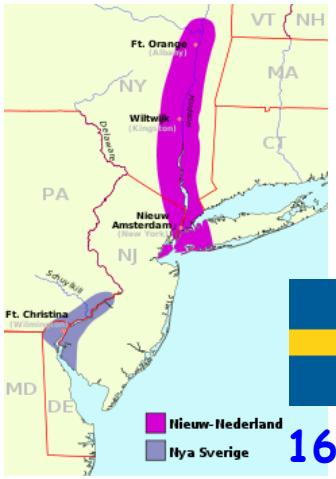
Spin-Orbit Torque in van der Waals Heterostructures of Magnetic Two-Dimensional Materials

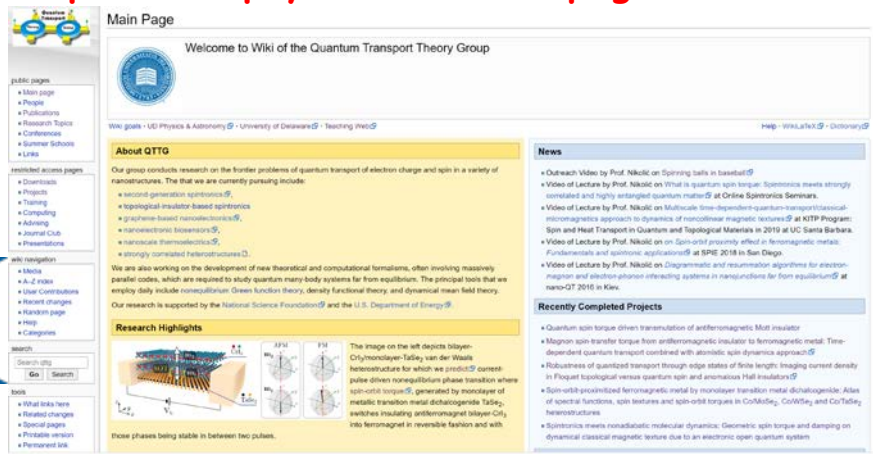
Branislav K. Nikolić

Department of Physics & Astronomy, University of Delaware, Newark, DE 19716, U.S.A.



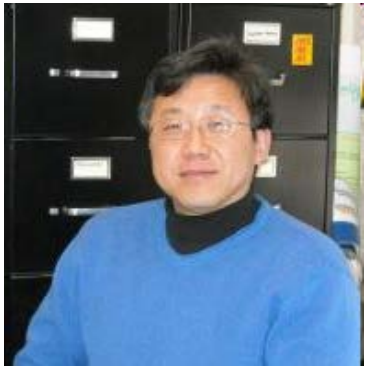
1638–1655

https://wiki.physics.udel.edu/qttg



Collaborators

Experiment



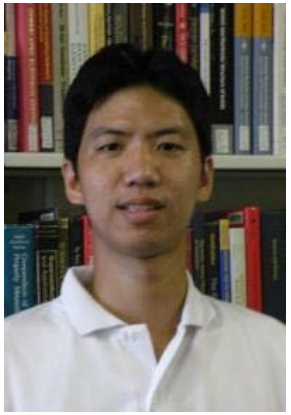
Prof. John Q. Xiao

Prof. Hyunsoo Yang

Theory & Computation

Dr. Kapildeb Dolui

Dr. J. M. Marmolejo-Tejada



Dr. Po-Hao Chang

Dr. Marko D. Petrović

Prof. Petr Plecháč

Prof. Jaroslav Fabian

Klaus Zollner

Watch Movies Throughout the Talk Carefully!

or talk

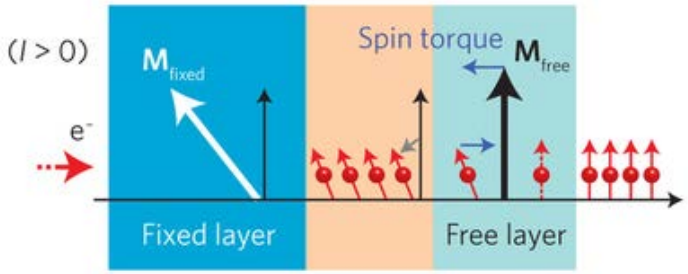
The Scientific Paper Is Obsolete

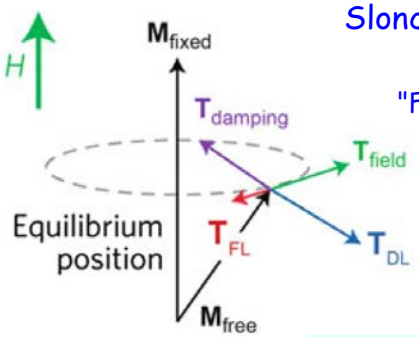
Here's what's next.

The Atlantic | James Somers

Spin-Transfer Torque (STT): Fundamentals and Applications

Fundamentals



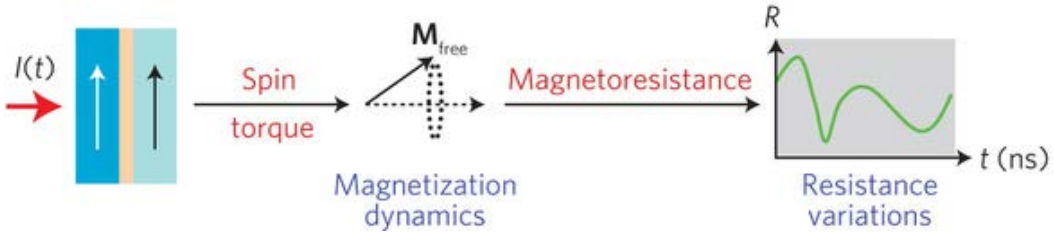


Slonczewski (1996), Berger (1996)

BUCKLEY CMP PRIZE:
"For predicting spin-transfer torque and opening the field of current-induced control over magnetic nanostructures."

$$T_{CD} = T_{DL} + T_{FL}$$

$$\mathbf{T}_{CD} \propto \langle \hat{\mathbf{s}} \rangle_{CD} \times \mathbf{M}_{free}$$



arXiv:1801.05793

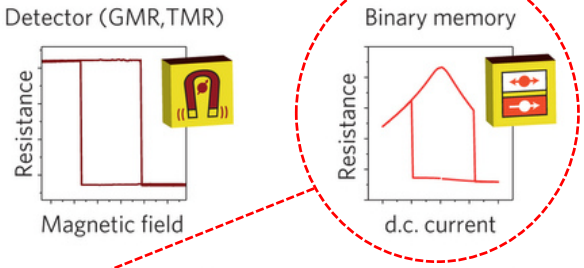
First-Principles Quantum Transport Modeling of Spin-Transfer and Spin-Orbit Torques in Magnetic Multilayers

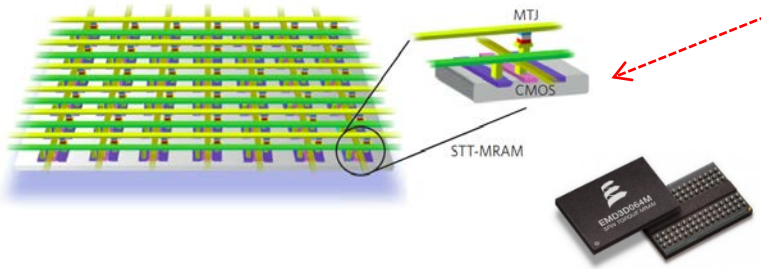
Branislav K. Nikolić, Kapildeb Dolui, Marko D. Petrović, Petr Plecháč, Troels Markussen, and Kurt Stokbro

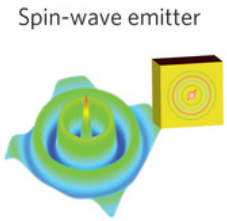
Applications

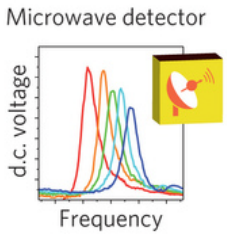
Spin-torque building blocks

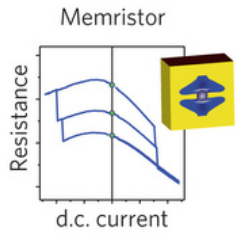
N. Locatelli, V. Cros and J. Grollier*







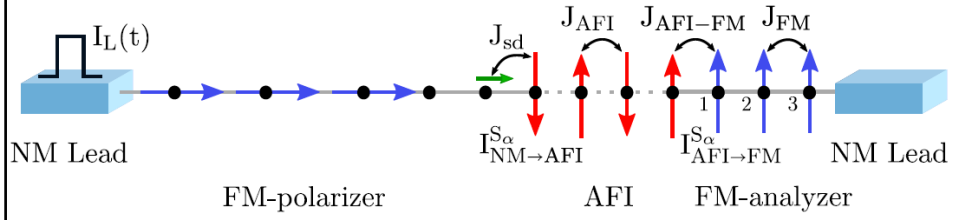




STT-Driven Magnetization Dynamics from Time-Dependent Quantum Transport + Atomistic Spin Dynamics

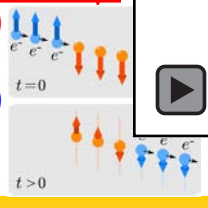
Electron-mediated STT

Magnon-mediated STT



TDNEGF+LLG formalism:
PRAppl. **15**, 034089 (2021)
PRAppl. **10**, 054038 (2018)
PRB **99**, 134409 (2019)
PRB **101**, 214412 (2020)
PRL **125**, 187202 (2020)

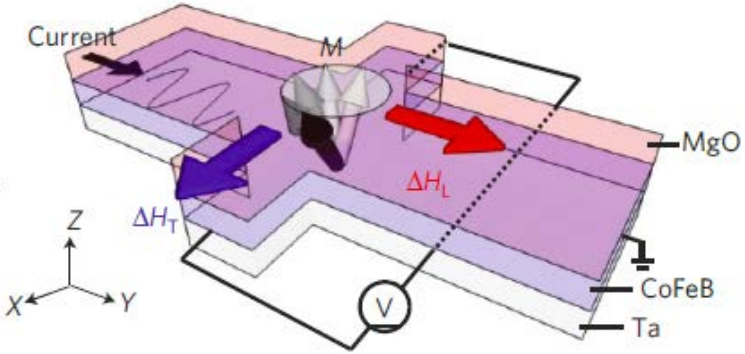
Quantum STT in collinear setup:
PRL **126**, 197202 (2021)
PRX (2021)
PRL **119**, 257201 (2017)



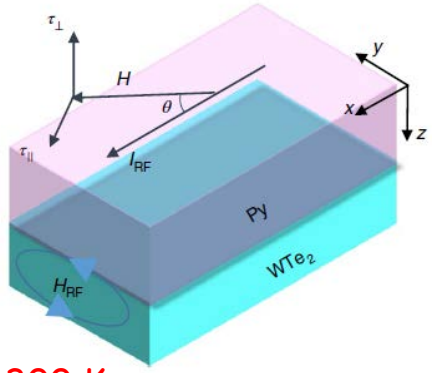
Spin-Orbit Torque (SOT): Fundamentals and Applications

Fundamentals

Nat. Mater. **9**, 230 (2010); Nature **476**, 189 (2011)
Science **336**, 555 (2012)
Nat. Mater. **12**, 240 (2013)

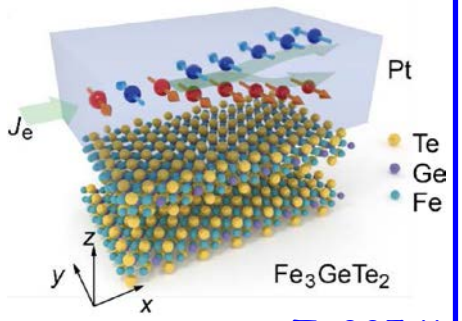


Nat. Nanotech. **14**, 945 (2019)



T=300 K
Magnetization switching with ultralow current density ~3×10^5 A/cm^2

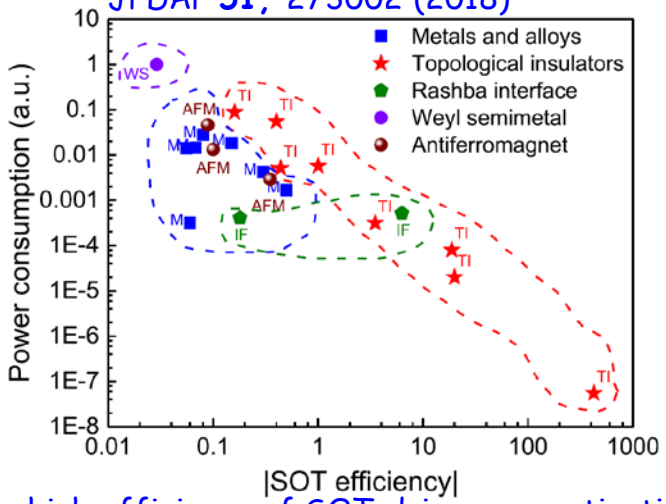
Nano Lett. **19**, 4400 (2019)
Sci. Adv. **5**, eaaw8904 (2019)



T~225 K
Switching with current density ~3×10^7 A/cm^2
but gate tunable

Applications

JPDAP **51**, 273002 (2018)



