

# Topological Proximity Effect in Ferromagnetic Metals: Fundamentals and Spintronic Applications

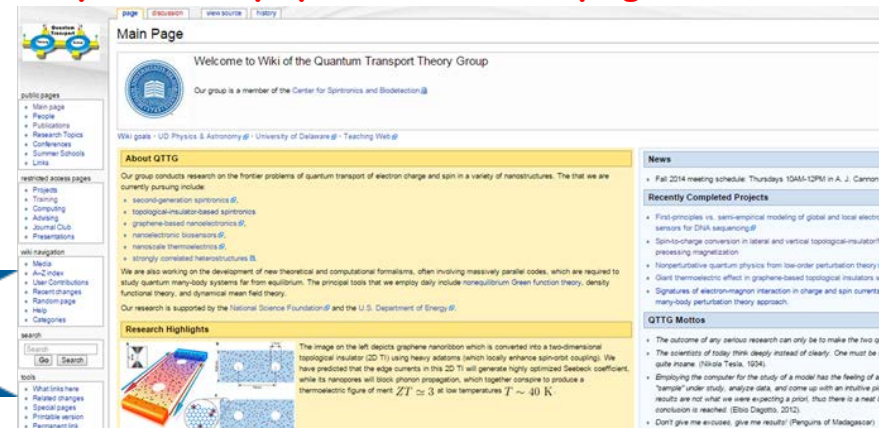
Branislav K. Nikolić

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



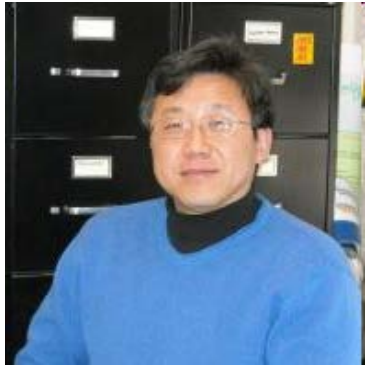
1638-1655

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



# Collaborators

## Experiment



Prof. J. Q. Xiao



Prof. J.-P. Wang

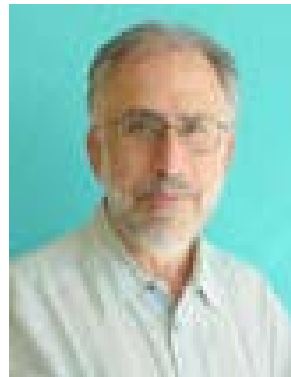
## Theory



Dr. Farzad Mahfouzi



Prof. N. Nagaosa



Prof. Nicholas Kioussis

## Computation



Dr. Kapildeb Dolui



J. M. Marmolejo-Tejada



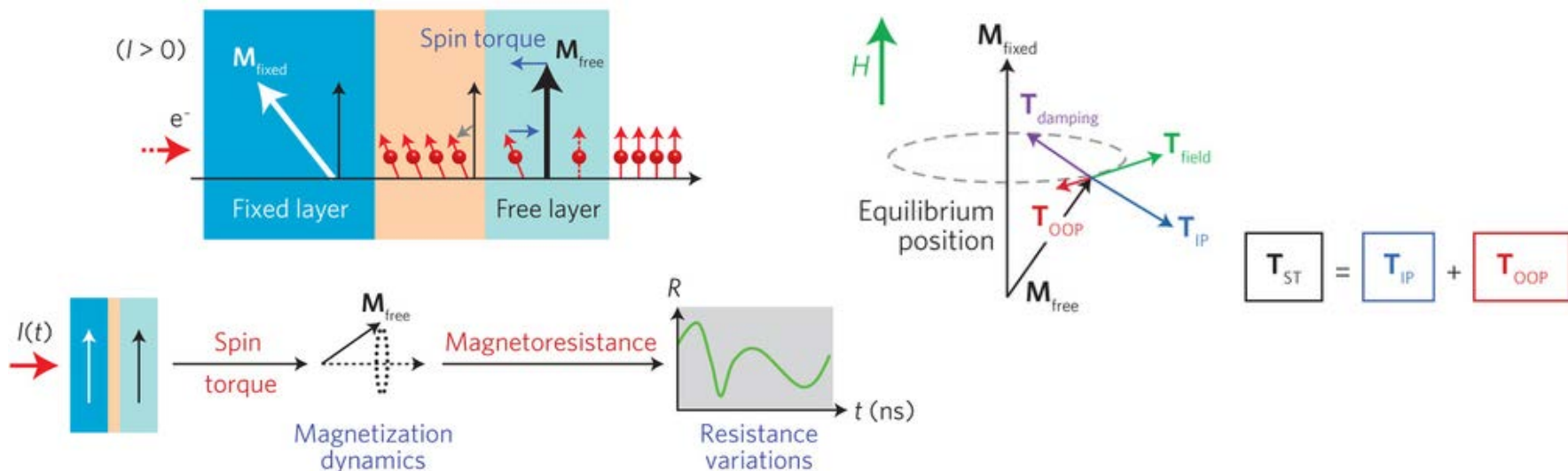
Dr. Po-Hao Chang



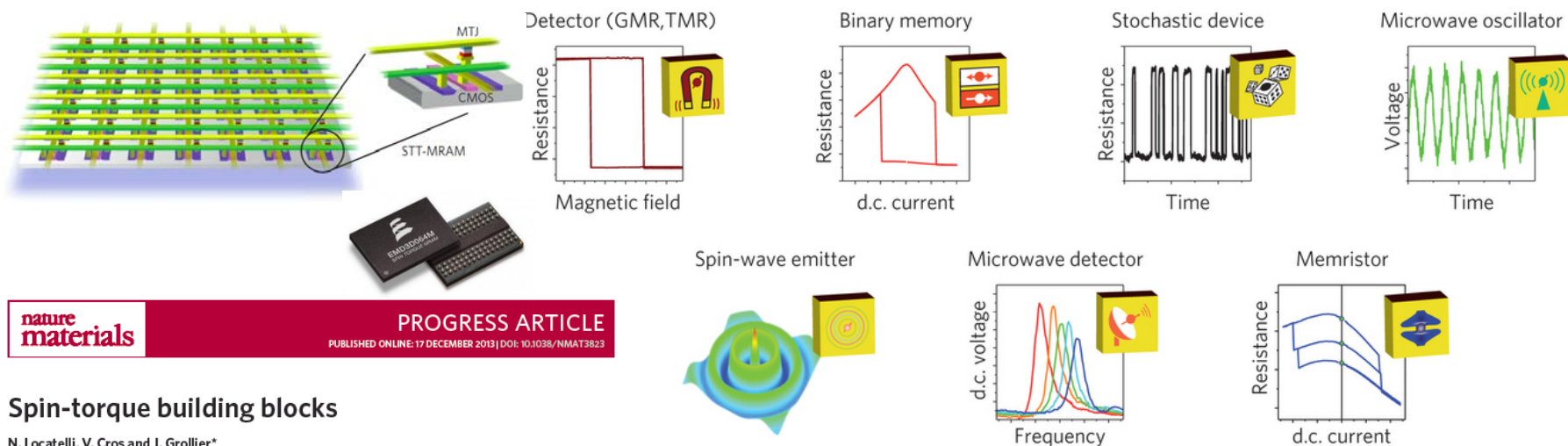
Dr. Kurt Stokbro

# Spin-Transfer Torque: Fundamentals and Applications

Fundamentals



Applications



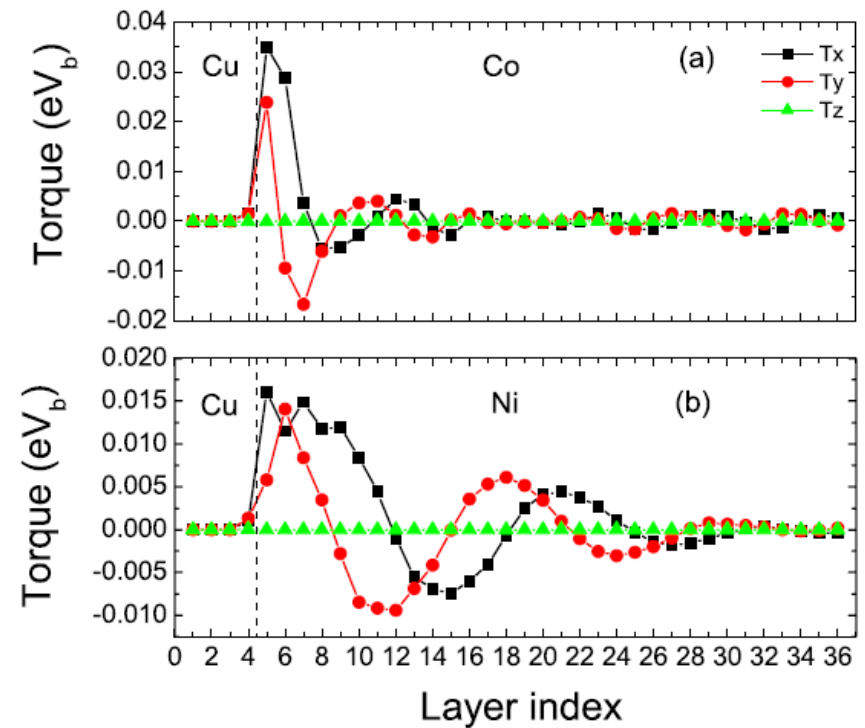
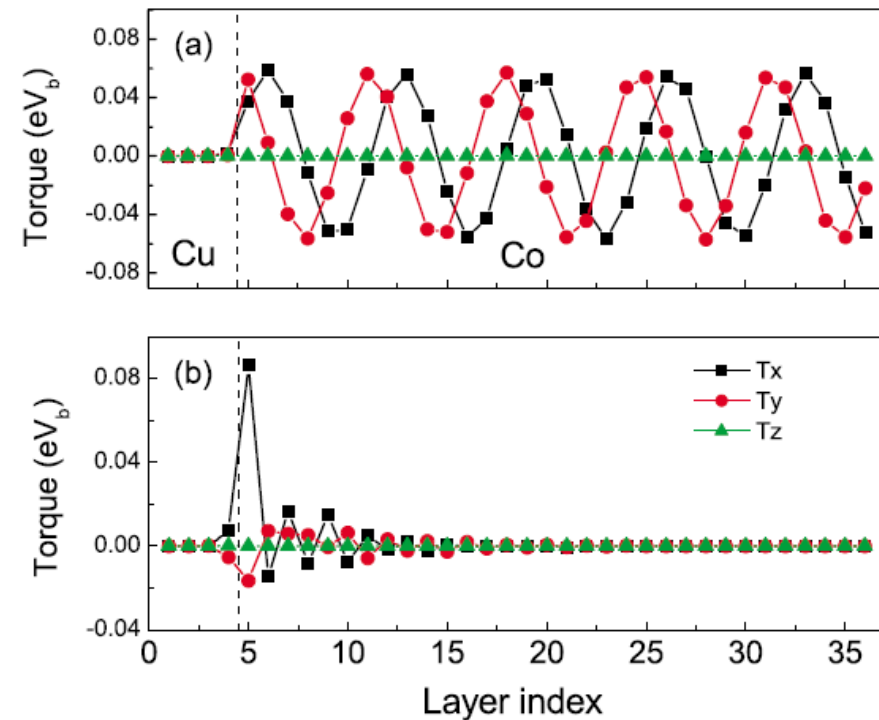
# Quantum Transport Theory is Needed to Describe STT

