferroelectric gate controls a channel with spin orbital coupling are described in the Supplementary material.

IV.   INDUCED POLARIZATION

While 2D materials are an attractive channel material choice, because of the reduced source to drain "cross-talk" or leakage current at very small spatial dimensions [59,60], in the devices discussed here, they are extremely attractive because they are atomically thin and the induced polarization in the channel is very high, as indicated in Figure 2. This is essential to the device concepts just discussed, but does not represent the limits imposed by the key challenges that must be addressed.

Another challenge lies in maintaining the ME spinFET device characteristics while scaling the device dimension to less than 10 nm. For this purpose, we favor HfS_3, In_4Se_3, In_4Te_3 or the electron gas that forms at the surface/interface of InP and InAs as spin-orbit coupling channel materials, because they are likely to be scalable to spatial channel widths of 10 nm or less. Concern about edge scattering has attracted the attention of theorists [61-66] and has been found to have a major influence in experiment [67-69]. The trichalcogenides, MX_3 and other transition metal *tri*chalcogenides (TMTCs) like In_4X_3 (X=Se, Te) possess a unique quasi-1D structure that makes devices scaled to dimensions less than 10 nm appear possible.

There are several reasons to seriously consider materials from the transition metal TMTC family. These trichalogenide materials are also layered materials but the edge structure and edge chemistry lend the ribbon greater fidelity and fewer imperfections. While the topological insulators may be suitable channel materials for the AFSOR logic device of Figure 1, as they do exhibit a topologically protected spin current, likely the better device performance will be achieved using TMTC's. The TMTC's not only possess a unique quasi-1D structure, but also have promising semiconductor properties. For example, TiS_3 has a band gap of ~ 1 eV [70], while In_4Se_3 has a direct band gap of about 1.3 eV [71-72] and an indirect gap of about 0.6 eV [73-75], making the band gaps of both TiS_3 and In_4Se_3 comparable to that of silicon (1.1 eV). Also, according to a recent theoretical study, in the direction along TiS_3 chains, titanium trisulfide is expected to have higher electron mobility of ~10,000 cm^2/Vs [71]. HfS_3, with a crystal structure similar to TiS_3, will also possess highly anisotropic crystal structure and might be a suitable choice TMTC material for the development of the AFSOR logic device of Figure 1, because of the expectation of large spin-orbit coupling (the Z of Hf is far larger than for Ti). This is extremely promising because

single layer titanium trisulfide, TiS_3 field effect transistors (FETs) have been fabricated [76]. These TMTC channel materials are viewed as advantageous as they combined significant spin orbit coupling and a minimum or edge scattering. It should be noted that in the case of various topological insulators, edge scattering will actually increase the influence of spin orbit coupling, and a thin layer TI will form a band gap [77] thus, should the chemical potential fall mid gap, retain the desire high on/off ratios. Without the band gap, the topological insulator material/channel will act more like a spin valve, and suffer from a decrease in on/off ratio and spin fidelity, in the limit of small spatial dimensions, in spite of the very large spin orbit coupling.