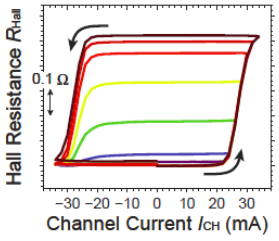
high efficiency of SOT-driven magnetization switching demonstrated: 60 fJ (vs. 150 fJ to 4 pJ with STT) energy consumed per bit writing

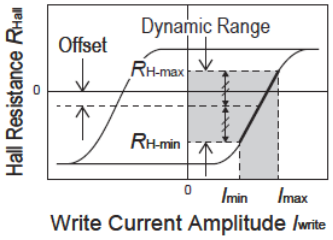
solid-state nonvolatile analogue memory with infinite read-write endurance

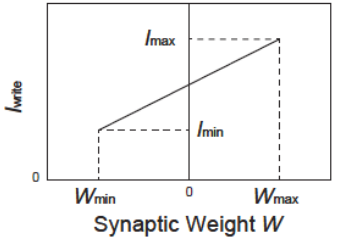
Applied Physics Express **10**, 013007 (2017)
https://doi.org/10.7567/APEX.10.013007

Analogue spin–orbit torque device for artificial-neural-network-based associative memory operation

William A. Borders[1], Hisanao Akima[1*], Shunsuke Fukami[1,2,3,4*], Satoshi Moriya[1], Shouta Kurihara[1], Yoshihiko Horio[1], Shigeo Sato[1], and Hideo Ohno[1,2,3,4,5]







This Talk in a Nutshell

Spectral functions and spin textures on metallic surfaces imaged by spin-ARPES

news & views

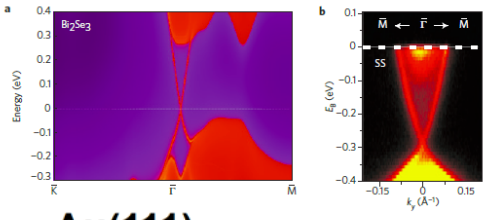
TEN YEARS OF NATURE PHYSICS

Not trivial to realize

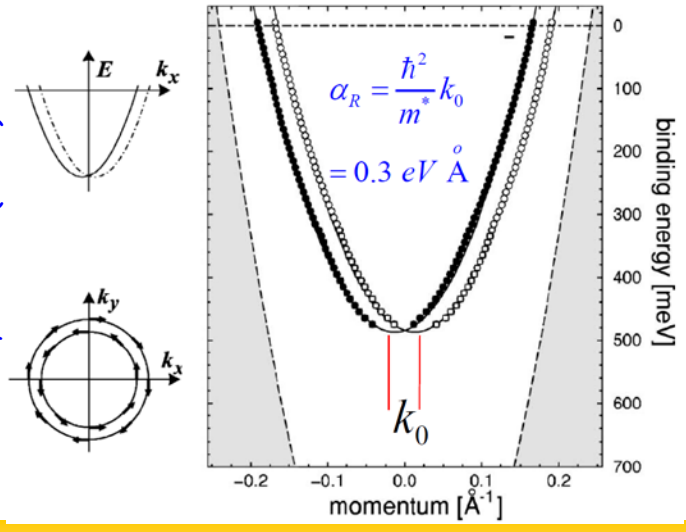
In 2009, two papers provided the first unambiguous examples of three-dimensional topological insulators — bulk insulators boasting metallic surface states with massless Dirac electrons. These now form just one of many classes of topological materials.

Joel E. Moore

An alternately compelling and frustrating fact about condensed-matter physics is that it takes place in actual materials. However beautiful a theoretical concept may be in the abstract, its ultimate appeal is limited until a material is found to realize it. Of course, condensed-matter physicists are not the only ones who live under the tyranny of the periodic table; nuclear physics and its interactions with society might have a much different history, for example, if either fewer or more isotopes could

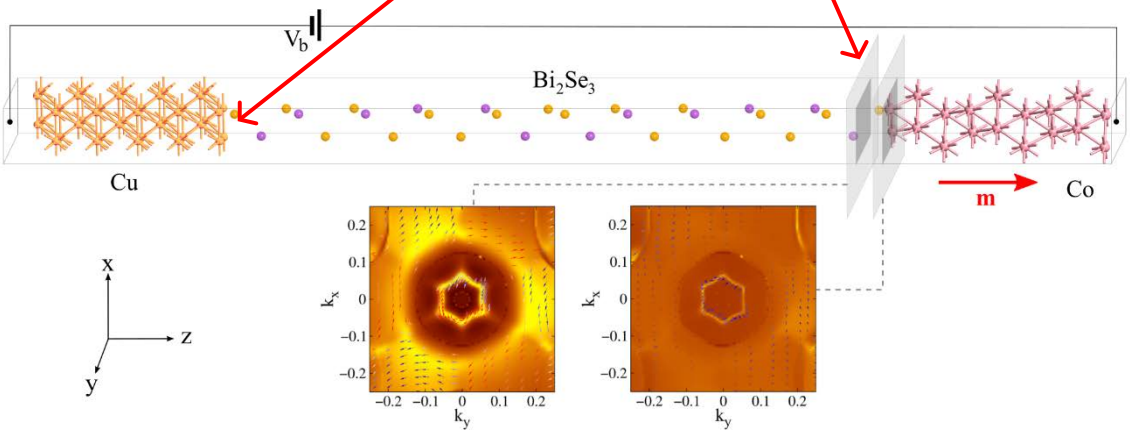


Au(111)



PRB 63, 115415 (2001)

What is the electronic and spin structure of states on both side of the interface and how they generate **nonequilibrium spin densities** upon spin-unpolarized current injection?



Crash Course on Spin-Orbit Coupling (SOC) in Vacuum

FORMALLY:

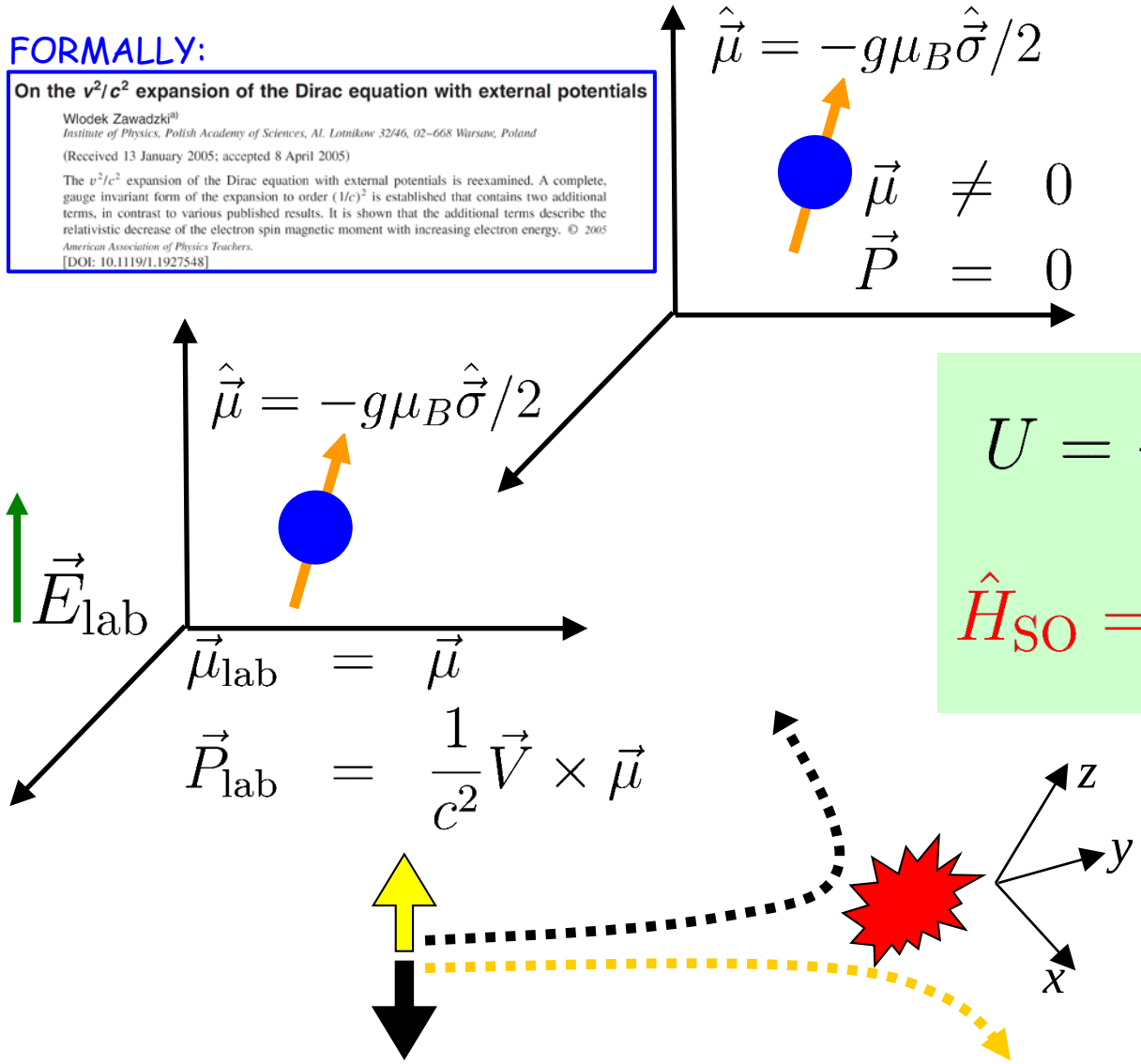
On the v^2/c^2 expansion of the Dirac equation with external potentials

Wlodek Zawadzki[a)]
Institute of Physics, Polish Academy of Sciences, Al. Lotnikow 32/46, 02–668 Warsaw, Poland

(Received 13 January 2005; accepted 8 April 2005)

The v^2/c^2 expansion of the Dirac equation with external potentials is reexamined. A complete, gauge invariant form of the expansion to order $(1/c)^2$ is established that contains two additional terms, in contrast to various published results. It is shown that the additional terms describe the relativistic decrease of the electron spin magnetic moment with increasing electron energy. © *2005 American Association of Physics Teachers.*

[DOI: 10.1119/1.1927548]



$$U = -\frac{1}{2}\vec{P}_{\rm lab} \cdot \vec{E}$$

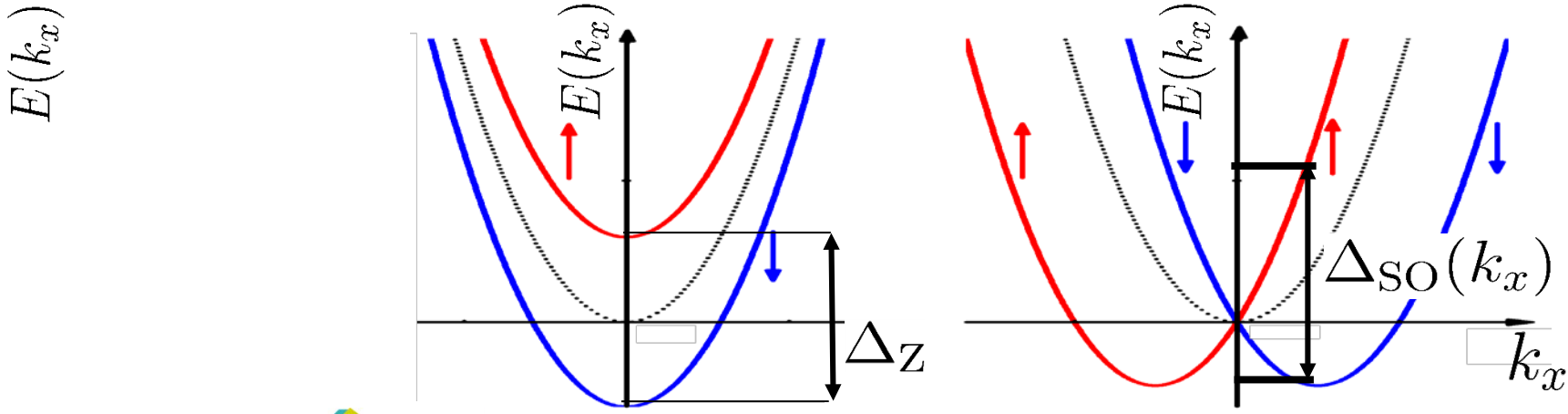
$$\hat{H}_{\rm SO} = \frac{e\hbar^2}{4m_0^2c^2}(\hat{\vec{\sigma}} \times \hat{\vec{p}}) \cdot \vec{E}$$