PHYSICAL REVIEW B 77, 184430 (2008)

## First-principles study of spin-transfer torques in layered systems with noncollinear magnetization

Shuai Wang, Yuan Xu, and Ke Xia

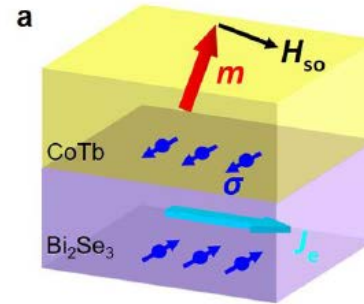
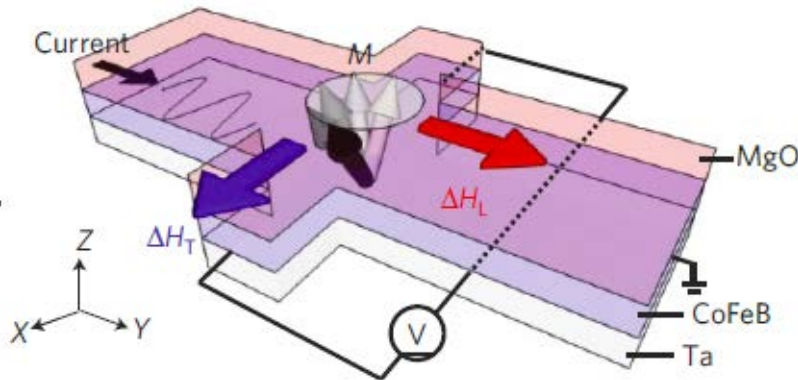
State Key Laboratory for Surface Physics, Institute of Physics, Chinese Academy of Sciences, P.O. Box 603, Beijing 100080, People's Republic of China





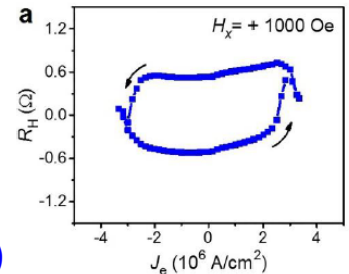
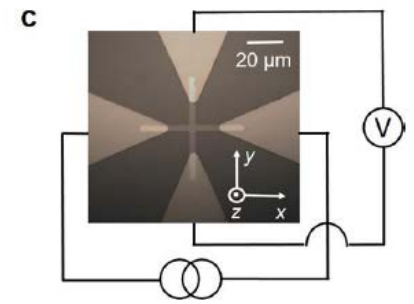
# Spin-Orbit Torque (SOT): Fundamentals and Applications

Nat. Mater. 12, 240 (2013)



T=300 K

PRL 119, 077702 (2017)

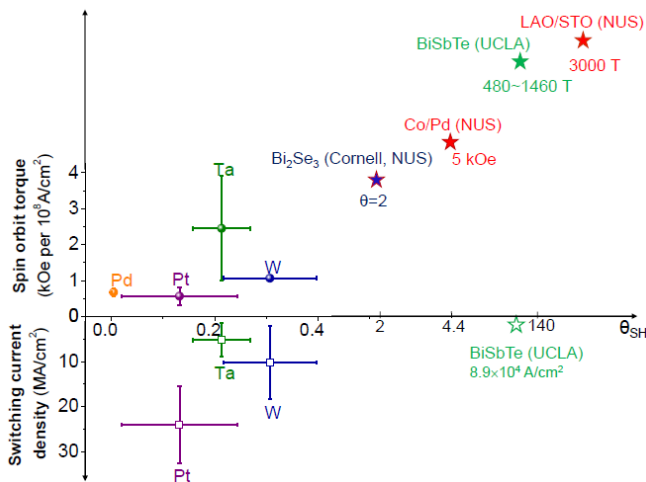
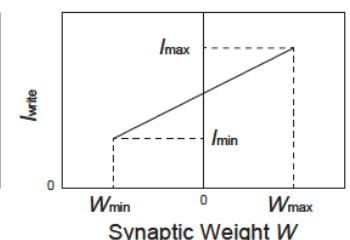
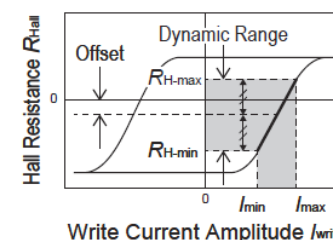
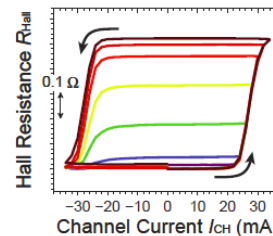


solid-state nonvolatile analogue memory  
with infinite read-write endurance

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<sup>1</sup>, Hisanao Akima<sup>1\*</sup>, Shunsuke Fukami<sup>1,2,3,4\*</sup>, Satoshi Moriya<sup>1</sup>, Shouta Kurihara<sup>1</sup>, Yoshihiko Horio<sup>1</sup>, Shigeo Sato<sup>1</sup>, and Hideo Ohno<sup>1,2,3,4,5</sup>



# Current-Driven Nonequilibrium Spin Density as the Origin of Fieldlike 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

nature  
materials

INSIGHT | PROGRESS ARTICLE  
PUBLISHED ONLINE: 23 APRIL 2012 | DOI: 10.1038/NMAT3305

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

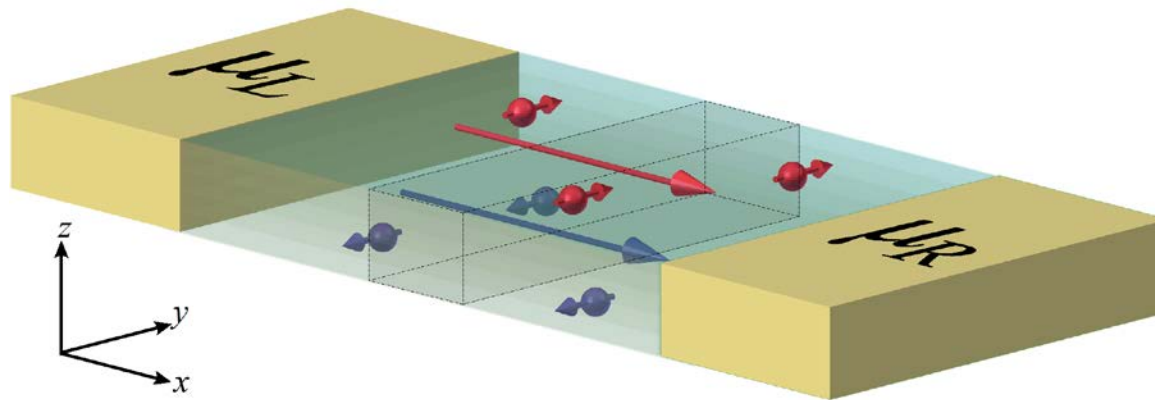
V.M. Edelstein

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

Spintronics and pseudospintronics in graphene  
and topological insulators

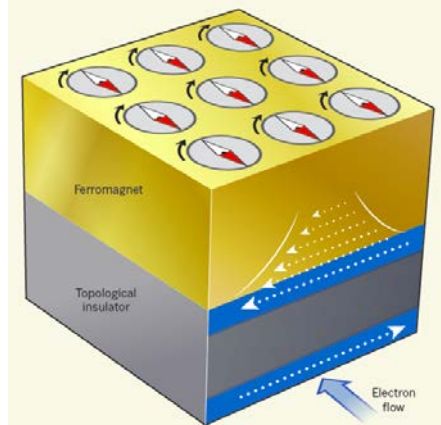
Dmytro Pesin and Allan H. MacDonald

$$S_y = \beta E_x$$



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

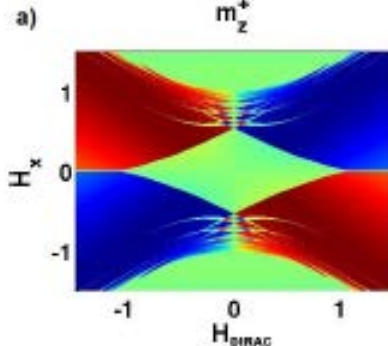
# Quantum Transport Theory (Which One?) is Needed to Describe Interfacially-Driven Antidamping SOT



Nature **511**, 449 (2014)  
PRB **93**, 125303 (2016)

Berry curvature  
antidamping torque

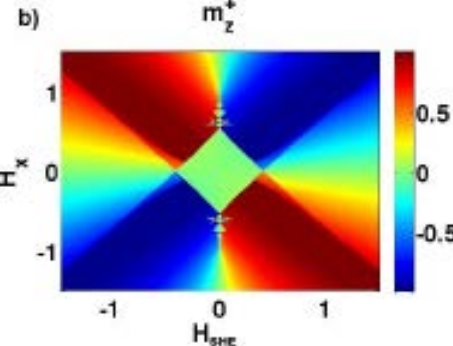
$$\propto m_z \mathbf{m} \times \hat{x}$$