As noted above, key to the magnetoelectric devices is the proximity induced polarization [16,24,41-42,77-79] in the narrow (2D) conduction channel. Not all of the proposed 2D semiconductor channel materials have been modeled, but as proof of principle, induced polarization in MoS_2 and WSe_2, in contact with chromia has been modeled, as indicated in Figure 5. We constructed a $Cr_2O_3(0001)$ slab model with 11 Cr layers and 10 O layers, in which the outmost layers are Cr ones, in accordance with the previous studies [16]. For the heterostructures of transition metal dichalcogenides (TMD) monolayer on top of $Cr_2O_3(0001)$ slab, we adopted a 3×3 TMD supercell to match the 2×2 $Cr_2O_3(0001)$ slab supercell. The lattice mismatch for WSe_2/Cr_2O_3 was 0.3%, which was applied to the lattice constant a of $Cr_2O_3(0001)$ slab in order to match the TMD supercells, since the electronic properties of TMDs are very sensitive to the lattice constant a, whereas the band gap changes of $Cr_2O_3(0001)$ slab on lattice constant a are negligible.
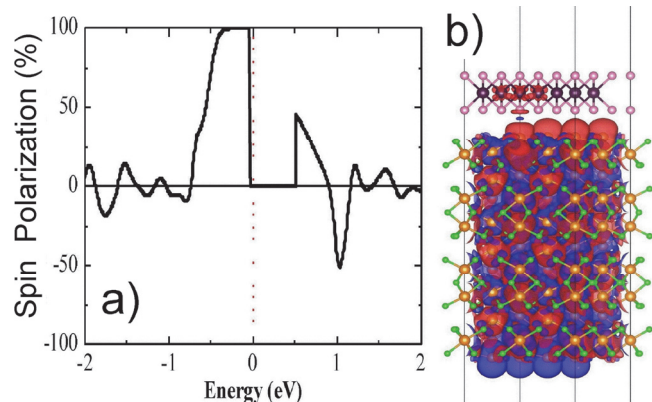

Figure 5. *The induced spin-polarization in WSe_2, by the boundary magnetization of chromia. The induced polarization is altered at $K+$ and $K-$ points of the Brillouin zone (Figure 2), by a Zeeman like effect, so the WSe_2 channel is nearly 100% at the top of the valence band (for hole conduction), as indicated by (a), through interaction with chromia as indicated by (b).*

All calculations were performed within the framework of the Vienna *ab initio* simulation package VASP [80-82], a first-principles plane-wave code based on spin-polarized density functional theory (DFT). The exchange correlation was treated with the Perdew-Burke-Ernzerhof (PBE) functional [82], and the projector augmented wave (PAW) method was used to describe the interaction of electron-ion. And the plane wave basis set with the energy cutoff of 400 eV was adopted in the calculations. The vdW corrections [83-84] and dipole corrections [85-86] were performed for both heterostructures. To correct the strong on-site electronic correlation, the DFT+U method was used for the Cr atoms with U – J = 4 eV. The Brillouin zone integration is performed using Monkhorst-Pack [87] 4×4×1 grid for geometry optimizations and 7×7×1 for static electronic structure calculations of TMD monolayers, and 3×3×1 for relaxation and static calculations of the $Cr_2O_3(0001)$ slab and heterostructures..

We found that there is a transfer of 0.36 electrons from chromia to the MoS_2 monolayer, but negligible charge transfer from chromia to a WSe_2 monolayer (0.04 electrons). In spite of the very small charge transfer, chromia induces a very high level of spin polarization in both a MoS_2 adlayer and a WSe_2 monolayer (Figure 5). The take-away message is that even for a large spin orbit coupling system like the WSe_2 monolayer, the boundary polarization of chromia induces a high level of polarization. This means that for small source drain bias voltages, the carriers that pass over the magnetoelectric gate are of necessity, highly spin polarized. Simulations (Figure 5) indicate an exchange splitting of ~0.5 eV, in the vicinity of the valence band maximum and the Brillouin zone edge, due to interface polarization. This is more significant than the 150 meV expected for MoS_2, but in both cases the result of the very high spin polarization of the chromia boundary layer

Induced polarization is evident in graphene on chromia [16,78] but graphene is unsuitable in the devices presented here because of edge scattering, as noted above, and an absence of spin-orbit coupling. The density function theory results are much larger but still consistent with the observed exchange coupling of WSe_2 on the ferromagnet semiconductor CrI_3 [79].