$$F_{\rm SO} = \pm P_{\rm lab} \nabla E_x$$

Crash Course on Rashba SOC in Solids

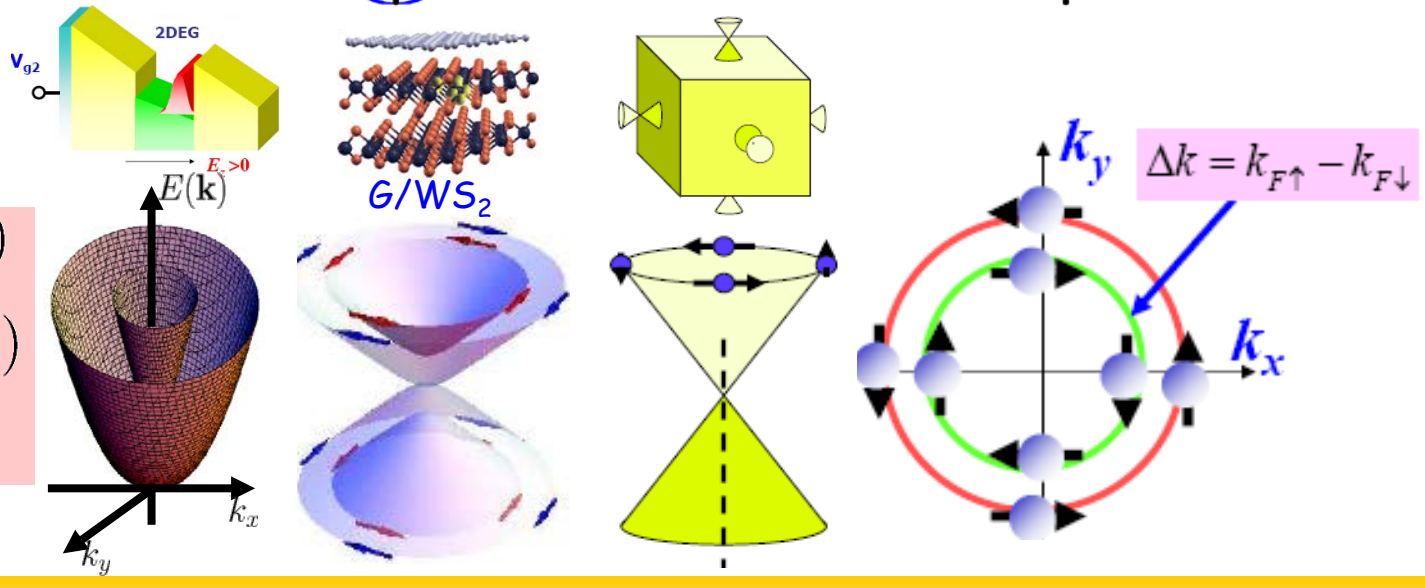
$$\hat{H}_{\mathrm{SO}}^{\mathrm{R}} = \frac{\alpha}{\hbar}(\hat{\boldsymbol{\sigma}} \times \hat{\mathbf{p}}) \cdot \mathbf{e}_z \equiv -\frac{g\mu_B}{2}\hat{\boldsymbol{\sigma}} \cdot \mathbf{B}_{\mathrm{R}}(\hat{\mathbf{p}})$$

1D:

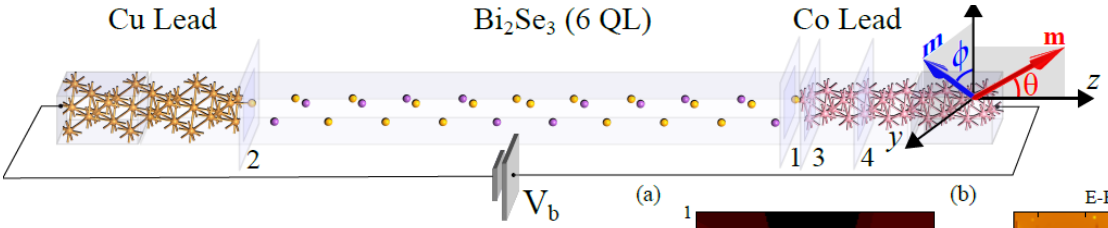


2D:

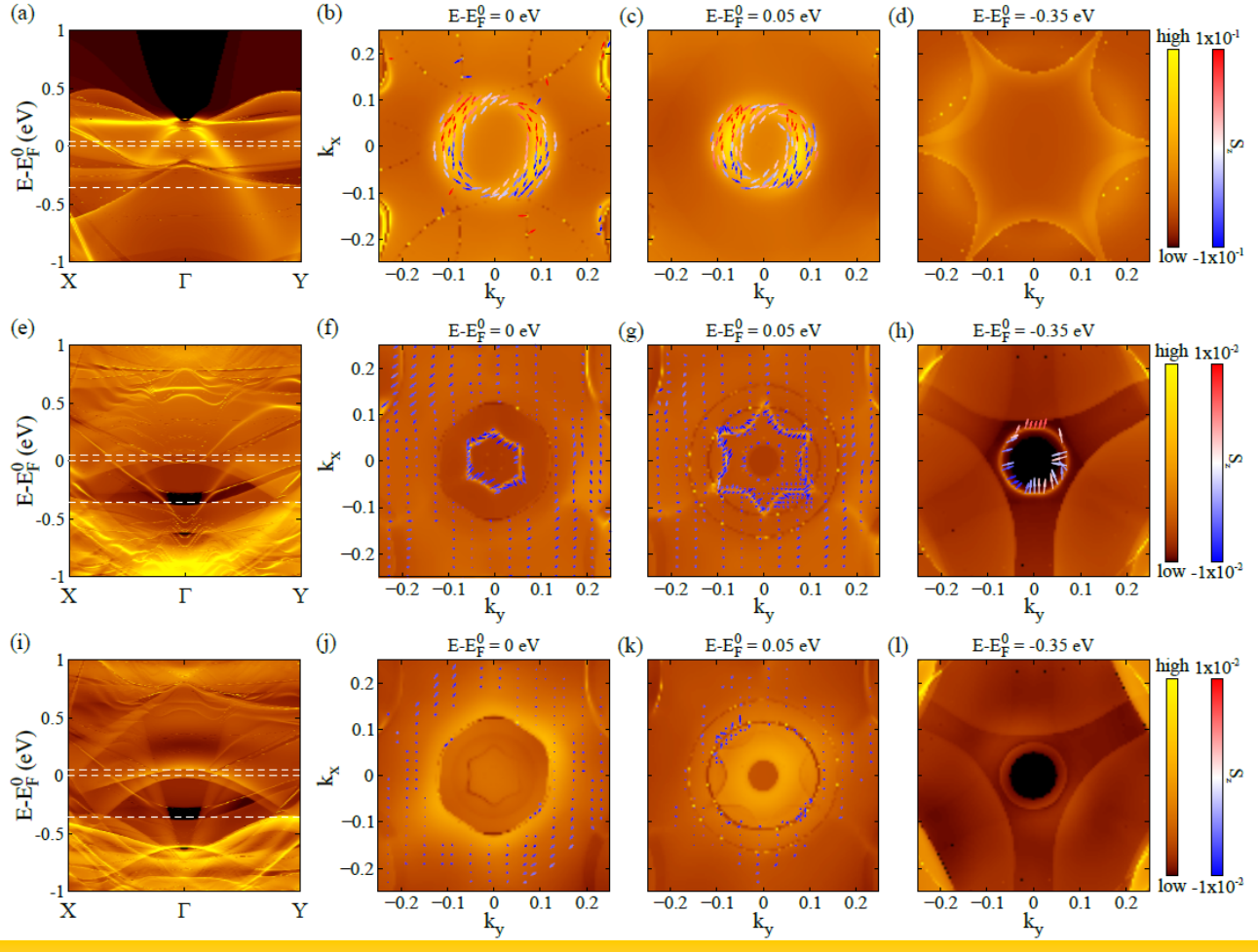
$$\varepsilon(\mathbf{k},\uparrow) = \varepsilon(-\mathbf{k},\downarrow)$$
$$\varepsilon(\mathbf{k},\uparrow) \neq \varepsilon(-\mathbf{k},\uparrow)$$
$$\varepsilon(\mathbf{k},\uparrow) \neq \varepsilon(\mathbf{k},\downarrow)$$



Spin-Orbit-Proximitized Ferromagnet: Co/Topological-Insulator-Bi_2Se_3



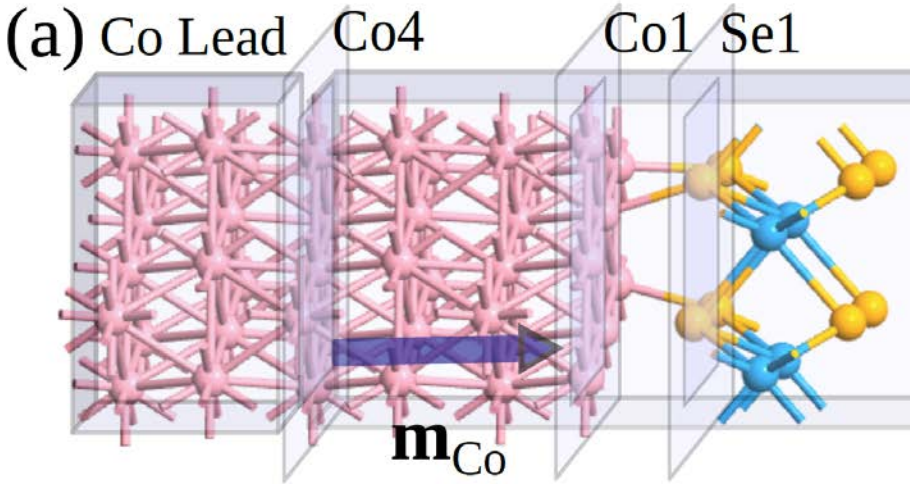
$$A(E;k_x,k_y,z) = -\frac{1}{\pi}\mathrm{Im}\left[G_{\mathbf{k}_{||}}(E;z,z)\right]$$

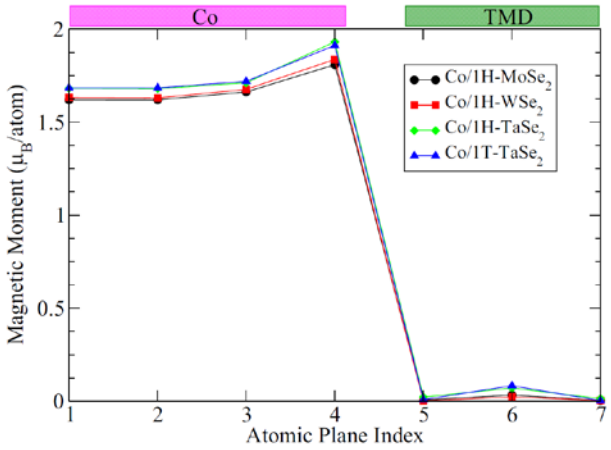


Nano Lett. **17**, 5626 (2017)

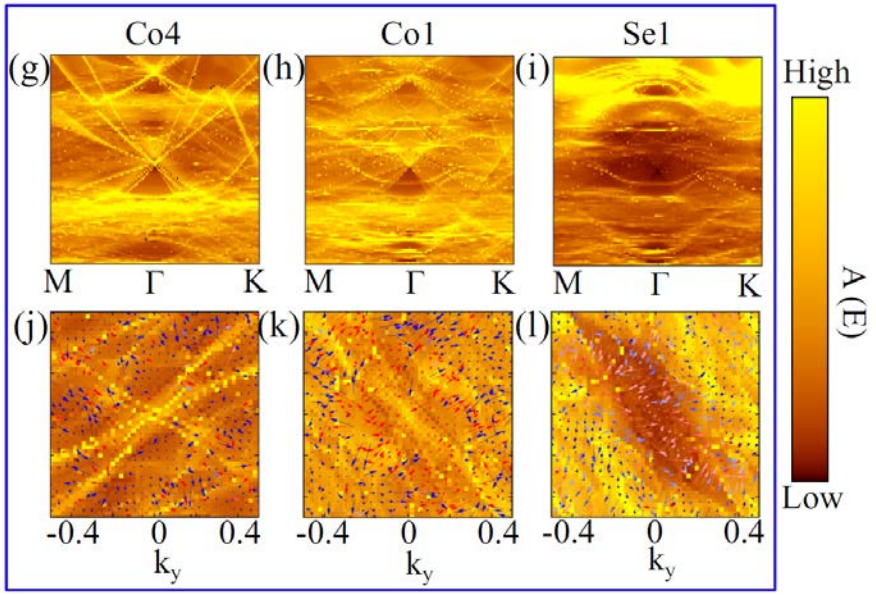
Spin-Orbit-Proximitized Ferromagnet: Co/Monolayer-Transition-Metal-Dichalcogenide

PRMater. **4**, 104007 (2020)