PRB **90**, 174423 (2014); PRB **96**, 014408 (2017)  
PRB **91**, 134402 (2015); Nat. Nanotech. **9**, 211 (2014)

SHE antidamping torque

$$\propto m_z \mathbf{m} \times \hat{x} - m_x \mathbf{m} \times \hat{z}$$



antidamping torque is zero  
in the absence of  
spin-dependent scattering

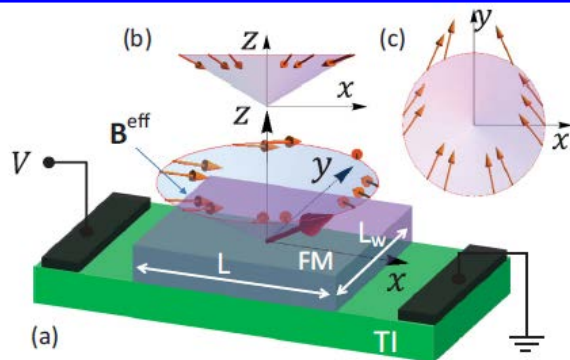
PRB **86**, 014416 (2012)

$$\hat{U}_{\text{dis}} = \sum_i \delta(\mathbf{r} - \mathbf{r}_i) (u_{\downarrow} P_{+}^0 + u_{\uparrow} P_{-}^0)$$

missing diagrams

PRB **95**, 094401 (2017)

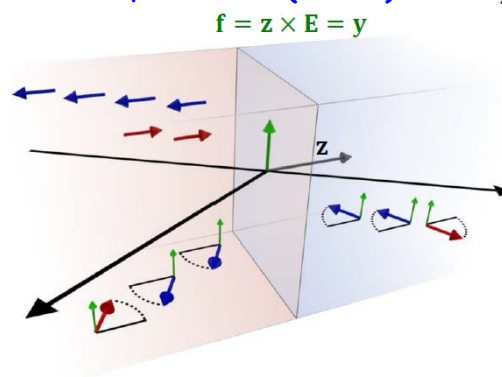
$$K_{\alpha\beta} = \alpha_{\alpha} \left[ \Gamma_{\beta}^{\alpha} + M_{\alpha} \left[ \Gamma_{\beta}^{\alpha} \Gamma_{\beta}^{\alpha} + \Gamma_{\beta}^{\alpha} \Gamma_{\beta}^{\alpha} \right] \right] + M_{\alpha}^2 \left[ \Gamma_{\beta}^{\alpha} \Gamma_{\beta}^{\alpha} + \Gamma_{\beta}^{\alpha} \Gamma_{\beta}^{\alpha} + \Gamma_{\beta}^{\alpha} \Gamma_{\beta}^{\alpha} + \Gamma_{\beta}^{\alpha} \Gamma_{\beta}^{\alpha} \right] + \dots$$



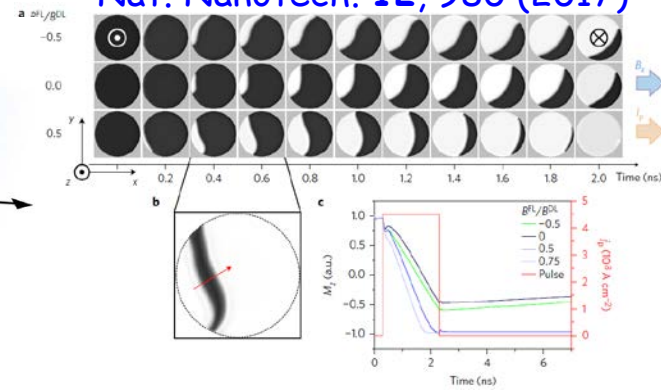
PRB **84**, 113407 (2011)  
PRB **86**, 161406(R) (2012)  
arXiv:1604.07885

MISSING INGREDIENTS: 3D geometry and switching at the boundaries

PRB **94**, 104420 (2016)  
PRB **94**, 104419 (2016)

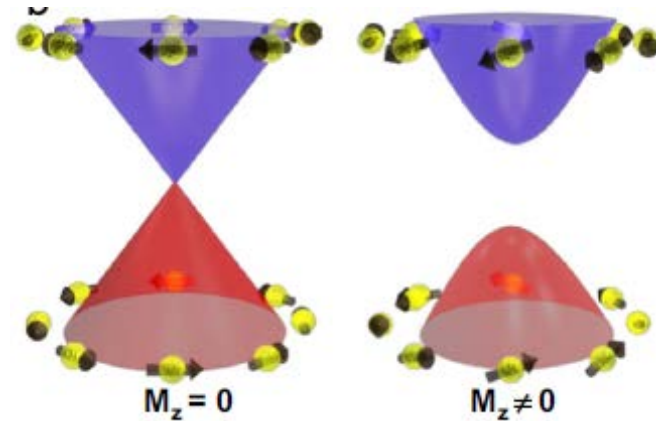
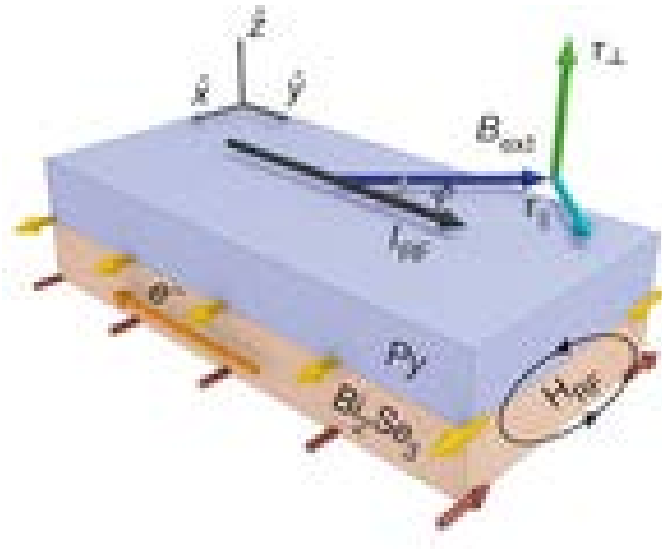


Nat. Nanotech. **12**, 980 (2017)



# Trouble with Simplistic Hamiltonians for Describing SOT Experiments

Nature **511**, 449 (2014)



“Our findings have potential importance for technology, in that the spin torque ratio for  $\text{Bi}_2\text{Se}_3$  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.”

**Table 1 | Comparison of room-temperature  $\sigma_{s,\parallel}$  and  $\theta_{s,\parallel}$  for  $\text{Bi}_2\text{Se}_3$  with other materials**

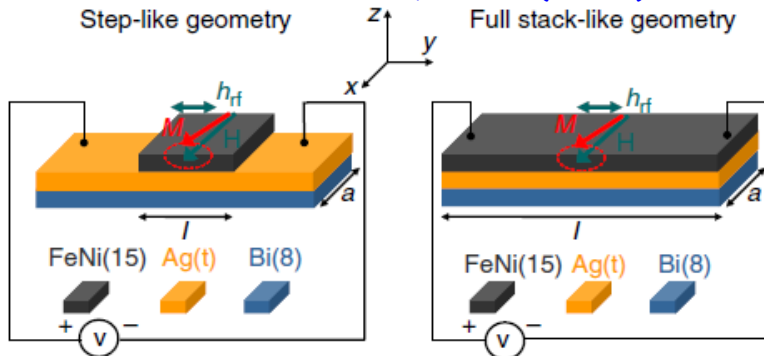
Parameter	$\text{Bi}_2\text{Se}_3$ (this work)	Pt (ref. 4)	$\beta\text{-Ta}$ (ref. 6)	Cu(Bi) (ref. 23)	$\beta\text{-W}$ (ref. 24)
$\theta_{\parallel}$	2.0–3.5	0.08	0.15	0.24	0.3
$\sigma_{s,\parallel}$	1.1–2.0	3.4	0.8	—	1.8

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

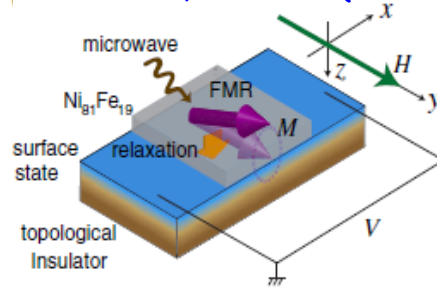


# Trouble with Simplistic Hamiltonians for Describing Spin-to-Charge Conversion Experiments

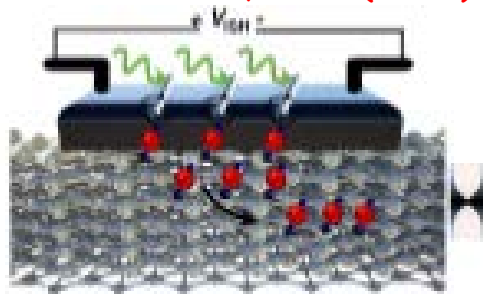
Nat. Comm. **4**, 2944 (2013)