V. CONCLUSION

There are multiple schemes for constructing a magnetoelectric FET, and the nonvolatility of such a device can be enhanced by combining the magnetoelectric with a channel with large spin-orbit coupling. Such devices, as described here have considerable added functionality. Some of these magnetoelectric FET devices are spintronic devices, without ferromagnetism. Because there is no need to reverse the magnetization of any ferromagnetic, even the most simple magnetoelectric FET [17,24] compares well with CMOS [88], with a comparable energy cost and reduced delay time. We acknowledge that materials other than chromia, exhibit magneto-electric switching, such as barium ferrite [89] and the rare earth ferrites [90] and these too, along with other like materials, could be used as the magneto-electric gate dielectric, in place of chromia, in the devices discussed here, so long as there is reliable isothermal switching at room temperature and above, at a low coercive voltage.

REFERENCES

[1] C. Binek and B. Doudin, "Magnetoelectronics with magnetoelectrics," *Journal of Physics-Condensed Matter,* vol. 17, pp. L39-L44, 2005.

[2] H. Dery, P. Dalal, L. Cywinski, and L. J. Sham, "Spin-based logic in semiconductors for reconfigurable large-scale circuits," *Nature,* vol. 447, pp. 573-576, 05/31/ 2007.

[3] A. Ney, C. Pampuch, R. Koch, and K. H. Ploog, "Programmable computing with a single magnetoresistive element," *Nature,* vol. 425, pp. 485-487, 10/02/ 2003.

[4] D. E. Nikonov and I. A. Young, "Overview of Beyond-CMOS Devices and a Uniform Methodology for Their Benchmarking," *Proceedings of the IEEE,* vol. 101, pp. 2498-2533, 2013.

[5] V. V. Zhirnov, J. A. Hutchby, G. I. Bourianoffls, and J. E. Brewer, "Emerging research logic devices," *IEEE Circuits and Devices Magazine,* vol. 21, pp. 37-46, 2005.

[6] F. Jonietz, S. Mühlbauer, C. Pfleiderer, A. Neubauer, W. Münzer, A. Bauer, *et al.*, "Spin Transfer Torques in MnSi at Ultralow Current Densities," *Science,* vol. 330, pp. 1648-1651, 2010.

[7] W. Porod and M. Niemier, "Better computing with magnets - The simple bar magnet, shrunk down to the nanoscale, could be a powerful logic device," *IEEE Spectrum,* vol. 52, pp. 44-60, 2015.

[8] X. He, Y. Wang, N. Wu, A. N. Caruso, E. Vescovo, K. D. Belashchenko, *et al.*, "Robust isothermal electric control of exchange bias at room temperature," *Nat Mater,* vol. 9, pp. 579-585, 07//print 2010.

[9] W. Echtenkamp and C. Binek, "Electric Control of Exchange Bias Training," *Physical Review Letters,* vol. 111, p. 187204, 10/31/ 2013.

[10] T. Ashida, M. Oida, N. Shimomura, T. Nozaki, T. Shibata, and M. Sahashi, "Isothermal electric switching of magnetization in Cr_2O_3/Co thin film system," *Applied Physics Letters,* vol. 106, p. 132407, Mar. 2015.

[11] T. Kosub, M. Kopte, F. Radu, O. G. Schmidt, and D. Makarov, "All-Electric Access to the Magnetic-Field-Invariant Magnetization of Antiferromagnets," *Physical Review Letters,* vol. 115, p. 097201, Aug. 2015.

[12] T. Kosub, M. Kopte, R. Huhne, P. Appel, B. Shields, P. Maletinsky, *et al.*, "Purely antiferromagnetic magnetoelectric random access memory," *Nature Communications,* vol. 8, p. 7, Jan 2017.

[13] K. Toyoki, Y. Shiratsuchi, A. Kobane, C. Mitsumata, Y. Kotani, T. Nakamura, *et al.*, "Magnetoelectric switching of perpendicular exchange bias in Pt/Co/alpha-Cr_2O_3/Pt stacked films," *Applied Physics Letters,* vol. 106, p. 162404, Apr 2015.