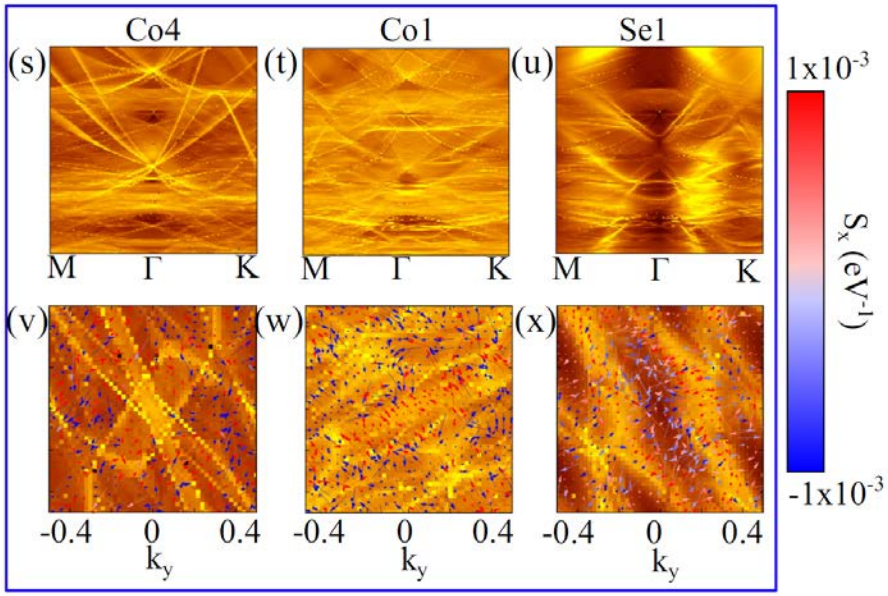




Co/WSe_2

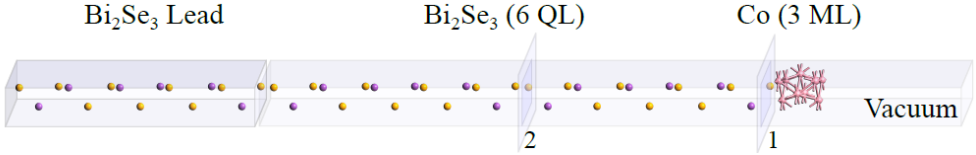


$Co/TaSe_2$

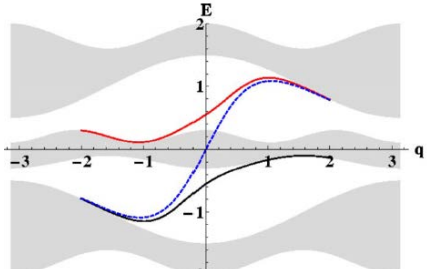


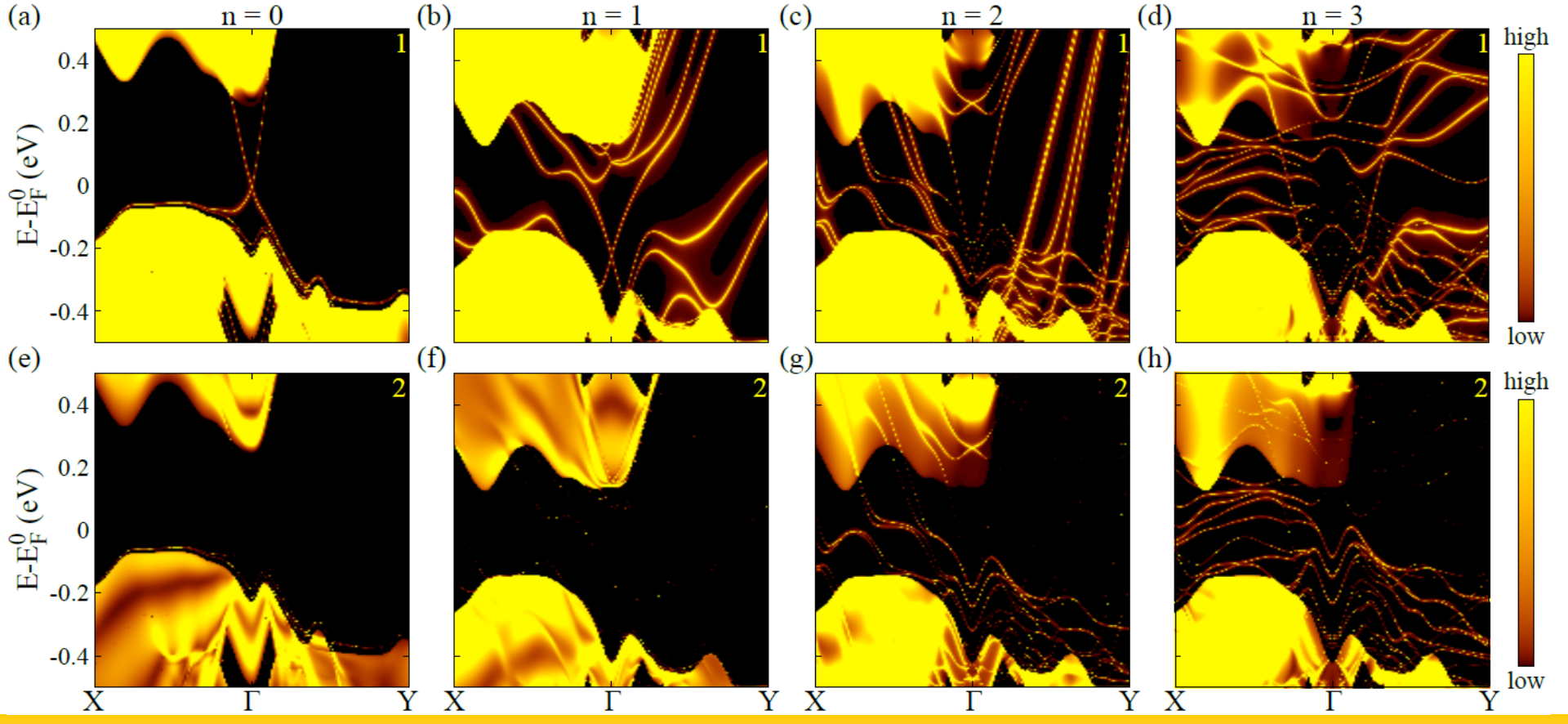
Spectral Function and Spin Textures on the TI Side of Co/TI Interface

Nano Lett. **17**, 5626 (2017)



PRB **82**, 195417 (2010)
PRB **96**, 235433 (2017)





Spin-Transfer and Spin-Orbit Torques from Nonequilibrium Green Functions (NEGF)

❑Fundamental quantities of NEGF formalism:

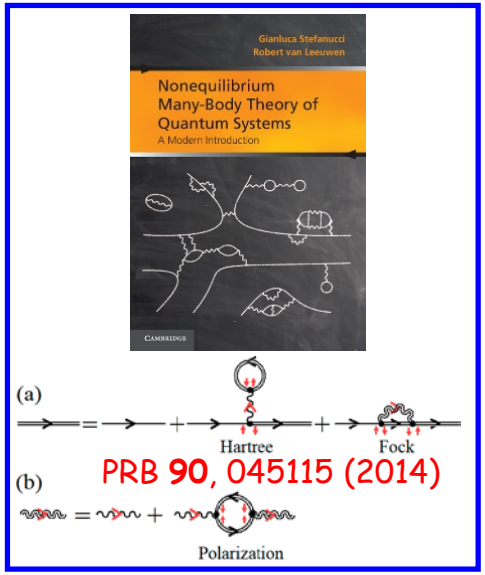
density of available quantum states:

$$G^r_{\sigma\sigma'}(t,t') = -\frac{i}{\hbar}\Theta(t-t')\langle\{\hat{c}_{\mathbf{r}\sigma}(t), \hat{c}^\dagger_{\mathbf{r}'\sigma'}(t')\}\rangle$$

how are those states occupied:

$$G^<_{\sigma\sigma'}(t,t') = \frac{i}{\hbar}\langle\hat{c}^\dagger_{\mathbf{r}'\sigma'}(t')\hat{c}_{\mathbf{r}\sigma}(t)\rangle$$

Learn more about NEGF from:



PRB **90**, 045115 (2014)

❑NEGFs for steady-state transport:

$$G^r(t,t') \to G^r(t-t') \xrightarrow{\text{FT}} G^r(E) \qquad G^<(t,t') \to G^<(t-t') \xrightarrow{\text{FT}} G^<(E)$$

$$\hat{\rho}_{\text{eq}} = \sum_n f(E_n)|E_n\rangle\langle E_n| = -\frac{1}{\pi}\int_{-\infty}^{+\infty} dE\, \text{Im}\, G^r(E) f(E)$$

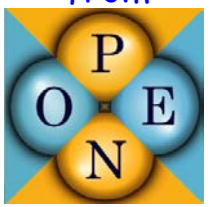
$$\hat{\rho}_{\text{neq}} = \frac{1}{2\pi i}\int_{-\infty}^{+\infty} dE\, G^<(E)$$

❑NEGF-based expression for spin-transfer torque:

$$\begin{aligned}
\hat{H}_{\text{ncDFT}} &= -\frac{\hbar^2\nabla^2}{2m} + V_{\text{Hartree}}(\mathbf{r}) + V_{\text{XC}}(\mathbf{r}) + V_{\text{ext}}(\mathbf{r}) - \hat{\boldsymbol{\sigma}}\cdot\mathbf{B}_{\text{XC}} \to \hat{\mathbf{T}} = \frac{d\hat{\mathbf{s}}}{dt} = \frac{1}{2i}\left[\hat{\boldsymbol{\sigma}}, \hat{H}_{\text{ncDFT}}\right] \\
\mathbf{T}_{\text{CD}} &= \text{Tr}[(\hat{\rho}_{\text{neq}} - \hat{\rho}_{\text{eq}})\hat{\mathbf{T}}_{\text{CD}}] \Leftrightarrow \mathbf{T}_{\text{CD}} = \int d^3r\, \mathbf{s}_{\text{CD}}(\mathbf{r}) \times \mathbf{B}_{\text{XC}}(\mathbf{r}) \\
\mathbf{s}_{\text{CD}}(\mathbf{r}) &= \text{Tr}_{\text{spin}}[(\hat{\rho}_{\text{neq}} - \hat{\rho}_{\text{eq}})\hat{\boldsymbol{\sigma}}]
\end{aligned}$$

most general torque formula valid in the presence of SOC and other spin-nonconserving processes

LCAO-ncDFT from:



SYNOPSYS | QuantumATK

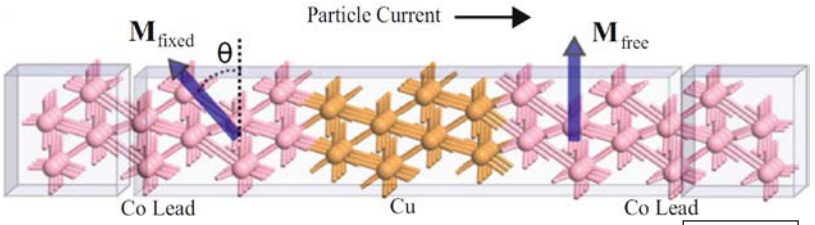
arXiv:1801.05793
PRMater. **3**, 011401 (2019)

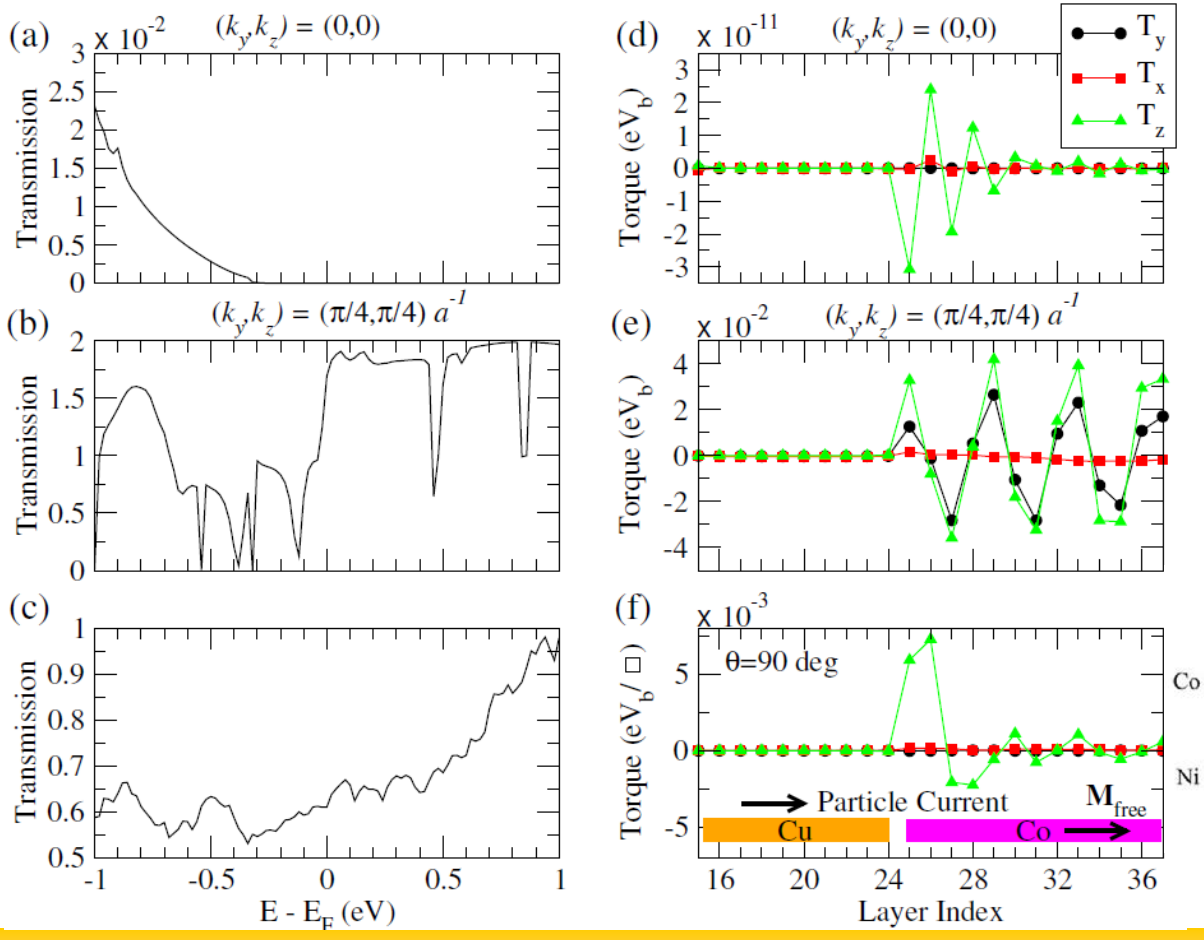
EXAMPLE: First-Principles Quantum Transport Theory of Conventional STT

arXiv:1801.05793

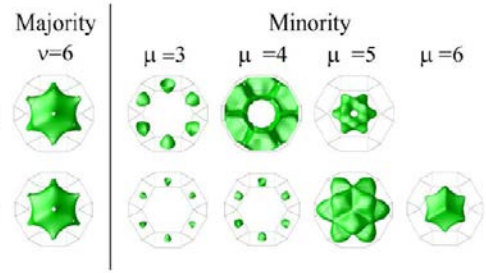
First-Principles Quantum Transport Modeling of Spin-Transfer and Spin-Orbit Torques in Magnetic Multilayers