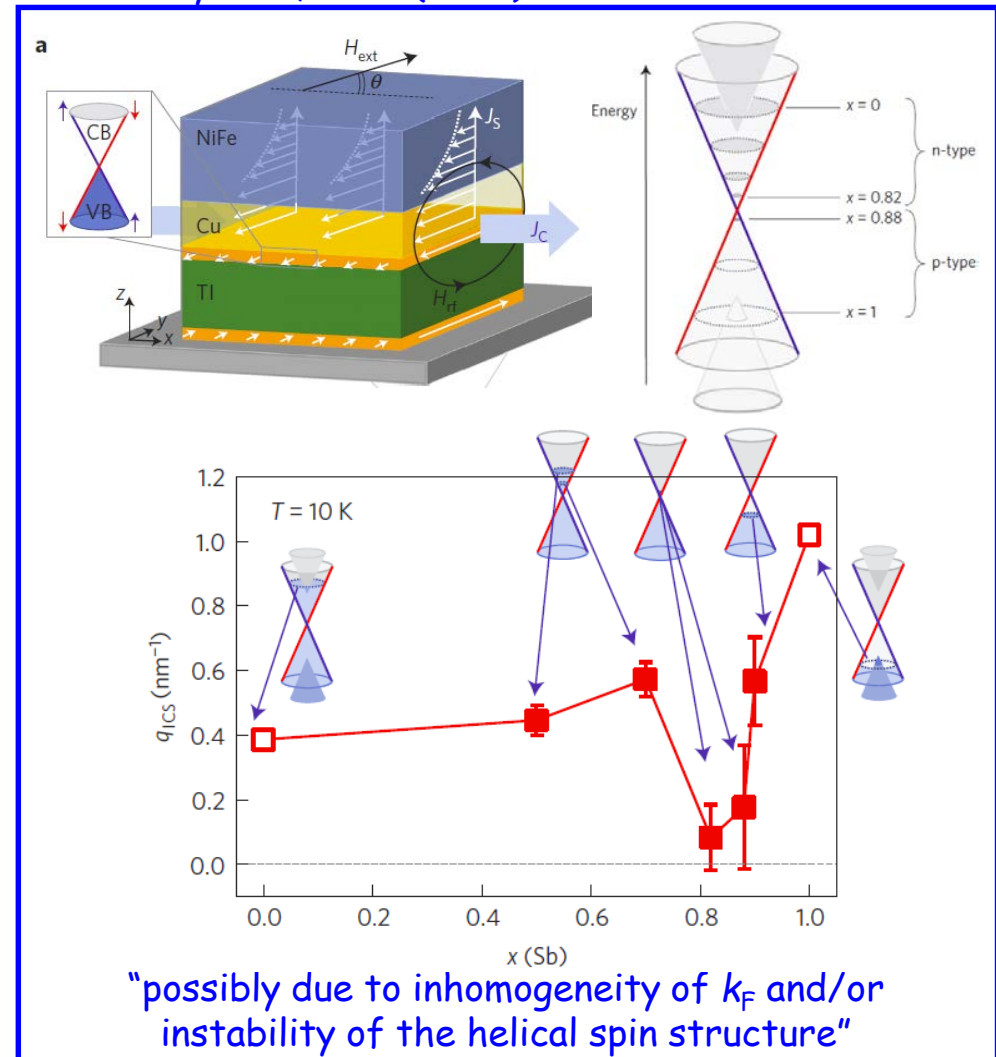
PRL **113**, 196601 (2014)



Nano Lett. **15**, 7126 (2015)



Nature Phys. **12**, 1027 (2016)



# This Talk in a Nutshell: $\Psi_{TM} + \Psi_{FM}$

news & views

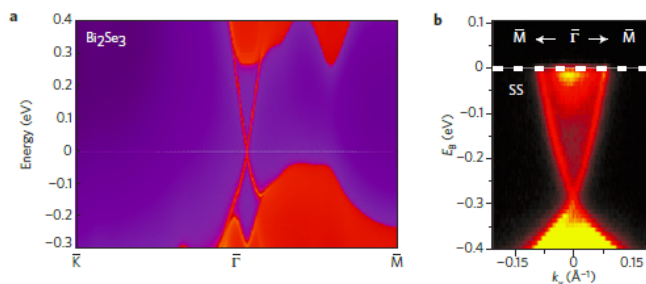
TEN YEARS OF NATURE PHYSICS

## Not trivial to realize

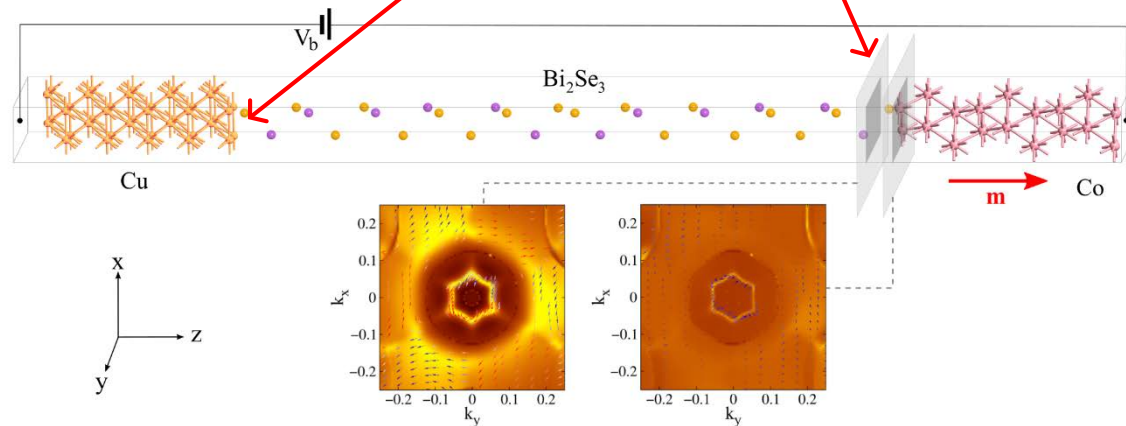
In 2009, two papers provided the first unambiguous examples of three-dimensional topological insulators — bulk insulators boasting metallic surface states with massless Dirac electrons. These now form just one of many classes of topological materials.

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 support chain reactions. In the same vein



What is the electronic and spin structure of interfacial states and how they affect SOT?



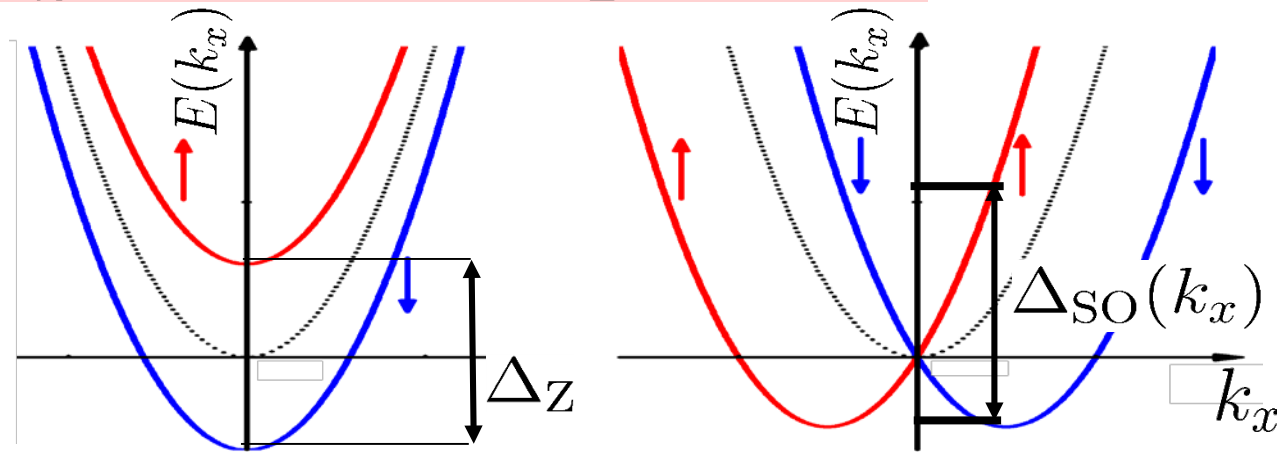
Nano Lett. 17, 5626 (2017)

# Crash Course on Rashba SO Coupling

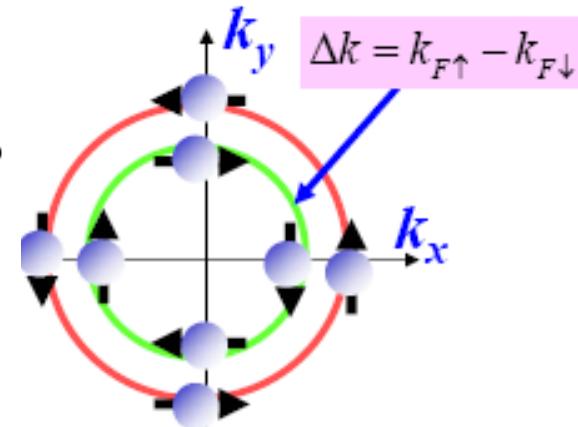
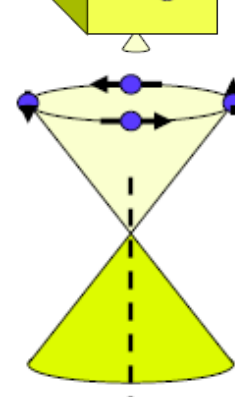
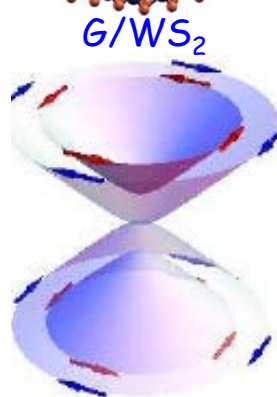
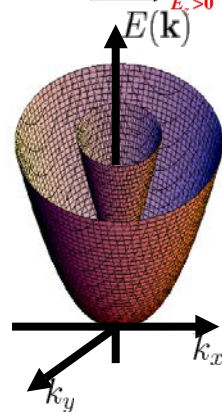
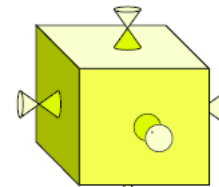
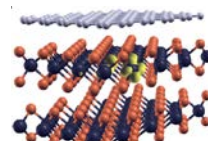
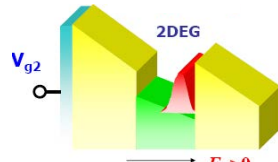
$$\hat{H}_{\text{SO}}^{\text{R}} = \frac{\alpha}{\hbar} (\hat{\boldsymbol{\sigma}} \times \hat{\mathbf{p}}) \cdot \mathbf{e}_z \equiv -\frac{g\mu_B}{2} \hat{\boldsymbol{\sigma}} \cdot \mathbf{B}_{\text{R}}(\hat{\mathbf{p}})$$

1D:

$E(k_x)$



2D:



$$\begin{aligned} \varepsilon(\mathbf{k}, \uparrow) &= \varepsilon(-\mathbf{k}, \downarrow) \\ \varepsilon(\mathbf{k}, \uparrow) &\neq \varepsilon(-\mathbf{k}, \uparrow) \\ \varepsilon(\mathbf{k}, \uparrow) &\neq \varepsilon(\mathbf{k}, \downarrow) \end{aligned}$$

# Spin Density and Torque from Nonequilibrium Green Function (NEGF) Formalism

## □ Fundamental quantities of NEGF formalism:

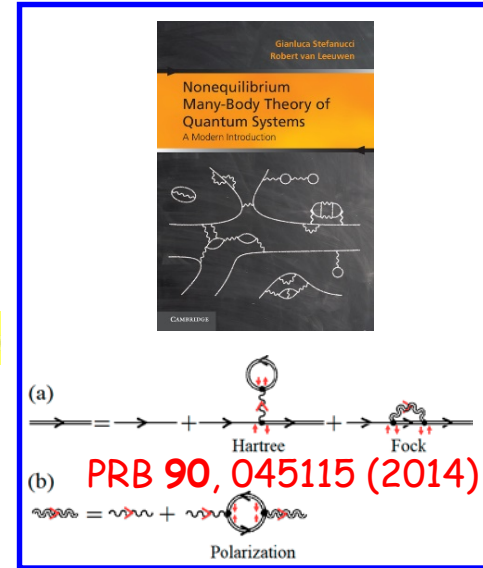
density of available quantum states:

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

how are those states occupied:

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

Learn more about NEGF from:



## □ NEGF for steady-state transport:

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

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

$$\rho_{\text{eq}} = -\frac{1}{\pi} \int_{-\infty}^{+\infty} dE \text{Im} \mathbf{G}^r(E) f(E - E_F)$$

$$\rho_{\text{neq}} = \frac{1}{2\pi i} \int_{-\infty}^{+\infty} dE \mathbf{G}^<(E)$$

## □ NEGF-based expression for spin-transfer torque:

SPIN 3, 1330002 (2013)

$$\hat{H} = -\frac{\hbar^2 \nabla^2}{2m} + V_H(\mathbf{r}) + V_{\text{XC}}(\mathbf{r}) + V_{\text{ext}}(\mathbf{r}) - \boldsymbol{\sigma} \cdot \mathbf{B}_{\text{XC}}(\mathbf{r}) \Rightarrow \hat{\mathbf{T}} = \frac{d\hat{\mathbf{S}}}{dt} = \frac{1}{2i} [\hat{\boldsymbol{\sigma}}, \hat{H}]$$

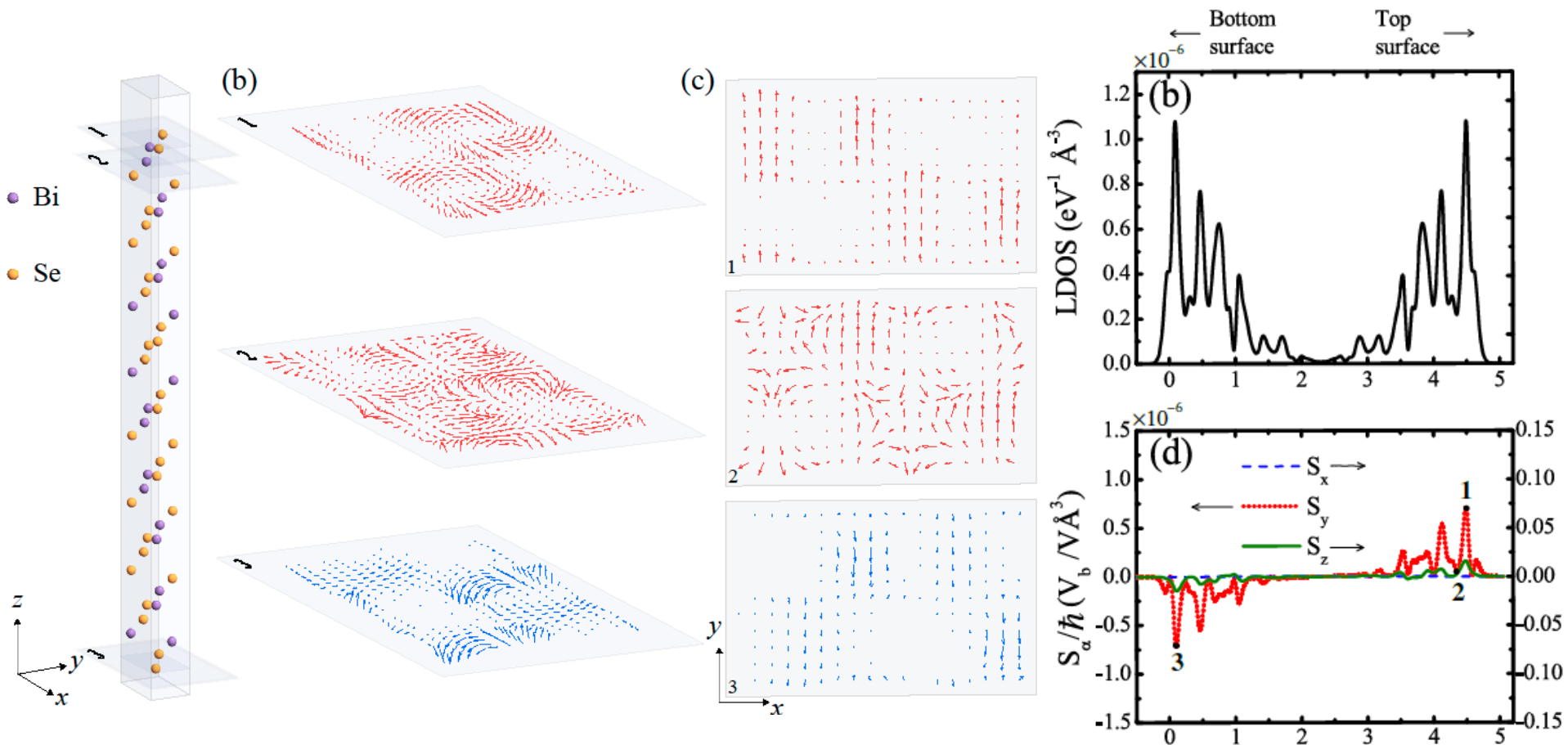
$$\mathbf{T} = \text{Tr} [\hat{\rho}_{\text{neq}} \hat{\mathbf{T}}] \Leftrightarrow \mathbf{T} = \int_F d^3r \mathbf{m}_{\text{neq}}(\mathbf{r}) \times \mathbf{B}_{\text{XC}}(\mathbf{r})$$

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



# Current-Driven Nonequilibrium Spin Texture on the Surface and in the Bulk of $\text{Bi}_2\text{Se}_3$

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



# Spectral Function and Spin Textures on the TI Side of TI/FM Heterostructures

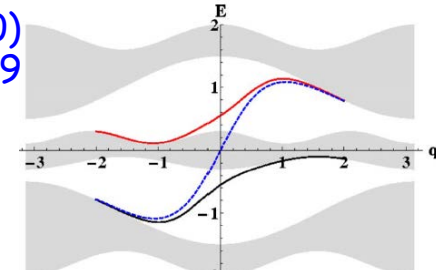
Bi<sub>2</sub>Se<sub>3</sub> Lead

Bi<sub>2</sub>Se<sub>3</sub> (6 QL)

Co (3 ML)