[14] N. Wu, X. He, A. L. Wysocki, U. Lanke, T. Komesu, K. D. Belashchenko, *et al.*, "Imaging and Control of Surface Magnetization Domains in a Magnetoelectric Antiferromagnet," *Physical Review Letters,* vol. 106, p. 087202, Feb 2011.

[15] N. Wu and P. A. Dowben, "Magnetic Surface States in High Polarization Materials," in *Spintronics Iv.* vol. 8100, H. J. M. Drouhin, J. E. Wegrowe, and M. Razeghi, Eds., ed Bellingham: Spie-Int Soc Optical Engineering, 2011.

[16] R. Choudhary, P. Kumar, P. Manchanda, D. J. Sellmyer, P. A. Dowben, A. Kashyap, *et al.*, "Interface-Induced Spin Polarization in Graphene on Chromia," *Ieee Magnetics Letters,* vol. 7, p. 4, 2016.

[17] J. A. Kelber, C. Binek, P. A. Dowben, and K. Belashchenko, "Magneto-electric voltage controlled spin transistors," U.S. Patent 9,718,700, August 1, 2017.

[18] Y. G. Semenov, K. W. Kim, and J. M. Zavada, "Spin field effect transistor with a graphene channel," *Applied Physics Letters,* vol. 91, p. 3, Oct 2007.

[19] S. C. Stuart, B. Gray, D. Nevola, L. Su, E. Sachet, M. Ulrich, *et al.*, "Magnetoelectric oxide films for spin manipulation in graphene," *Physica Status Solidi-Rapid Research Letters,* vol. 10, pp. 242-247, Mar 2016.

[20] S. Manipatruni, D. E. Nikonov, and I. A. Young, "Spin-Orbit Logic with Magnetoelectric Nodes: A Scalable Charge Mediated Nonvolatile Spintronic Logic," available online http://arxiv.org/abs/1512.05428, 2015.

[21] B. Doudin, C. Binek, "Magnetic spin valve with a magnetoelectric element", U.S. Patent 7,358,846, April 15, 2008.

[22] M. Bibes and A. Barthelemy, "Multiferroics: Towards a magnetoelectric memory," *Nature Materials,* vol. 7, pp. 425-426, Jun 2008.

[23] X. Chen, A. Hochstrat, P. Borisov, and W. Kleemann, "Magnetoelectric exchange bias systems in spintronics," *Applied Physics Letters,* vol. 89, p. 202508, Nov 2006.

[24] P. A. Dowben, C. Binek, and D. E. Nikonov, "Potential of Nonvolatile Magnetoelectric Devices for Spintronic Applications," in *Nanoscale Silicon Devices,* ed: CRC Press, 2015, pp. 255-278.

[25] A. Jaiswal and K. Roy, "MESL: Proposal for a Non-volatile Cascadable Magneto-Electric Spin Logic," *Scientific Reports,* vol. 7, p. 9, Jan 2017.

[26] A. Jaiswal, I. Chakraborty, and K. Roy, "Energy-Efficient Memory Using Magneto-Electric Switching of Ferromagnets," *Ieee Magnetics Letters,* vol. 8, p. 5, 2017.

[27] M. P. Anantram, M. S. Lundstrom, and D. E. Nikonov, "Modeling of Nanoscale Devices", Proceedings of the IEEE, v. 96, no. 9, pp. 1511 - 1550 (2008).

[28] D. E. Nikonov and I. A. Young, "Benchmarking spintronic logic devices based on magnetoelectric oxides," *Journal Of Materials Research,* vol. 29, pp. 2109-2115, Sep 2014.

[29] D. E. Nikonov and I. A. Young, "Benchmarking of Beyond-CMOS Exploratory Devices for Logic Integrated Circuits," *IEEE Journal on Exploratory Solid-State Computational Devices and Circuits,* vol. 1, pp. 3-11, 2015.

[30] N. Sharma, A. Marshall, J. Bird, and P. Dowben, "Magneto-Electric Magnetic Tunnel Junction as Process Adder for Non-Volatile Memory Applications," *IEEE Dallas Circuits And Systems Conference (Dcas),* p. 4, 2015.