Branislav K. Nikolić, Kapildeb Dolui, Marko D. Petrović, Petr Plecháč, Troels Markussen, and Kurt Stokbro



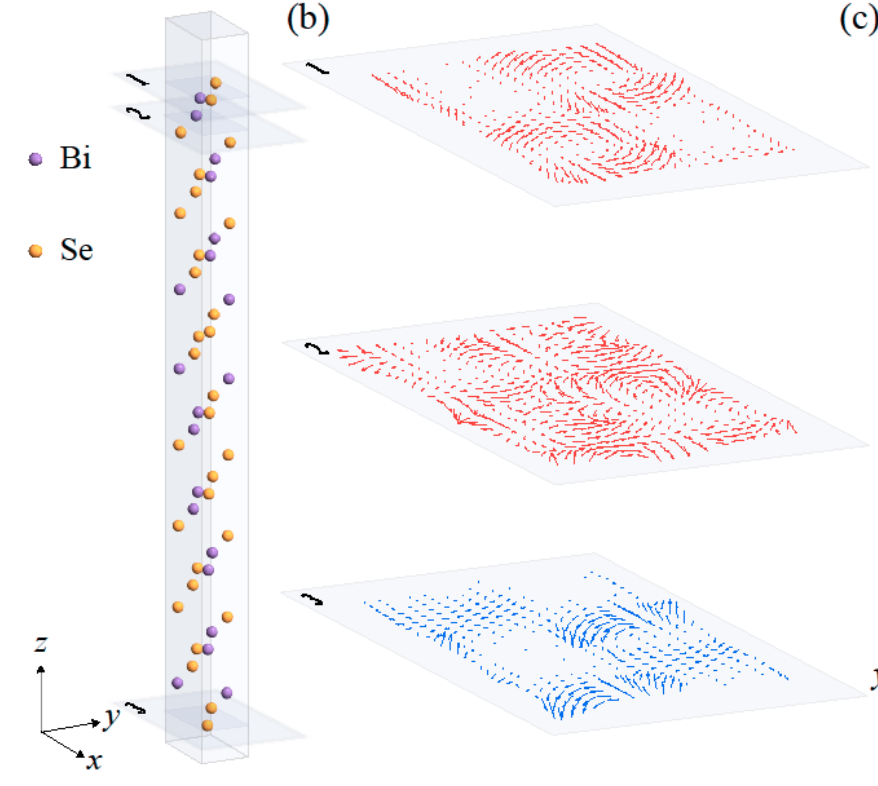


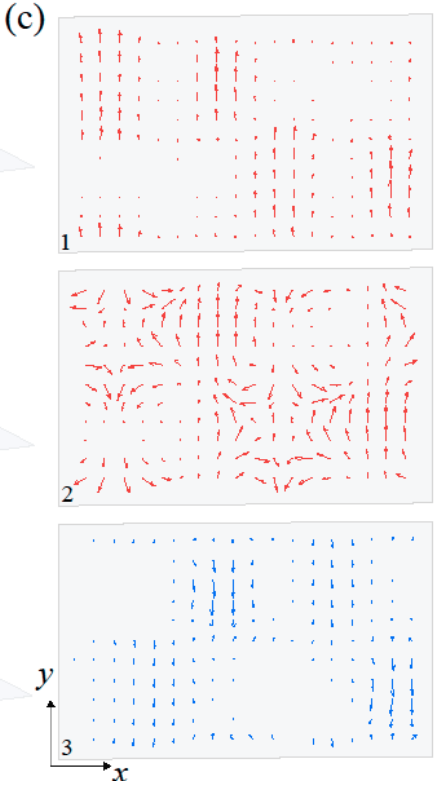
PRB **77**, 184430 (2008)

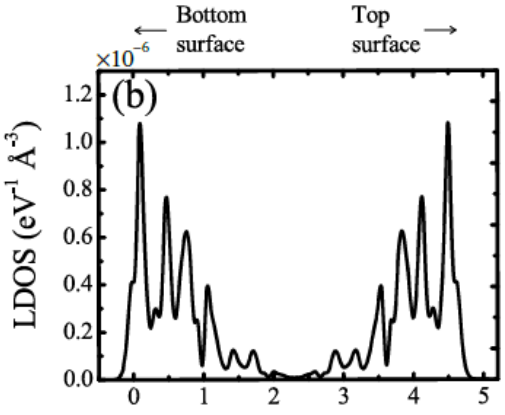


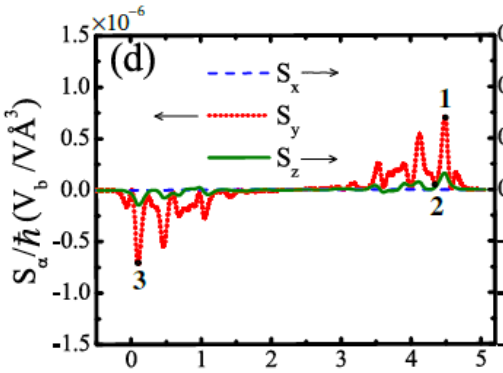
EXAMPLE: Current-Driven Nonequilibrium Spin Textures around the Surface of Bi_2Se_3

PRB **92**, 201406(R) (2015)



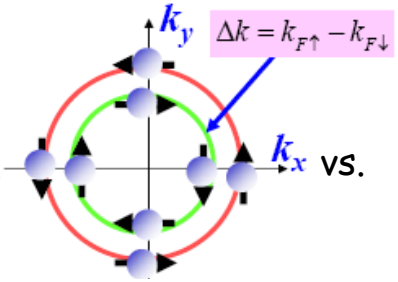




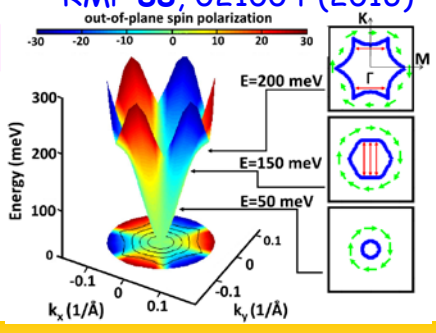


$$\frac{S_y^{\text{Rashba}}}{n} = \frac{e\tau E_x}{p_F}\frac{\alpha}{\hbar v_F} \quad \text{vs.} \quad \frac{S_y^{\text{TI}}}{n} = \frac{e\tau E_x}{p_F}$$

due to spin-momentum locking

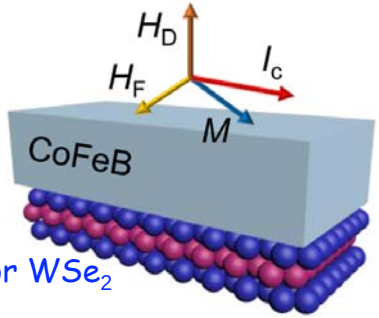


RMP **88**, 021004 (2016)



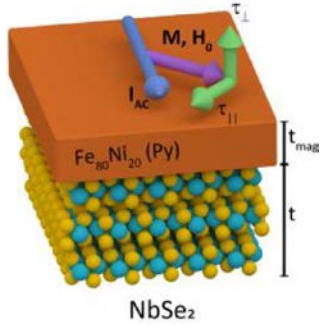
Computational Screening for Optimal SOT in Co/TMD Heterostructures

Nano Lett. **16**, 7514 (2018)



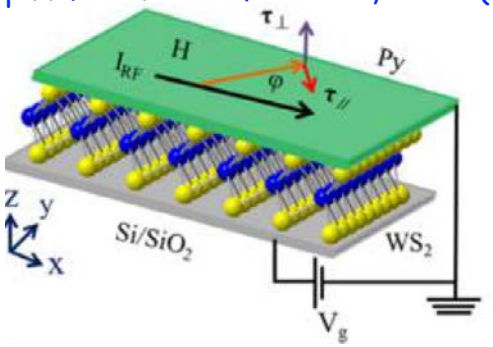
MoS_2 or WSe_2

Nano Lett. **18**, 1311 (2018)

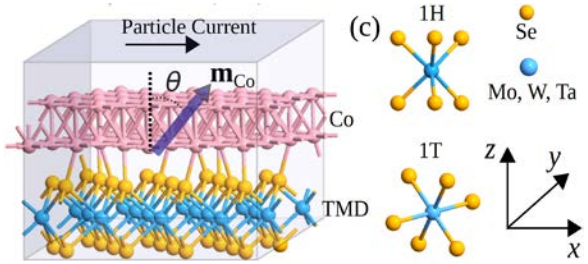


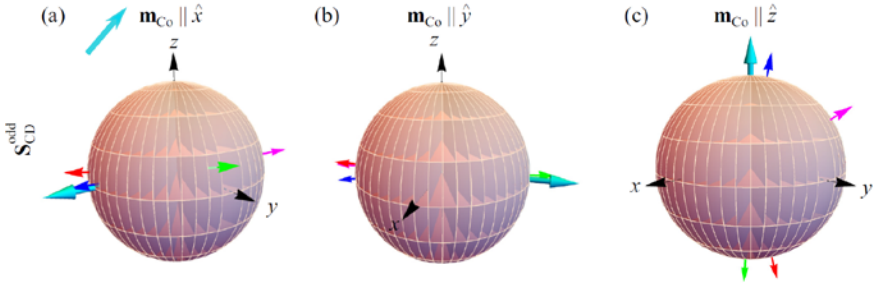
$NbSe_2$

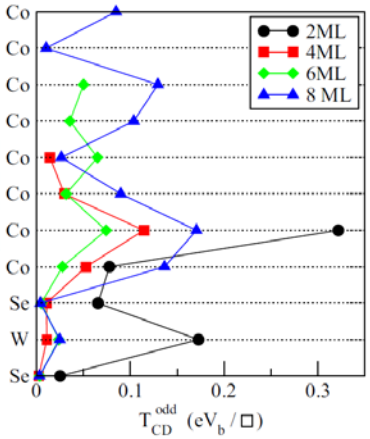
ACS Appl. Mater. Interfaces **10**, 2843 (2018)



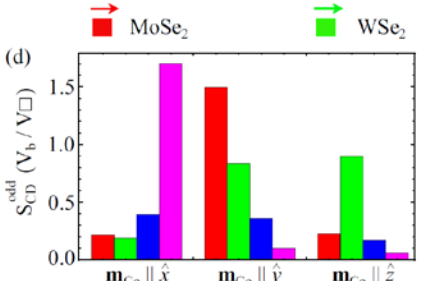
PRMater. **4**, 104007 (2020)







$$\mathbf{T}_{CD}^{odd} = (\mathbf{p} \times \mathbf{m}_{Co}) \left[\sum_{n=0}^{\infty} T_{n\alpha} |\hat{z} \times \mathbf{m}_{Co}|^{2n} \right] + \mathbf{m}_{Co} \times (\hat{z} \times \mathbf{m}_{Co})(\mathbf{m}_{Co} \cdot \hat{x}) \left[\sum_{n=0}^{\infty} T_{n\beta} |\hat{z} \times \mathbf{m}_{Co}|^{2n} \right]$$



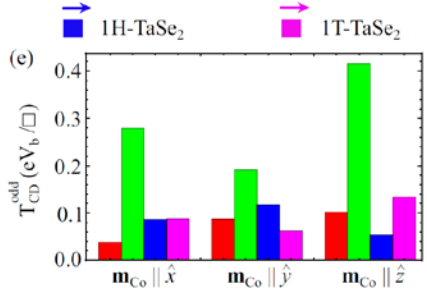
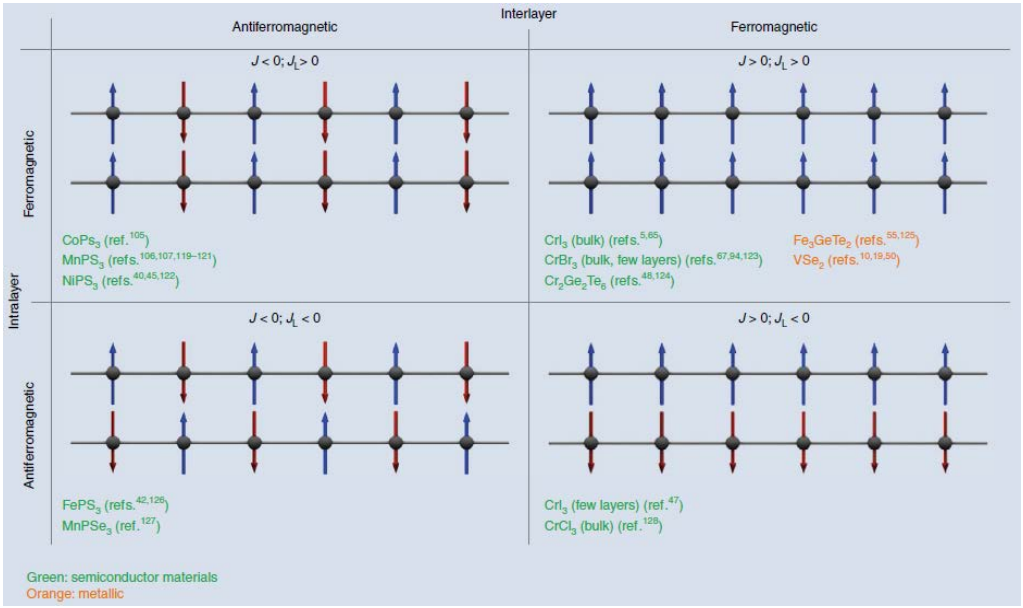


TABLE I. Fitted coefficients (in the units of $eV_b/\square$) in the angular dependence [Eq. (13)] of the odd component of SO torque for 2ML-Co/monolayer-1H-WSe_2 heterostructure. The SO coupling of WSe_2 is either switched on ($\zeta_{WSe_2} \neq 0$) or off ($\zeta_{WSe_2} = 0$) in ncDFT calculations. The unit vector $\mathbf{p}$ in Eq. (13) is given in the second column for which $\mathbf{m}_{Co} || \mathbf{p}$ leads to $\mathbf{T}_{CD}^{odd} = 0$.