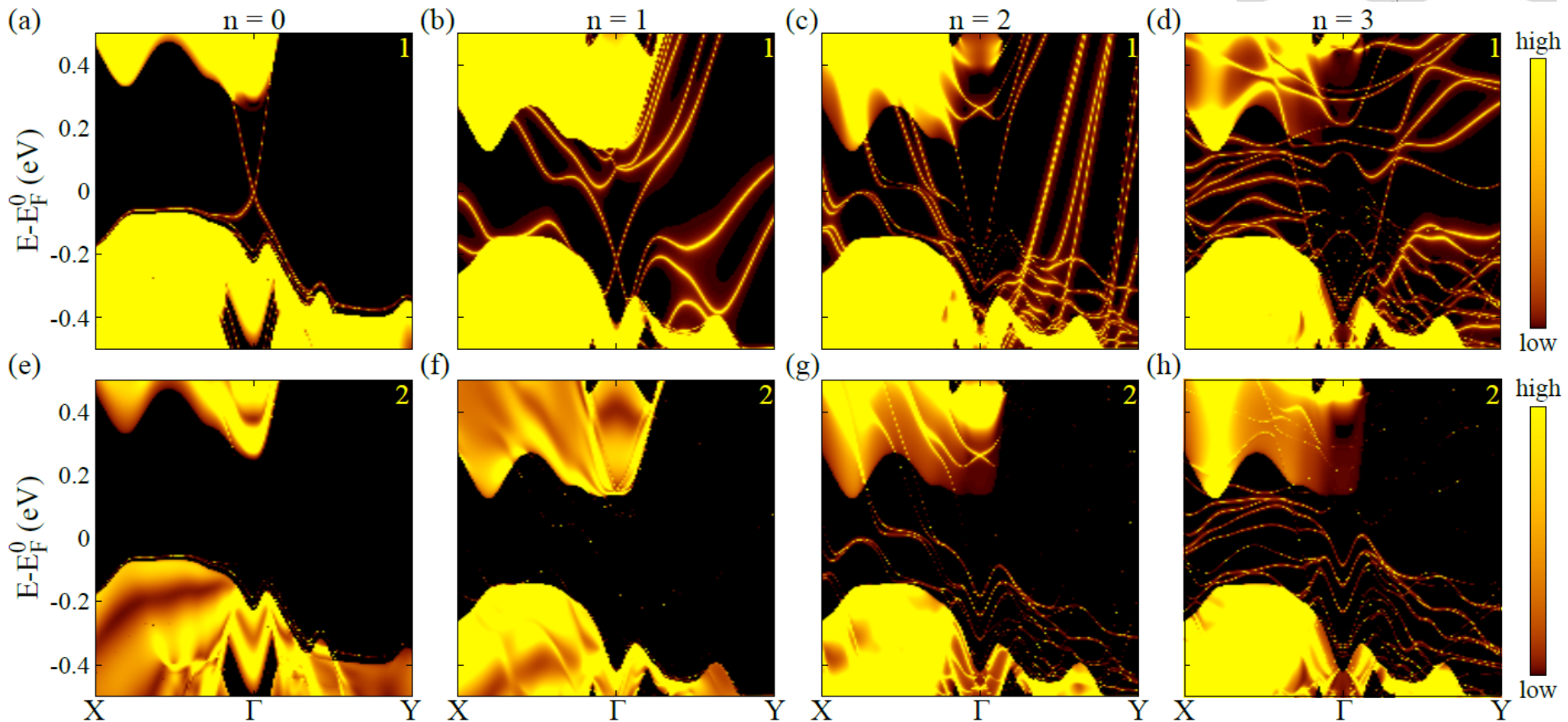
Vacuum

PRB **82**, 195417 (2010)  
arXiv:1707.06319



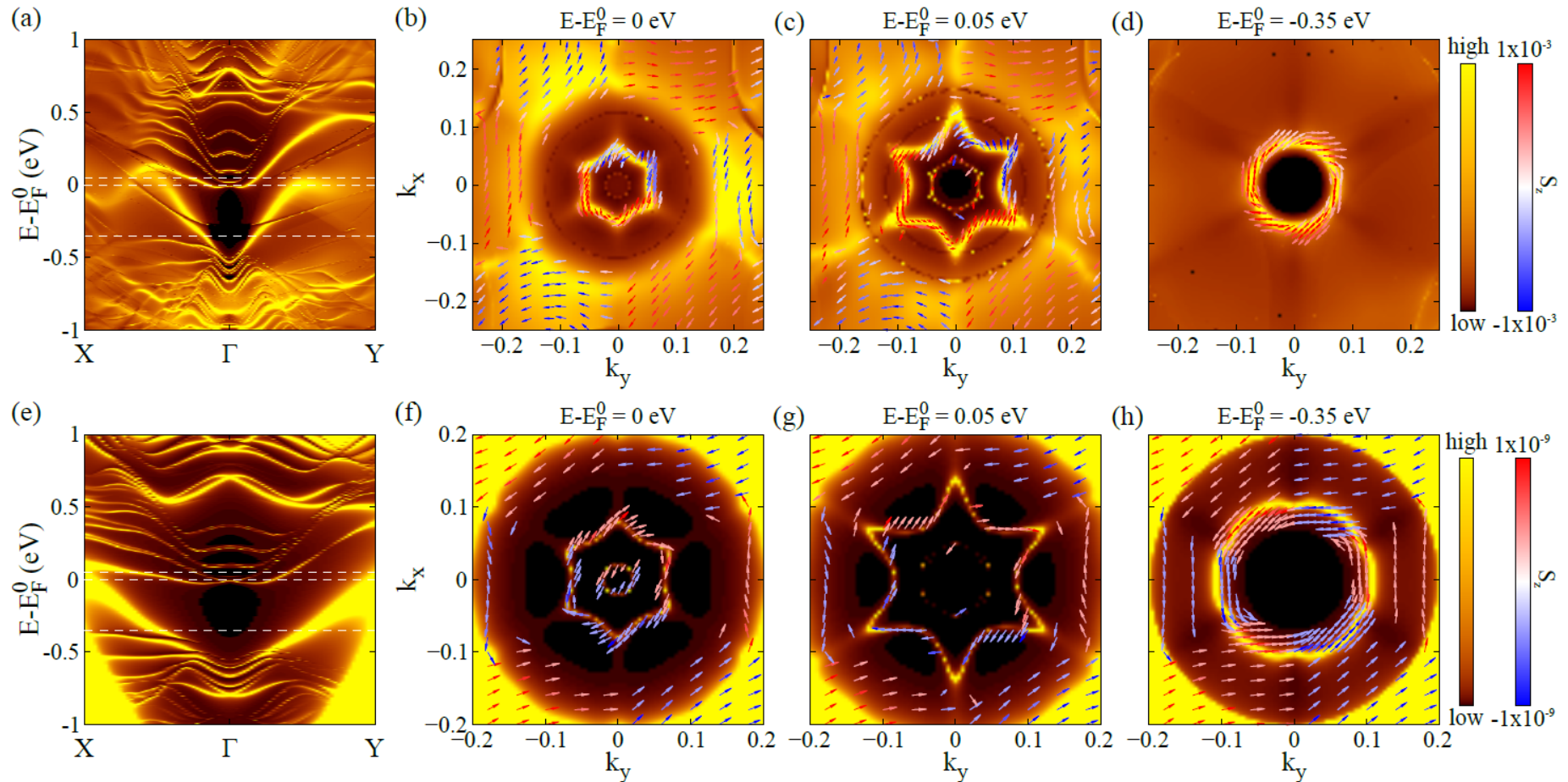
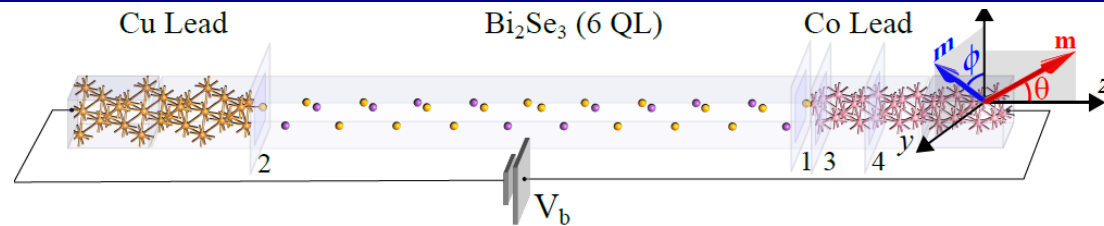
Nano Lett. **17**, 5626 (2017)

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



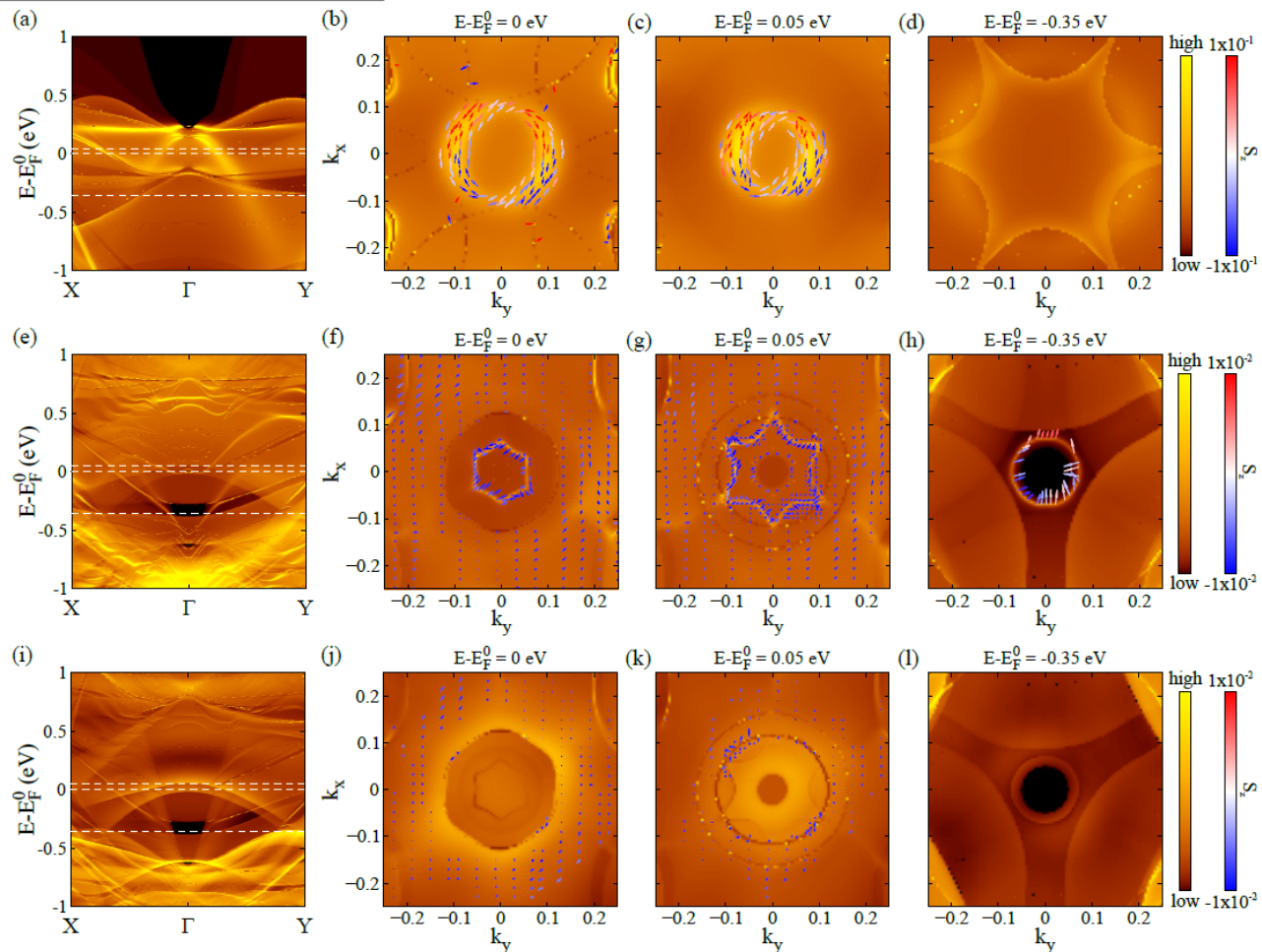
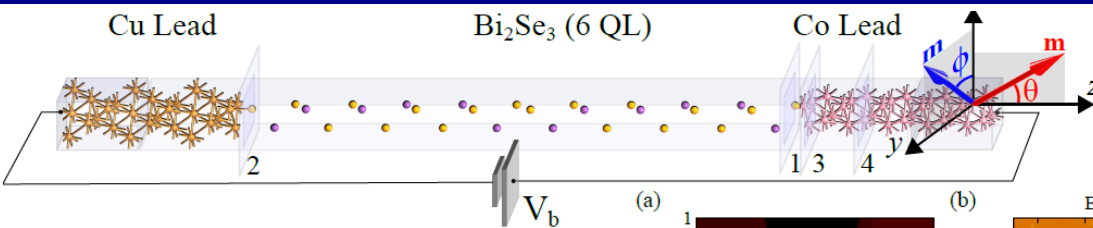
# Spectral Function and Spin Textures on the TI Side of NM/TI/FM Heterostructures