[31] N. Sharma, A. Marshall, J. Bird, and P. Dowben, "Magneto-electric magnetic tunnel junction logic devices," in *Fourth Berkeley Symposium on Energy Efficient Electronic Systems (E3S),* 2015, pp. 1-3.

[32] N. Sharma, A. Marshall, J. Bird, and P. Dowben, "Magneto-electric magnetic tunnel junction logic devices," in *Berkeley Symposium on Energy Efficient Electronic Systems (E3S),* 2015, pp. 1-3.

[33] N. Sharma, A. Marshall, J. Bird, and P. Dowben, "Multi-bit adder design using ME-MTJ technology," in *11th International Conference on Advanced Semiconductor Devices & Microsystems (ASDAM),* 2016, pp. 89-92.

[34] N. Sharma, A. Marshall, and J. Bird, "VerilogA based Compact model of a three-terminal ME-MTJ device," *IEEE 16th International Conference on Nanotechnology (Ieee-Nano),* pp. 145-148, 2016.

[35] N. Sharma, A. Marshall, and P. A. Dowben, "Unipolar Magnetoelectric Magnetic Tunnel Junction (UMMTJ) Devices and Circuits," *17th IEEE International Conference on Nanotechnology (IEEE NANO 2017), IEEE Xplore* p. in press, 2017.

[36] N. Sharma, J. P. Bird, P. Dowben, and A. Marshall, "Compact-device model development for the energy-delay analysis of magneto-electric magnetic tunnel junction structures," *Semiconductor Science and Technology,* vol. 31, p. 8, Jun 2016.

[37] N. Sharma, et. al, "VerilogA Compact Model of a ME-MTJ Based XNOR/NOR Gate," *2016 IEEE 16th International Conference on Nanotechnology (IEEE-Nano),* Nanoscale Architectures, 2017. NANOARCH 2017. IEEE International Symposium on. IEEE, 2017 (in press).

[38] J. P. Velev, P. A. Dowben, E. Y. Tsymbal, S. J. Jenkins, and A. N. Caruso, "Interface effects in spin-polarized metal/insulator layered structures," *Surface Science Reports,* vol. 63, pp. 400-425, Sep 2008.

[39] H. Liu, D. Bedau, D. Backes, J. A. Katine, J. Langer, and A. D. Kent, "Ultrafast switching in magnetic tunnel junction based orthogonal spin transfer devices," *Applied Physics Letters,* vol. 97, p. 242510, 2010.

[40] A. Iyama and T. Kimura, "Magnetoelectric hysteresis loops in Cr2O3 at room temperature," *Physical Review B,* vol. 87, p. 180408, May 2013.

[41] J. Mathon, "Magnetisation of a strongly paramagnetic layer in contact with a ferromagnetic substrate," *Journal of Physics F: Metal Physics,* vol. 16, p. L217, 1986.

[42] D. Schwenk, F. Fishman, and F. Schwabl, "Ferromagnetic multilayers: Statics and dynamics," *Physical Review B,* vol. 38, pp. 11618-11638, 12/01/ 1988.

[43] K. Hart and A. Slob, "INTEGRATED INJECTION LOGIC - NEW APPROACH TO LSI," *Ieee Journal of Solid-State Circuits,* vol. SC 7, pp. 346-&, 1972.

[44] Y. Lv, J. Kally, D. Zhang, J. S. Lee, M. Jamali, N. Samarth, *et al.*, "Unidirectional spin Hall magnetoresistance in topological insulator/ferromagnetic layer heterostructures," *arXiv:1701.06505,* 2017.

[45] C. O. Avci, K. Garello, A. Ghosh, M. Gabureac, S. F. Alvarado, and P. Gambardella, "Unidirectional spin Hall magnetoresistance in ferromagnet/normal metal bilayers," *Nature Physics,* vol. 11, pp. 570-575, Jul 2015.