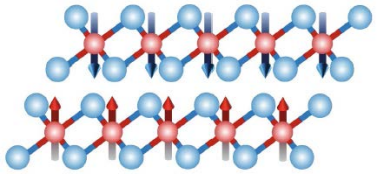
	$\mathbf{p} = (\theta, \phi)$	$T_{0\alpha}$	$T_{1\alpha}$	$T_{2\alpha}$	$T_{3\alpha}$	$T_{0\beta}$	$T_{1\beta}$
$\zeta_{WSe_2} \neq 0$	(75°, 60°)	0.416	−0.254	0.192	0.001	−0.092	0.105
$\zeta_{WSe_2} = 0$	(105°, 120°)	0.079	−0.038	0.063	−0.001	0.067	−0.014

What Can Two-Dimensional (2D) Magnetic Materials do for Spintronics?

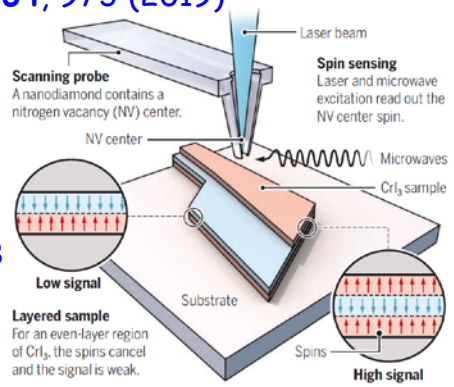
Nat. Nanotech. **14**, 408 (2019)

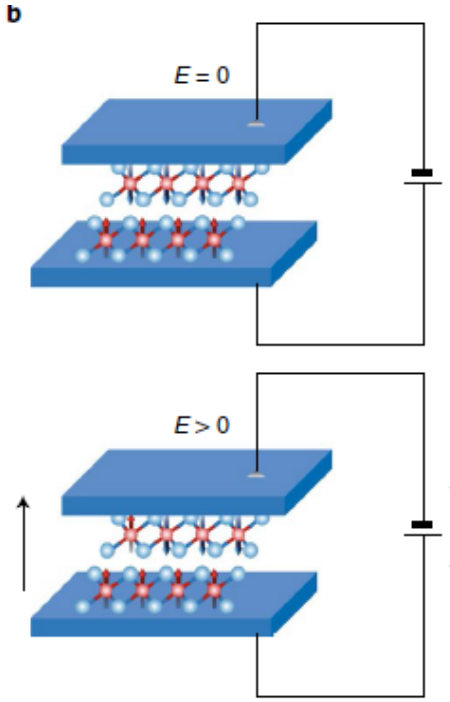


Science **364**, 973 (2019)

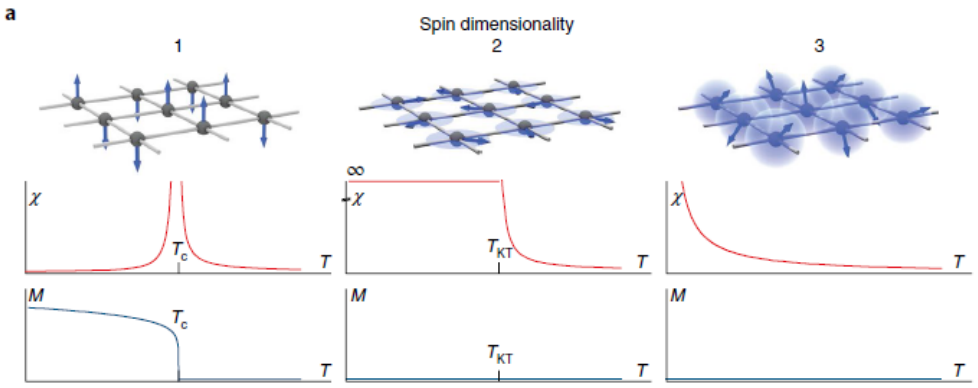


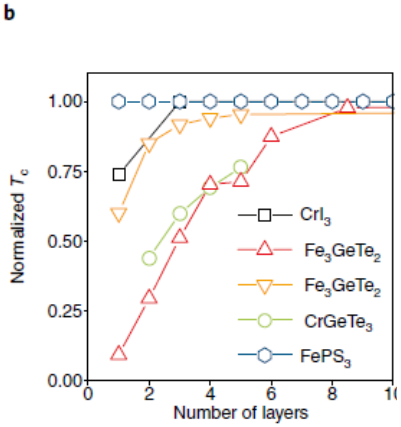
CrI_3





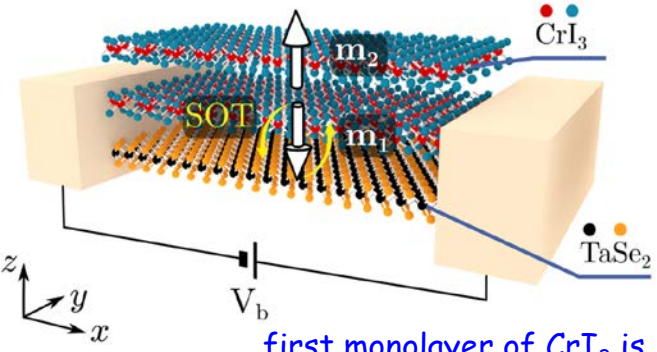
Nat. Mater. **14**, 406 (2018)

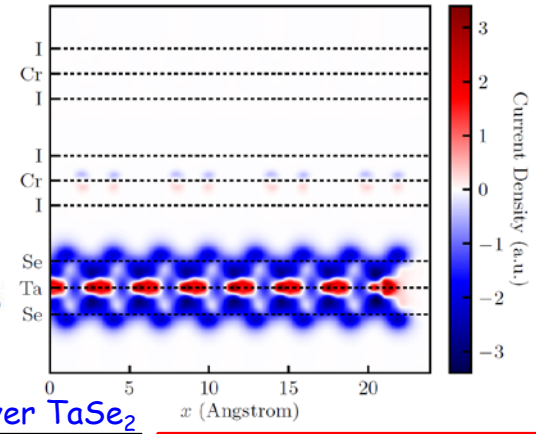




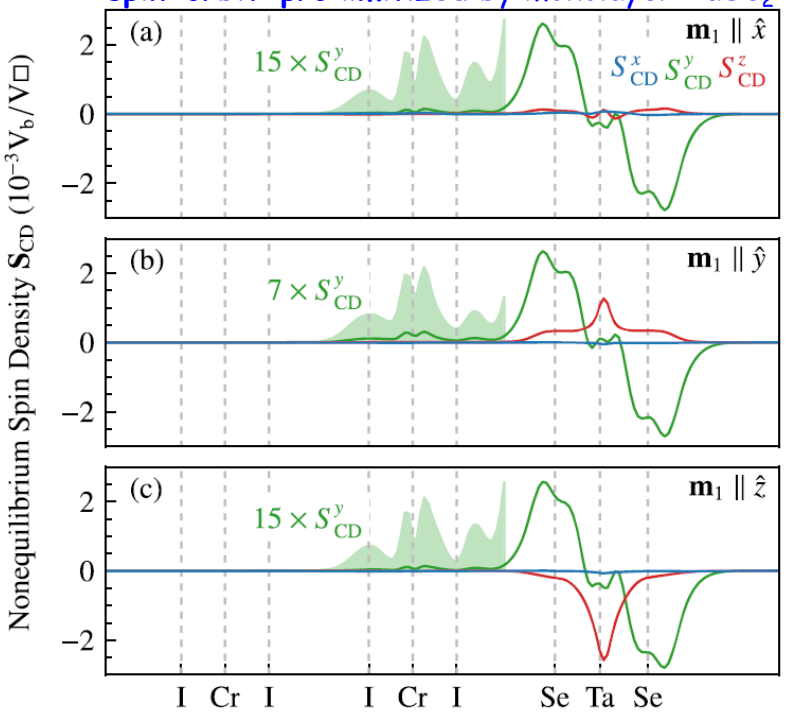
SOT in bilayer-CrI_3/monolayer-$TaSe_2$ vdW Heterostructures

Nano Lett. **20**, 2288 (2020)

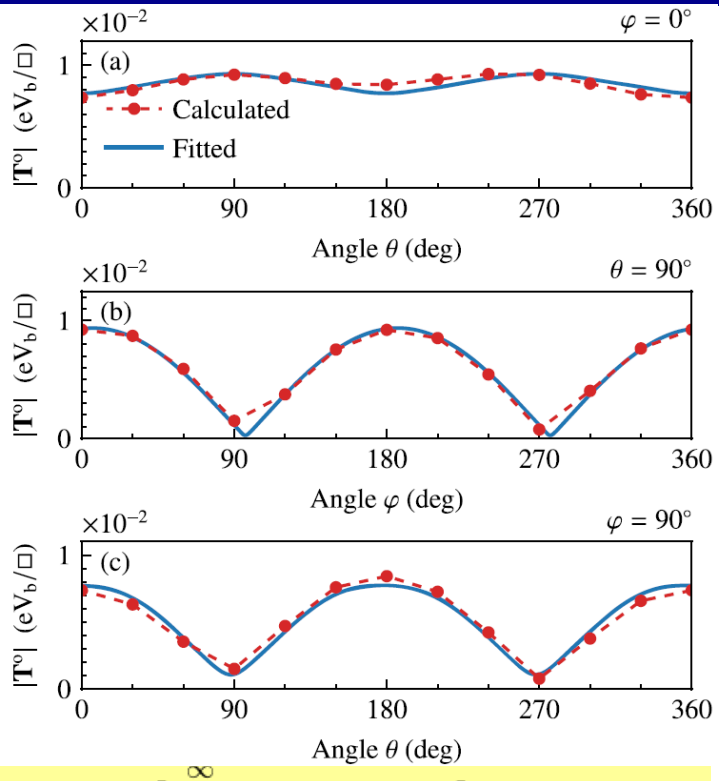




first monolayer of CrI_3 is **spin-orbit-proximitized** by monolayer $TaSe_2$



SOT occurs around interfaces, so the bulk of spin-orbit-materials is of little use and could be detrimental to the energy efficiency

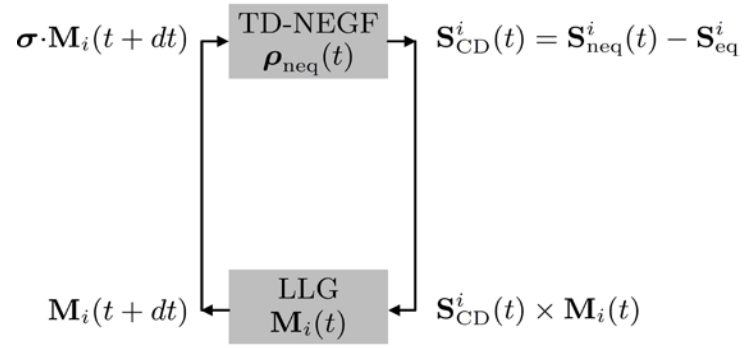


$$\mathbf{T}^o = (\mathbf{p} \times \mathbf{m}_1)\left[\sum_{n=0}^{\infty} \tau^o_{n\alpha} |\hat{z} \times \mathbf{m}_1|^{2n}\right] + \mathbf{m}_1 \times (\hat{z} \times \mathbf{m}_1)(\mathbf{m}_1 \cdot \hat{x})\left[\sum_{n=0}^{\infty} \tau^o_{n\beta} |\hat{z} \times \mathbf{m}_1|^{2n}\right]$$