Nano Lett. 17, 5626 (2017)



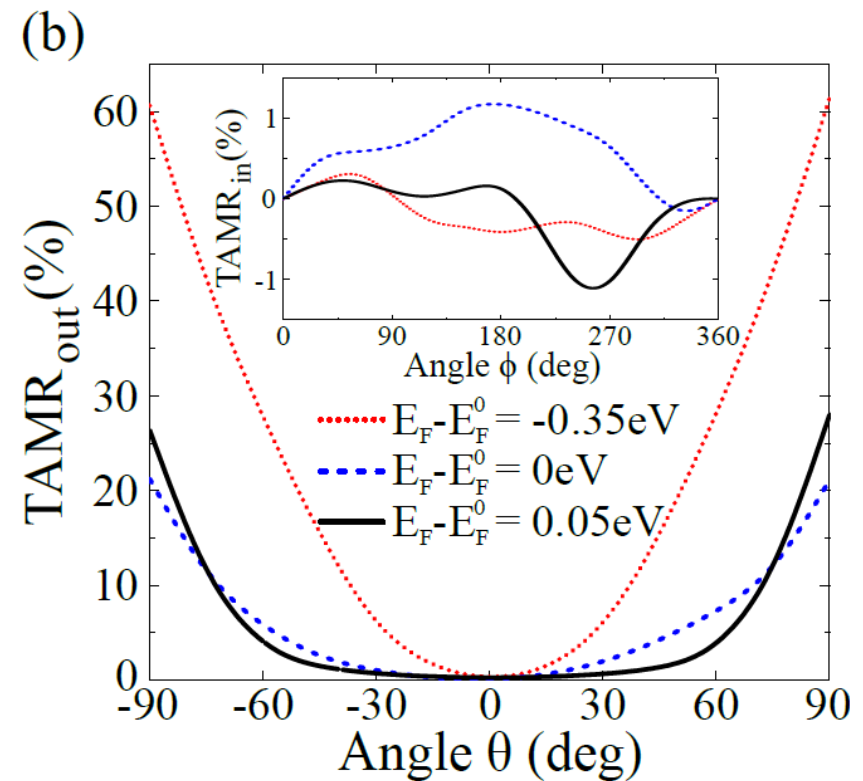
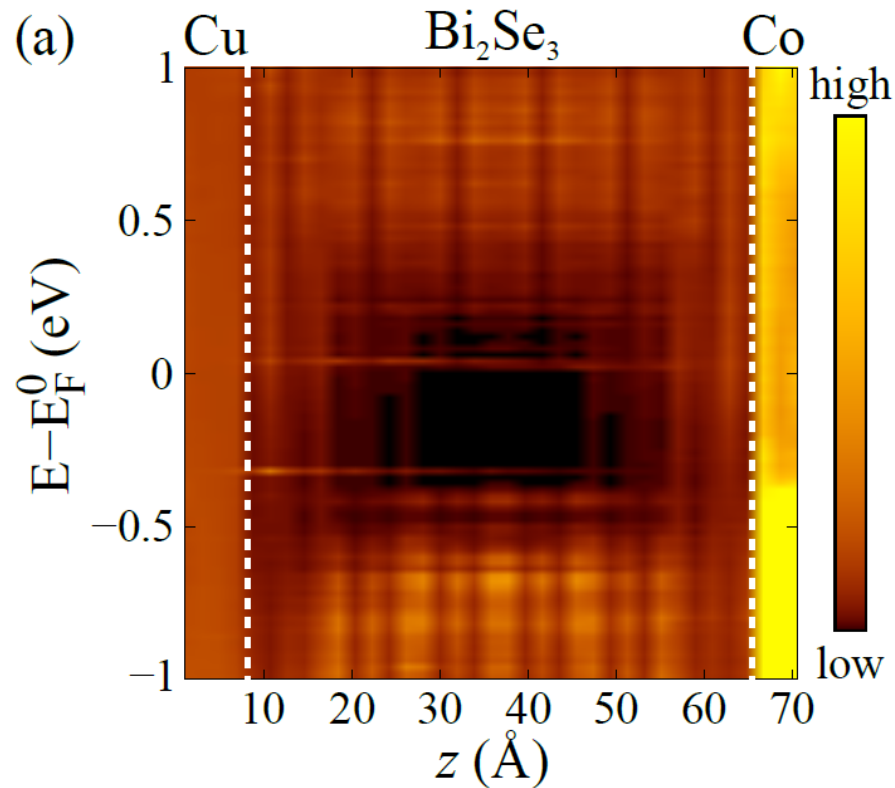
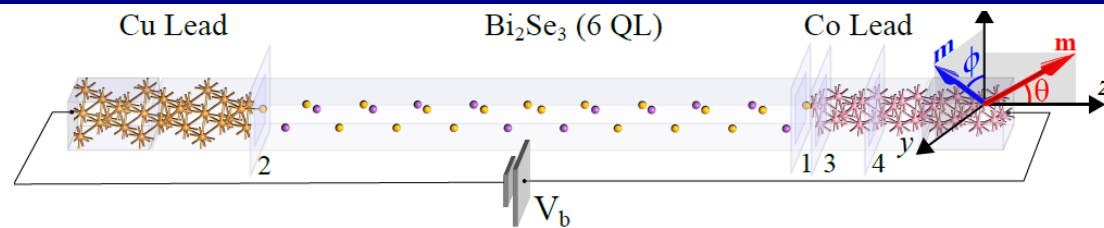
# Spectral Function and Spin Textures on the FM Side of TI/FM Heterostructures

Nano Lett. 17, 5626 (2017)





# Tunneling Anisotropic Magnetoresistance (TAMR) as a Probe of Interfacial Spin Texture



Nano Lett. 17, 5626 (2017)

# Adiabatic Expansion of NEGF Spits Out Expressions for Torque, Pumping and Gilbert Damping

$$\begin{aligned}\mathbf{G}(E, t) &\simeq \mathbf{G}_t + i(\partial \mathbf{G}_t / \partial E)(\partial \mathbf{U}_t / \partial t) \mathbf{G}_t \\ \mathbf{G}^<(t, t) &\simeq \int \frac{dE}{2\pi} [\mathbf{G}(E, t) - \mathbf{G}^\dagger(E, t)] f + i \sum_{\alpha=L,R} f' e V_\alpha \mathbf{G}_t \boldsymbol{\Gamma}_\alpha \mathbf{G}_t^\dagger + i f' \mathbf{G}_t \frac{\partial \mathbf{U}_t}{\partial t} \mathbf{G}_t^\dagger \\ \rho(t) &= \frac{1}{i} \mathbf{G}^<(t, t)\end{aligned}$$