[46] M. D'yakonov and V. Perel, "Possibility of orienting electron spins with current," *Soviet Journal of Experimental and Theoretical Physics Letters,* vol. 13, p. 467, 1971.

[47] M. Dyakonov and V. Perel, "Current-induced spin orientation of electrons in semiconductors," *Physics Letters A,* vol. 35, pp. 459-460, 1971.

[48] W. M. Saslow, "Spin Hall effect and irreversible thermodynamics: Center-to-edge transverse current-induced voltage," *Physical Review B,* vol. 91, p. 014401, 01/05/ 2015.

[49] Y. K. Kato, R. C. Myers, A. C. Gossard, and D. D. Awschalom, "Observation of the spin hall effect in semiconductors," *Science,* vol. 306, pp. 1910-1913, Dec 2004.

[50] S. O. Valenzuela and M. Tinkham, "Direct electronic measurement of the spin Hall effect," *Nature,* vol. 442, pp. 176-179, Jul 2006.

[51] J. Wunderlich, B. Kaestner, J. Sinova, and T. Jungwirth, "Experimental Observation of the Spin-Hall Effect in a Two-Dimensional Spin-Orbit Coupled Semiconductor System," *Physical Review Letters,* vol. 94, p. 047204, 02/04/ 2005.

[52] D. E. Nikonov, C. Binek, X. Hong, J. P. Bird, K. L. Wang, and P. A. Dowben, "Anti-Ferromagnetic Magneto-electric Spin-Orbit Read Logic," *U.S. Patent,* pp. Application No.: 62/460,164, 2017.

[53] M. Tosun, S. Chuang, H. Fang, A. B. Sachid, M. Hettick, Y. Lin, *et al.,* "High-Gain Inverters Based on WSe₂ Complementary Field-Effect Transistors," *ACS Nano,* vol. 8, pp. 4948-4953, 2014/05/27 2014.

[54] M. O. Li, D. Esseni, J. J. Nahas, D. Jena, and H. G. Xing, "Two-Dimensional Heterojunction Interlayer Tunneling Field Effect Transistors (Thin-TFETs)," *IEEE Journal of the Electron Devices Society,* vol. 3, pp. 200-207, 2015.

[55] D. E. Nikonov, G. I. Bourianoff, G. Rowlands, and I. N. Krivorotov, "Strategies and tolerances of spin transfer torque switching," *Journal of Applied Physics,* vol. 107, p. 9, Jun 2010.

[56] B. Radisavljevic, A. Radenovic, J. Brivio, V. Giacometti, and A. Kis, "Single-layer MoS₂ transistors," *Nature Nano,* vol. 6, pp. 147-150, 03//print 2011.

[57] H. Fang, S. Chuang, T. C. Chang, K. Takei, T. Takahashi, and A. Javey, "High-Performance Single Layered WSe2 p-FETs with Chemically Doped Contacts," *Nano Letters,* vol. 12, pp. 3788-3792, Jul 2012.

[58] G. Schmidt, D. Ferrand, L. W. Molenkamp, A. T. Filip, and B. J. van Wees, "Fundamental obstacle for electrical spin injection from a ferromagnetic metal into a diffusive semiconductor," *Physical Review B,* vol. 62, pp. R4790-R4793, Aug 2000.

[59] D. Jena, "Tunneling transistors based on graphene and 2-D Crystals," *Proc. IEEE,* vol. 101, no. 7, pp. 1585–1602, 2013.

[60] J. H. Kang, W. Cao, X. J. Xie, D. Sarkar, W. Liu, and K. Banerjee, "Graphene and Beyond-Graphene 2D Crystals for Next-Generation Green Electronics," in *Micro- And Nanotechnology Sensors, Systems, and Applications VI* vol. 9083, T. George, M. S. Islam, and A. K. Dutta, Eds., ed Bellingham: Spie-Int Soc Optical Engineering, 2014.