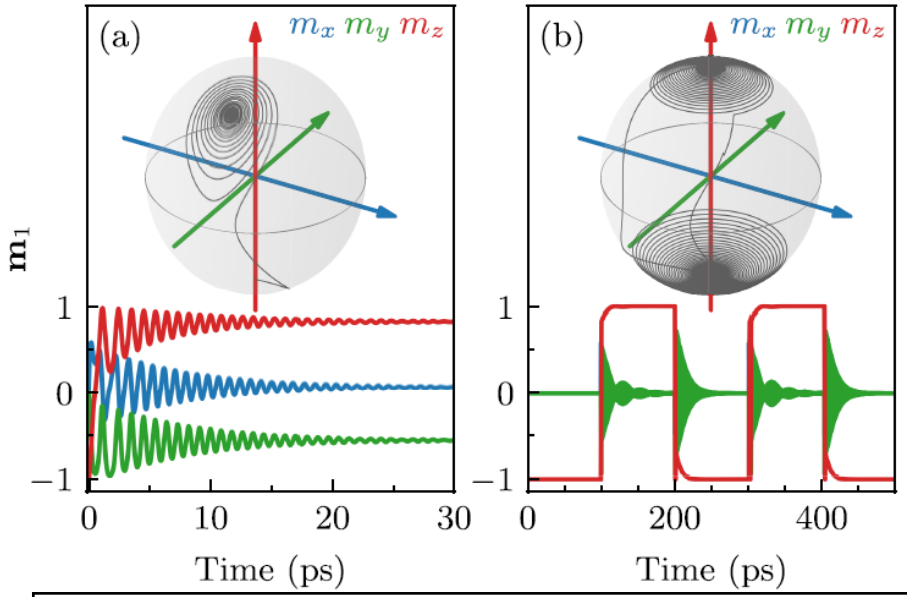
$\mathbf{p}(\theta, \phi)$	$\tau^o_{0\alpha}$	$\tau^o_{1\alpha}$	$\tau^o_{2\alpha}$	$\tau^o_{3\alpha}$	$\tau^o_{0\beta}$	$\tau^o_{1\beta}$
(88°, 98°)	77.22	17.32	-30.32	13.54	-9.19	-6.88

SOT-Driven AFM-FM Nonequilibrium Phase Transition in bilayer-CrI_3/monolayer-$TaSe_2$

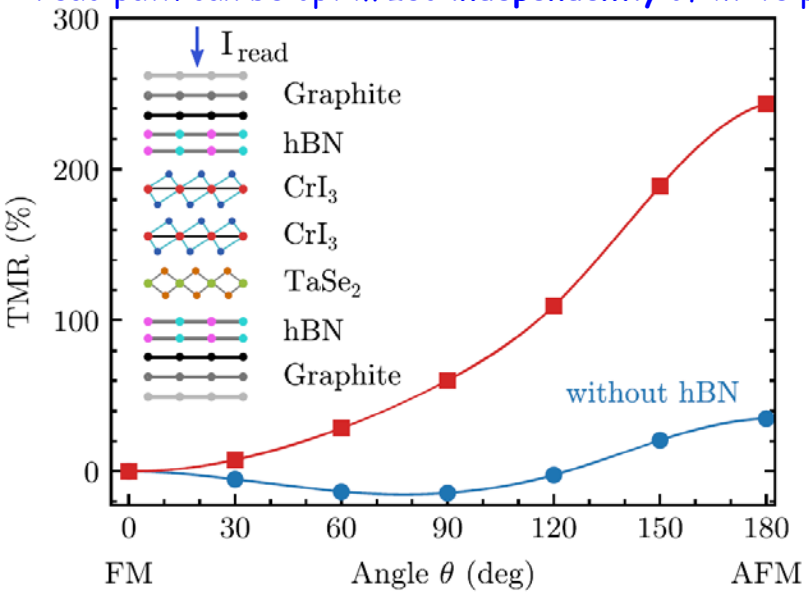
PRAppl. **10**, 054038 (2018)



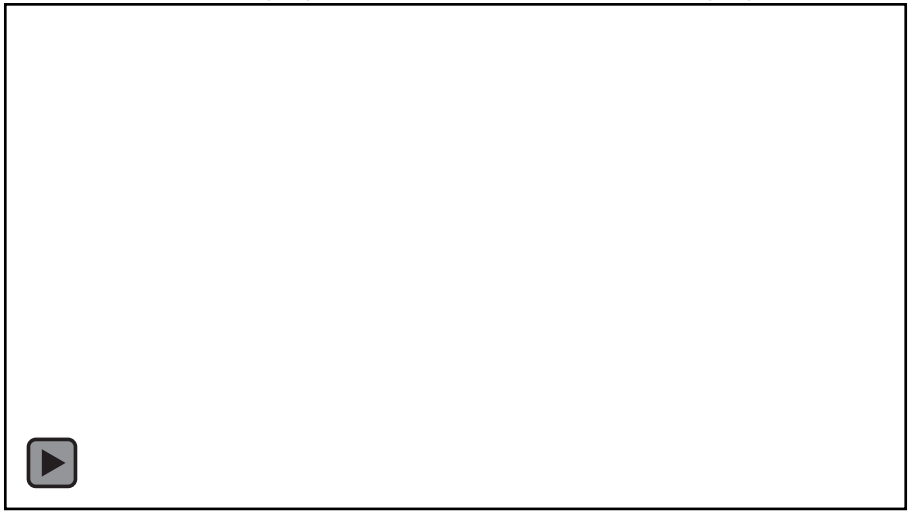
$$\frac{d\mathbf{m}_1}{dt}=-\gamma\mathbf{m}_1\times\mathbf{B}_1^{\rm eff}+\lambda\mathbf{m}_1\times\frac{d\mathbf{m}_1}{dt}+\frac{\gamma}{\mu_M}\mathbf{T}^{\rm o}$$



read path can be optimized **independently** of write path

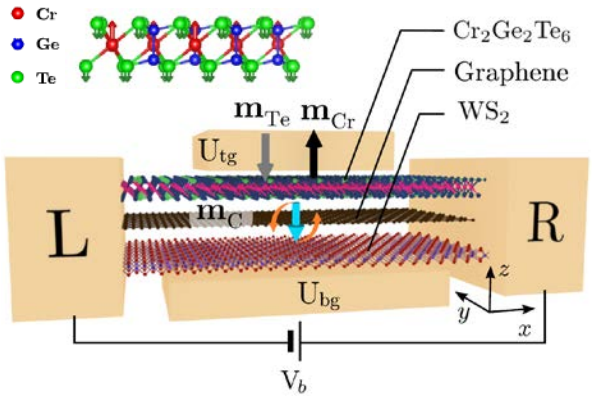


Nano Lett. **20**, 2288 (2020)

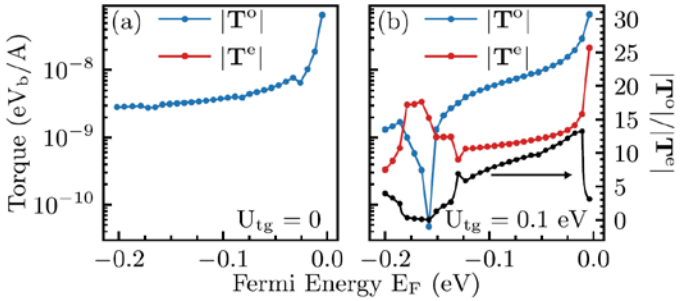


Scattering-Induced, Purely Interfacial and Gate-Tunable DL SOT in Doubly Proximitized Graphene

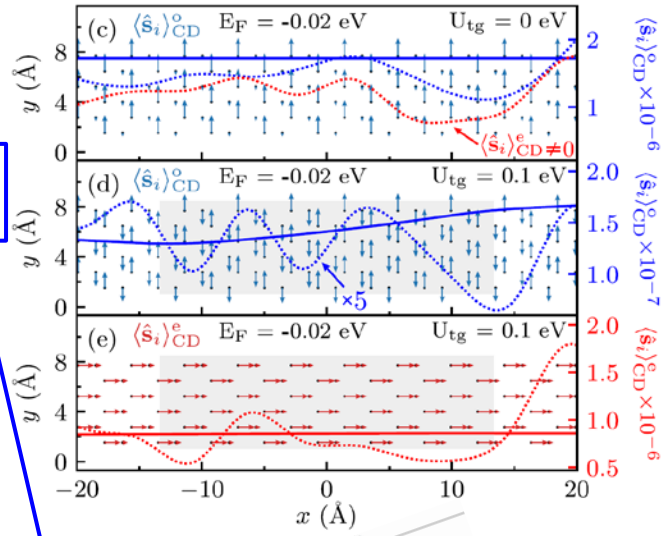
PRRes. **2**, 043057 (2020)

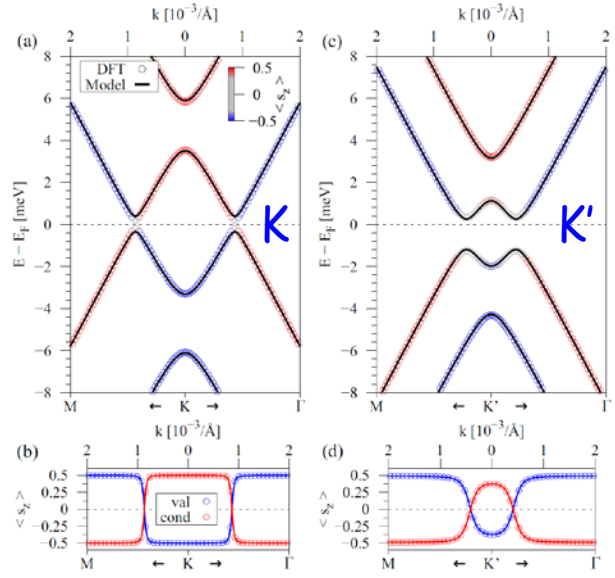


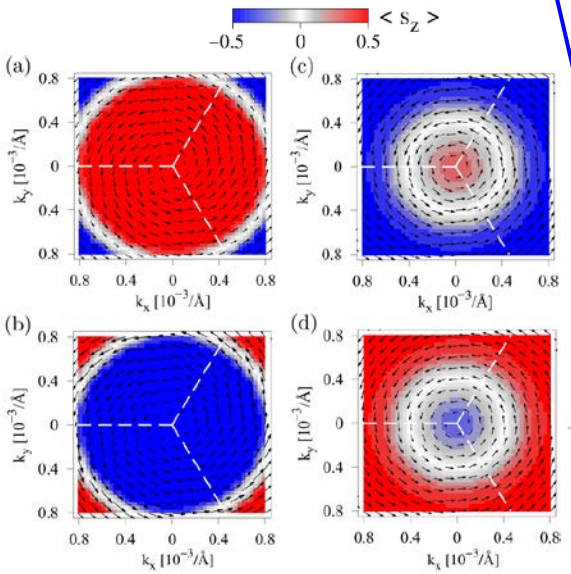
$$
\begin{aligned}
\hat{H} &= \hat{H}_0 + \hat{H}_\Delta + \hat{H}_{\rm I} + \hat{H}_{\rm R} + \hat{H}_{\rm ex} + \hat{H}_\xi, \\
\hat{H}_0 &= \hbar v_{\rm F}(\tau k_x \hat{\sigma}_x - k_y \hat{\sigma}_y) \otimes \hat{s}_0, \\
\hat{H}_\Delta &= \Delta \hat{\sigma}_z \otimes \hat{s}_0, \\
\hat{H}_{\rm I} &= \tau(\lambda_{\rm I}^{\rm A}\hat{\sigma}_+ + \lambda_{\rm I}^{\rm B}\hat{\sigma}_-) \otimes \hat{s}_z, \\
\hat{H}_{\rm R} &= -\lambda_{\rm R}(\tau\hat{\sigma}_x \otimes \hat{s}_y + \hat{\sigma}_y \otimes \hat{s}_x), \\
\hat{H}_{\rm ex} &= (-\lambda_{\rm ex}^{\rm A}\hat{\sigma}_+ + \lambda_{\rm ex}^{\rm B}\hat{\sigma}_-) \otimes \hat{s}_z, \\
\hat{H}_\xi &= \tau\xi\hat{\sigma}_0 \otimes \hat{s}_0.
\end{aligned}
$$



the out-of-plane component of the spin texture can be triggered by an exchange field, spin-valley locking, or competition between Rashba and orbital effects

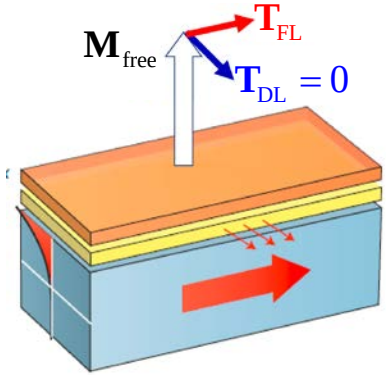






Resolving Key Unsettled Issue for SOT->**Role of Interfacial Mechanisms**->with vdW Heterostructures

INTERFACE: Edelstein (or inverse spin galvanic) effect for FL SOT



Solid State Communications, Vol. 73, No. 3, pp. 233–235, 1990. Printed in Great Britain. 0038–1098/90 $3.00 + .00 Pergamon Press plc

SPIN POLARIZATION OF CONDUCTION ELECTRONS INDUCED BY ELECTRIC CURRENT IN TWO-DIMENSIONAL ASYMMETRIC ELECTRON SYSTEMS

V.M. Edelstein

USSR Academy of Sciences, Institute of Solid State Physics, Chernogolovka 142432, USSR