[61] X. Blase, C. Adessi, B. Biel, A. Lopez-Bezanilla, M. V. Fernandez-Serra, E. R. Margine, *et al.,* "Conductance of functionalized nanotubes, graphene and nanowires: from ab initio to mesoscopic physics," *Physica Status Solidi B-Basic Solid State Physics,* vol. 247, pp. 2962-2967, Dec 2010.

[62] V. K. Dugaev and M. I. Katsnelson, "Edge scattering of electrons in graphene: Boltzmann equation approach to the transport in graphene nanoribbons and nanodisks," *Phys. Rev. B,* vol. 88, p. 235432, 2013.

[63] E. R. Mucciolo and C. H. Lewenkopf, "Disorder and electronic transport in graphene," *Journal of Physics: Condensed Matter,* vol. 22, p. 273201, 2010.

[64] M. Wimmer, İ. Adagideli, S. Berber, D. Tománek, and K. Richter, "Spin Currents in Rough Graphene Nanoribbons: Universal Fluctuations and Spin Injection," *Physical Review Letters,* vol. 100, p. 177207, 05/02/ 2008.

[65] J. Wurm, K. Richter, and İ. Adagideli, "Edge effects in graphene nanostructures: From multiple reflection expansion to density of states," *Physical Review B,* vol. 84, p. 075468, 08/12/ 2011.

[66] V. Y. Oleg, "Emergence of magnetism in graphene materials and nanostructures," *Reports on Progress in Physics,* vol. 73, p. 056501, 2010.

[67] M. Y. Han, J. C. Brant, and P. Kim, "Electron Transport in Disordered Graphene Nanoribbons," *Physical Review Letters,* vol. 104, p. 056801, 02/01/ 2010.

[68] S. A. Jensen, R. Ulbricht, A. Narita, X. Feng, K. Müllen, T. Hertel, *et al.,* "Ultrafast Photoconductivity of Graphene Nanoribbons and Carbon Nanotubes," *Nano Letters,* vol. 13, pp. 5925-5930, 2013/12/11 2013.

[69] Y. J. Shi, J. Lan, E. J. Ye, W. Q. Sui, and X. A. Zhao, "Four-terminal impedance of a graphene nanoribbon based structure," *European Physical Journal B,* vol. 87, p. 251, Oct 2014.

[70] J. Dai and X. C. Zeng, "Titanium Trisulfide Monolayer: Theoretical Prediction of a New Direct-Gap Semiconductor with High and Anisotropic Carrier Mobility," *Angewandte Chemie-International Edition,* vol. 54, pp. 7572-7576, Jun 2015.

[71] N. Benramdane and R. H. Misho, "Structural and optical properties of In₄Se₃ thin films obtained by flash evaporation," *Solar Energy Materials and Solar Cells,* vol. 37, pp. 367-377, 1995.

[72] Y. B. Losovyj, M. Klinke, E. Cai, I. Rodriguez, J. Zhang, L. Makinistian, *et al.,* "The electronic structure of surface chains in the layered semiconductor In₄Se₃(100)," *Applied Physics Letters,* vol. 92, p. 122107, 2008.

[73] K. Fukutani, Y. Miyata, I. Matsuzaki, P. V. Galiy, P. A. Dowben, T. Sato, *et al.,* "High-Resolution Angle-Resolved Photoemission Study of Quasi-One-Dimensional Semiconductor In4Se3," *Journal Of the Physical Society Of Japan,* vol. 84, p. 6, Jul 2015.

[74] Y. S. Lim, M. Jeong, S. Won-Seon, J.-H. Lee, C.-H. Park, M. Sznajder, *et al.,* "Condenson state and its effects on thermoelectric properties in In₄Se₃," *Journal of Physics D: Applied Physics,* vol. 46, p. 275304, 2013.

[75] V. P. Savchin, "Characteristics of the Transport-Properties of Layer In₄Se₃ Crystals " *Soviet Physics Semiconductors-USSR,* vol. 15 p. 827, 1981.

[76] A. Lipatov, P. M. Wilson, M. Shekhirev, J. D. Teeter, R. Netusil, and A. Sinitskii, "Few-layered titanium trisulfide (TiS₃) field-effect transistors," *Nanoscale,* vol. 7, pp. 12291-12296, 2015.

[77] M. Neupane, A. Richardella, J. Sánchez-Barriga, S. Xu, N. Alidoust, I. Belopolski, *et al.,* "Observation of quantum-tunnelling-modulated spin texture in ultrathin topological insulator Bi₂Se₃ films," *Nature Communications* vol. 5, p. 3841, 05/12/online 2014.

[78] S. Cao, Z. Xiao, C.-P. Kwan, K. Zhang, J. P. Bird, W. Lu, *et al.,* "Moving towards the Magnetoelectric Graphene Transistor," *Applied Physics Letters,* vol. 111, 182402, 2017.

[79] D. Zhong, K. L. Seyler, X. Linpeng, R. Cheng, N. Sivadas, B. Huang, E. Schmidgall, T. Taniguchi, K. Watanabe, M. A. McGuire, W. Yao, D. Xiao, K.-M. C. Fu, X. Xu1, "Van der Waals engineering of ferromagnetic semiconductor heterostructures for spin and valleytronics," *Science Advances* vol. 3: e1603113, 2017.

[80] G. Kresse and J. Hafner, "Ab initio molecular dynamics for liquid metals," *Physical Review B,* vol. 47, pp. 558-561, 01/01/ 1993.

[81] G. Kresse and J. Hafner, "Ab initio molecular-dynamics simulation of the liquid-metal–amorphous-semiconductor transition in germanium," *Physical Review B,* vol. 49, pp. 14251-14269, 05/15/ 1994.

[82] J. P. Perdew, K. Burke, and M. Ernzerhof, "Generalized Gradient Approximation Made Simple," *Physical Review Letters,* vol. 77, pp. 3865-3868, 10/28/ 1996.

[83] J. Klimes, D. R. Bowler, and A. Michaelides, "Chemical accuracy for the van der Waals density functional," *Journal oOf Physics-Condensed Matter,* vol. 22, p. 5, Jan 2010.

[84] J. Klimeš, D. R. Bowler, and A. Michaelides, "Van der Waals density functionals applied to solids," *Physical Review B,* vol. 83, p. 195131, 05/25/ 2011.

[85] G. Makov and M. C. Payne, "Periodic boundary conditions in ab initio calculations," *Physical Review B,* vol. 51, pp. 4014-4022, 02/15/ 1995.

[86] J. Neugebauer and M. Scheffler, "Adsorbate-substrate and adsorbate-adsorbate interactions of Na and K adlayers on Al(111)," *Physical Review B,* vol. 46, pp. 16067-16080, 12/15/ 1992.

[87] H. J. Monkhorst and J. D. Pack, "Special points for Brillouin-zone integrations," *Physical Review B,* vol. 13, pp. 5188-5192, 06/15/ 1976.

[88] N. Sharma, A. Marshall, J. Bird, and P. Dowben, *"Verilog-A based Compact Modeling of the ME-FET device", submitted E3S Symposium & Steep Transistors Workshop*

[89] J. T. Heron, M. Trassin, K. Ashraf, M. Gajek, Q. He, S. Y. Yang, et al., "Electric field induced magnetization reversal in a ferromagnet-multiferroic heterostructure," *Physical Review Letters,* vol. 107, p. 217202 , Nov. 2011.

[90] Y. Tokunaga, Y. Taguchi, T. Arima and Y. Tokura, "Electric field induced generation and reversal of ferromagnetic moment in ferrites," Nature Physics vol. 8, pp. 838–844, Aug. (2012)