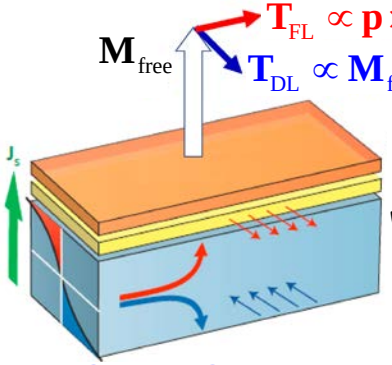
$$S_y = \beta E_x$$

PHYSICAL REVIEW B **78**, 212405 (2008)

Theory of nonequilibrium intrinsic spin torque in a single nanomagnet

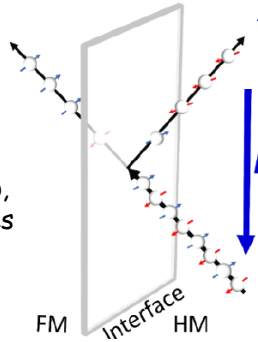
A. Manchon and S. Zhang

BULK: Spin Hall effect for DL SOT



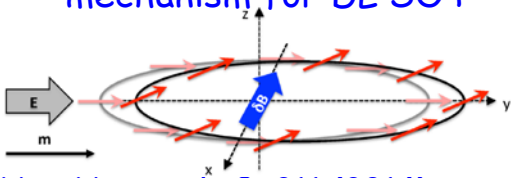
DL SOT directs the magnetization toward **p**, whereas FL SOT induces magnetization precessions around **p**

INTERFACE: Spin-orbit filtering for DL SOT



PRL **121**, 136805 (2018)

INTERFACE: Berry curvature mechanism for DL SOT

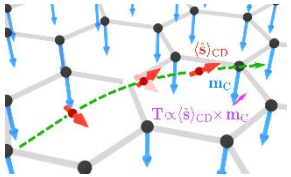


Nat. Nanotech. **9**, 211 (2014)

PRL **121**, 017202 (2018)

in $CuO_x/Ni_{81}Fe_{19}$ efficiency is 2–3 orders of magnitude smaller than that from the bulk SHE of Pt

INTERFACE: Skew-scattering off nonmagnetic impurities in the presence of noncoplanar spin texture for DL SOT



PRRes. **2**, 043057 (2020)

PRRes. **2**, 043401 (2020)

in standard FM/HM bilayers interfacial SOC is often detrimental for SOT

PHYSICAL REVIEW LETTERS **122**, 077201 (2019)

Spin-Orbit Torques in Heavy-Metal–Ferromagnet Bilayers with Varying Strengths of Interfacial Spin-Orbit Coupling

Lijun Zhu,[1,*] D. C. Ralph,[1,2] and R. A. Buhrman[1]

PHYSICAL REVIEW APPLIED **15**, L031001 (2021)

Absence of Significant Spin-Current Generation in Ti/Fe-Co-B Bilayers with Strong Interfacial Spin-Orbit Coupling

Lijun Zhu[1,2,*] and Robert A. Buhrman[1]

arXiv:2007.09817

Interfacial Dzyaloshinskii-Moriya interaction and spin-orbit torque in $Au_{1-x}Pt_x$/Co bilayers with varying interfacial spin-orbit coupling

Lijun Zhu[1], Xin Ma[2], Xiaoqin Li[2], Robert A. Buhrman[1]

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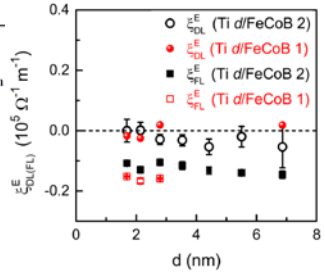
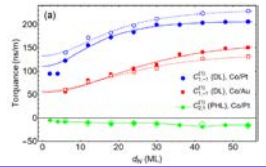


PHYSICAL REVIEW B **101**, 020407(R) (2020)

Interfacial contributions to spin-orbit torque and magnetoresistance in ferromagnet/heavy-metal bilayers

K. D. Belashchenko,[1] Alexey A. Kovalev,[1] and M. van Schilfgaarde[2]



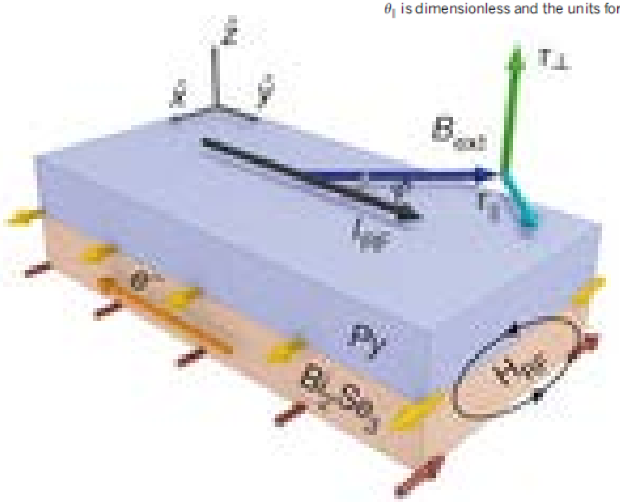
Resolving Trouble with Simplistic Hamiltonians and Intuitive Picture of How Current Flows to Drive SOT

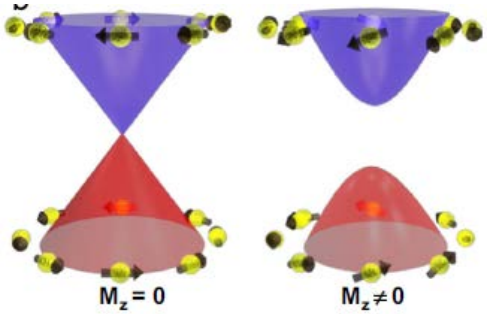
Nature **511**, 449 (2014)

Table 1 | Comparison of room-temperature $\sigma_{s,\parallel}$ and $\theta_{s,\parallel}$ for Bi_2Se_3 with other materials

Parameter	Bi_2Se_3 (this work)	Pt (ref. 4)	β-Ta (ref. 6)	Cu(Bi) (ref. 23)	β-W (ref. 24)
$\theta_\parallel$	2.0–3.5	0.08	0.15	0.24	0.3
$\sigma_{S,\parallel}$	1.1–2.0	3.4	0.8	—	1.8

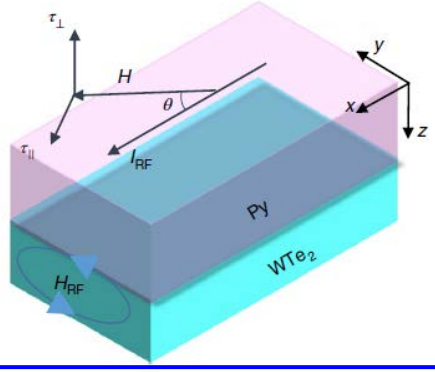
$\theta_\parallel$ is dimensionless and the units for $\sigma_{S,\parallel}$ are $10^5\hbar/2e\ \Omega^{-1}\,m^{-1}$.





"Our findings have potential importance for technology, in that the spin torque ratio for Bi_2Se_3 at room temperature is larger than that for any previously measured spin current source material. However, as noted above, for practical applications the specific layer structure of our devices (topological insulator/metallic magnet) does not make good use of this high intrinsic efficiency because most of the applied current is shunted through the metallic magnet and does not contribute to spin current generation within the topological insulator. Applications will probably require coupling topological insulators to insulating (or high-resistivity) magnets so that the majority of the current will flow in the topological insulator."

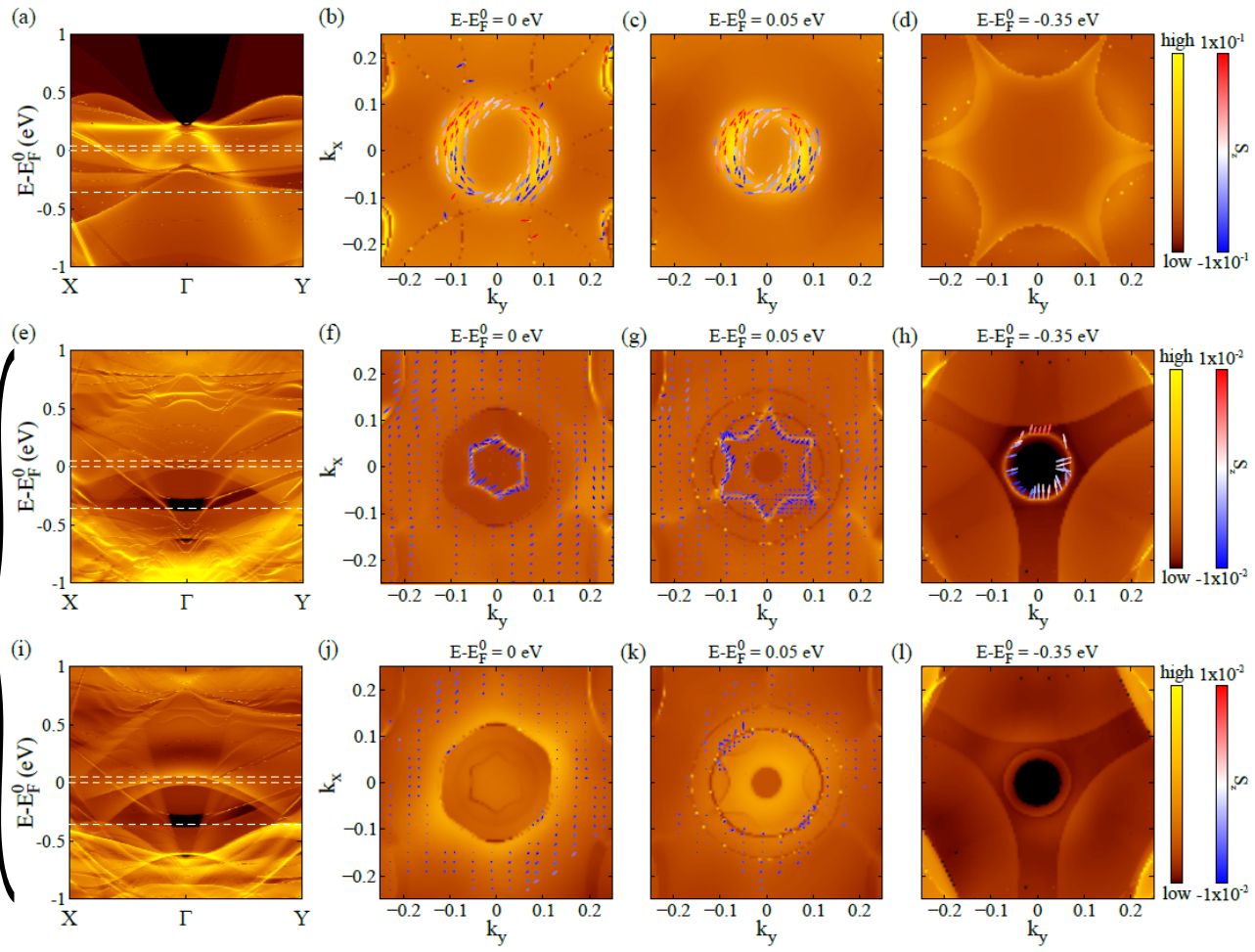
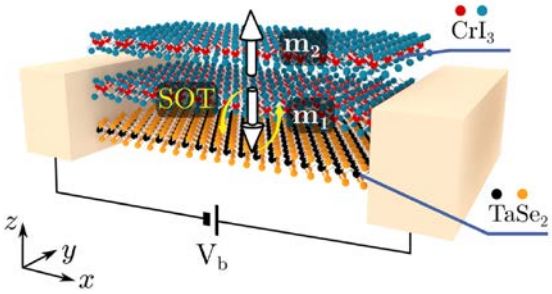
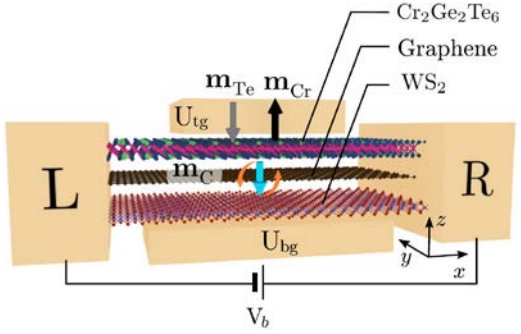
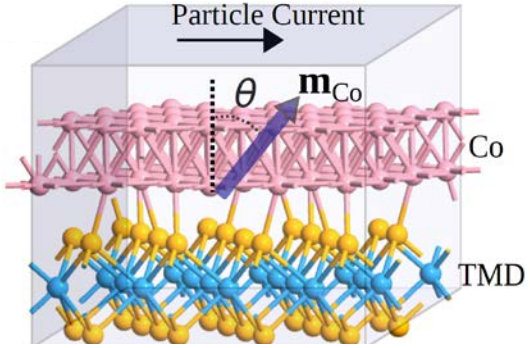
Nat. Nanotech. **14**, 945 (2019)



Magnetization switching with ultralow current density ~3×10^5 A/cm^2 at T=300 K

one would miss later developments

"Physics comes in two parts: the precise mathematical formulation of the laws, and the conceptual interpretation of the mathematics. **However, if words of conceptual interpretation actually convey the wrong meaning of the mathematics, they must be replaced by more accurate words."** (W. J. Mullin)

Conclusions in Pictures

SO-proximitized ferromagnet can be very far away from the original