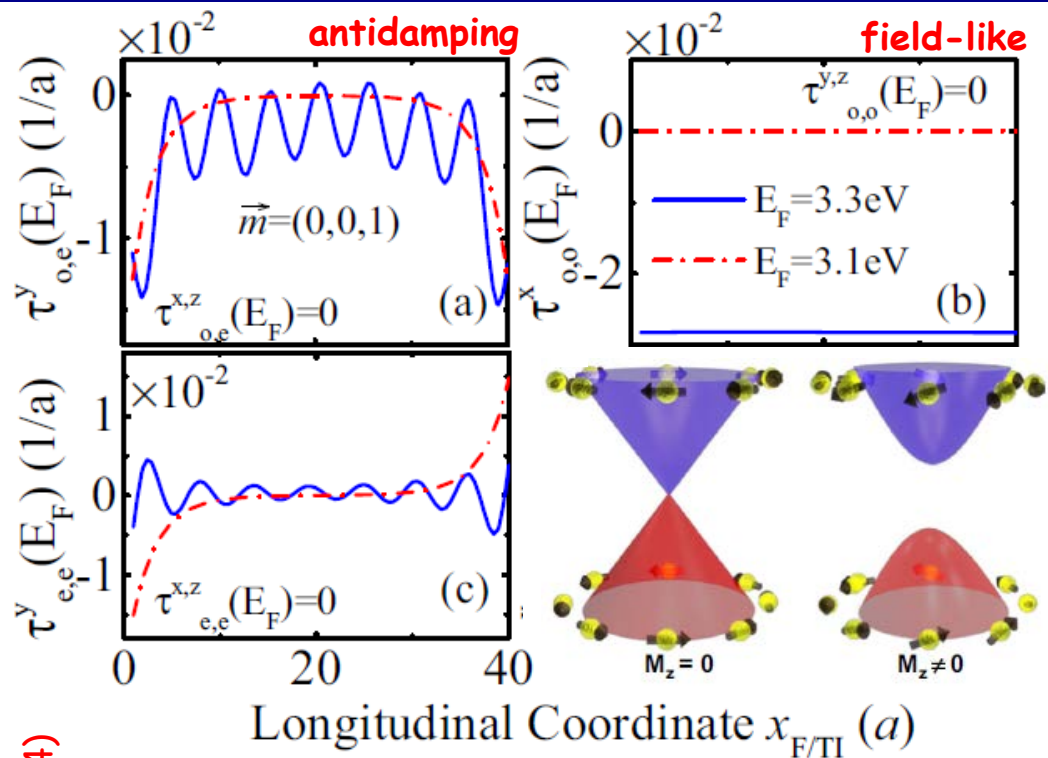
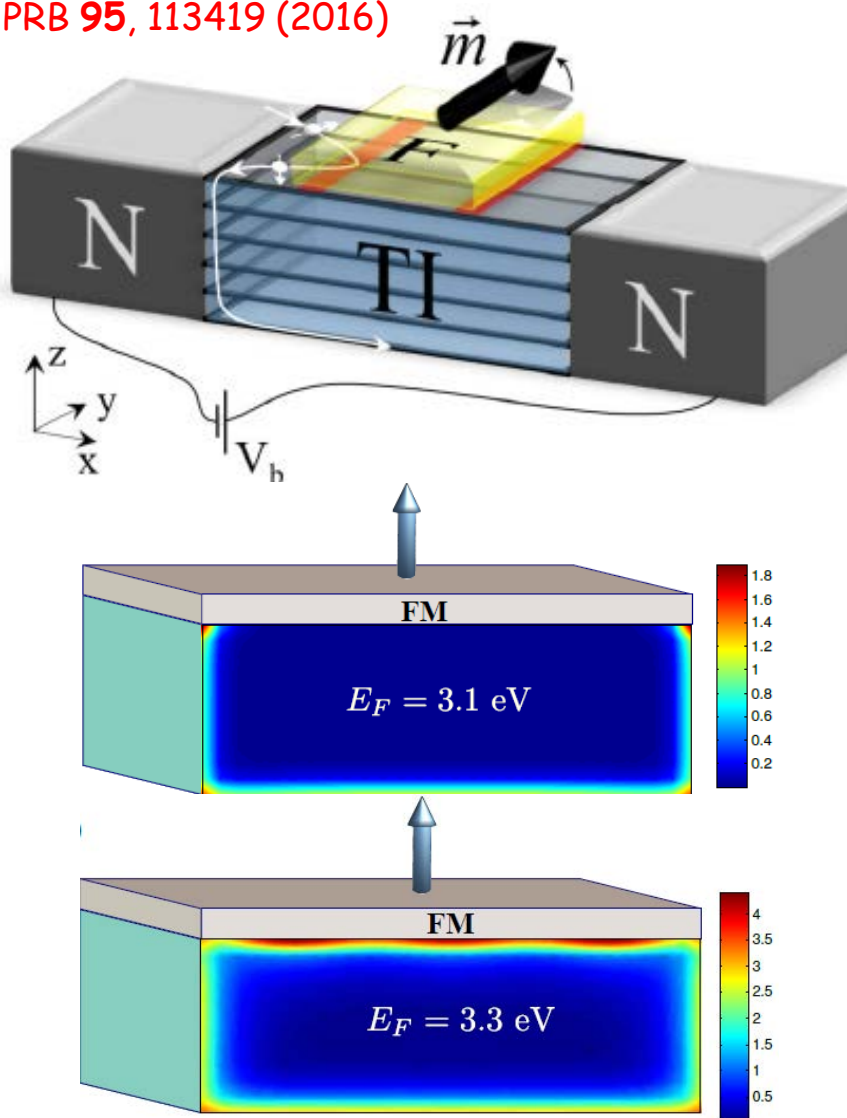
$$\begin{aligned}T^{\alpha\beta}(E) &= \text{Tr} [\boldsymbol{\Gamma}_\alpha \mathbf{G}_t \boldsymbol{\Gamma}_\beta \mathbf{G}_t^\dagger] \text{ charge current} \\ T^{\alpha i}(E) &= \text{Tr} [\mathbf{1}_m \boldsymbol{\sigma}_i \mathbf{G}_t^\dagger \boldsymbol{\Gamma}_\alpha \mathbf{G}_t] \text{ spin torque} \\ T^{i\alpha}(E) &= \text{Tr} [\mathbf{1}_m \boldsymbol{\sigma}_i \mathbf{G}_t \boldsymbol{\Gamma}_\alpha \mathbf{G}_t^\dagger] \text{ charge pumping} \\ T^{ij}(E) &= \text{Tr} [\mathbf{1}_m \boldsymbol{\sigma}_i (\mathbf{G}_t^\dagger - \mathbf{G}_t) \mathbf{1}_m \boldsymbol{\sigma}_j (\mathbf{G}_t - \mathbf{G}_t^\dagger)] \text{ Gilbert damping}\end{aligned}$$

PRB 95, 113419 (2016)

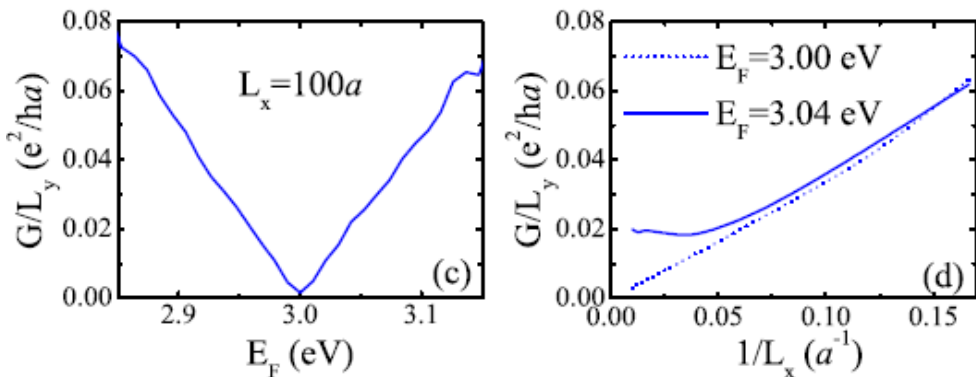
$$\rho \left\{ \begin{aligned} \rho_{oo} &= \int dE (f_L - f_R) [\mathbf{G} \boldsymbol{\Gamma}_L \mathbf{G}^\dagger - \mathbf{G}^\dagger \boldsymbol{\Gamma}_L \mathbf{G} - \mathbf{G} \boldsymbol{\Gamma}_R \mathbf{G}^\dagger + \mathbf{G}^\dagger \boldsymbol{\Gamma}_R \mathbf{G}] / 8\pi && \text{gives antidamping STT or field-like SOT} \\ + \\ \rho_{oe} &= \int dE (f_L - f_R) [\mathbf{G} \boldsymbol{\Gamma}_L \mathbf{G}^\dagger + \mathbf{G}^\dagger \boldsymbol{\Gamma}_L \mathbf{G} - \mathbf{G} \boldsymbol{\Gamma}_R \mathbf{G}^\dagger - \mathbf{G}^\dagger \boldsymbol{\Gamma}_R \mathbf{G}] / 8\pi && \text{gives field-like STT or antidamping SOT} \\ + \\ \rho_{ee} &= \int dE (f_L + f_R) [-\text{Im} \mathbf{G}] / 2\pi && \text{contains both equilibrium (should be subtracted) and nonequilibrium contributions} \\ + \\ \rho_{eo} &\equiv 0 \end{aligned} \right. \quad \text{SPIN 3, 1330002 (2013)}$$

# Spatial Profile of Antidamping SOT in TI/FI Heterostructures and the Role of Evanescent States

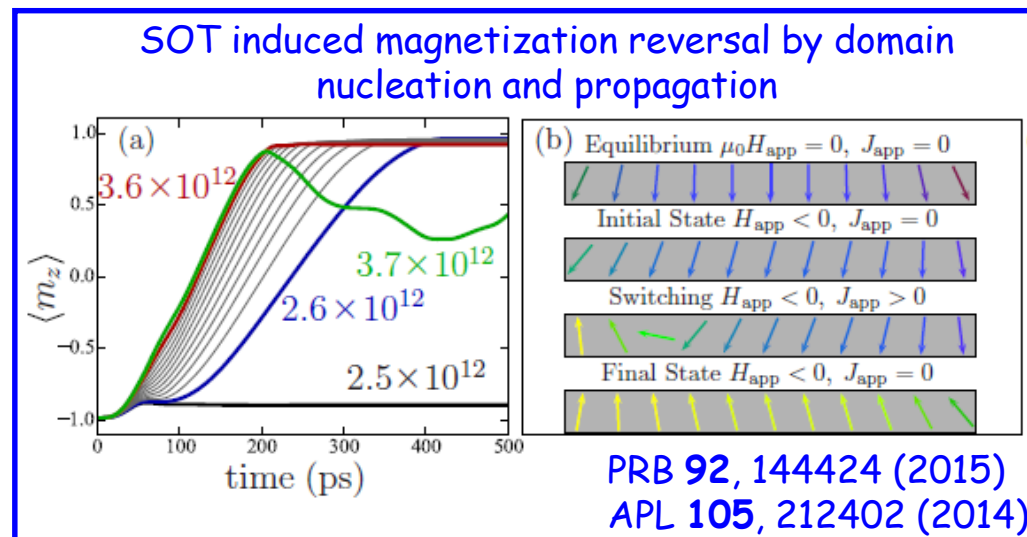
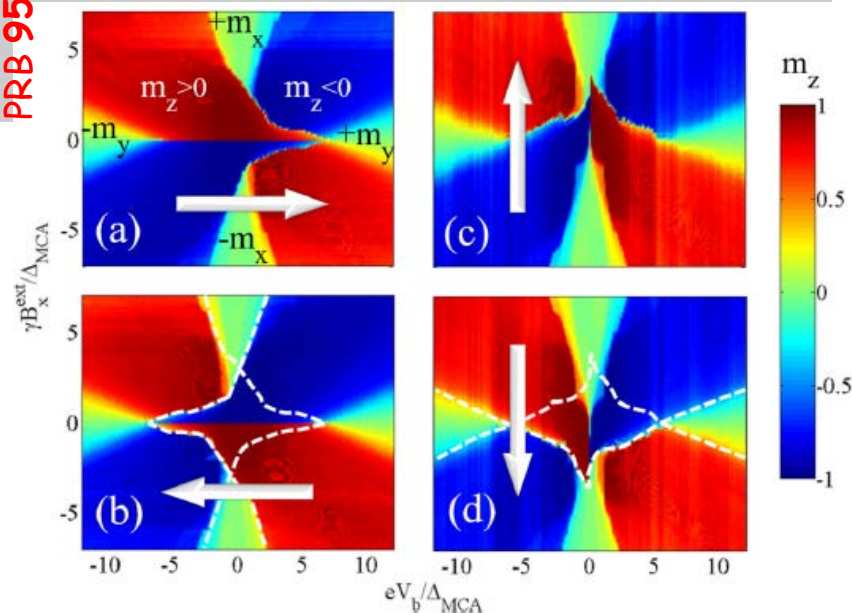
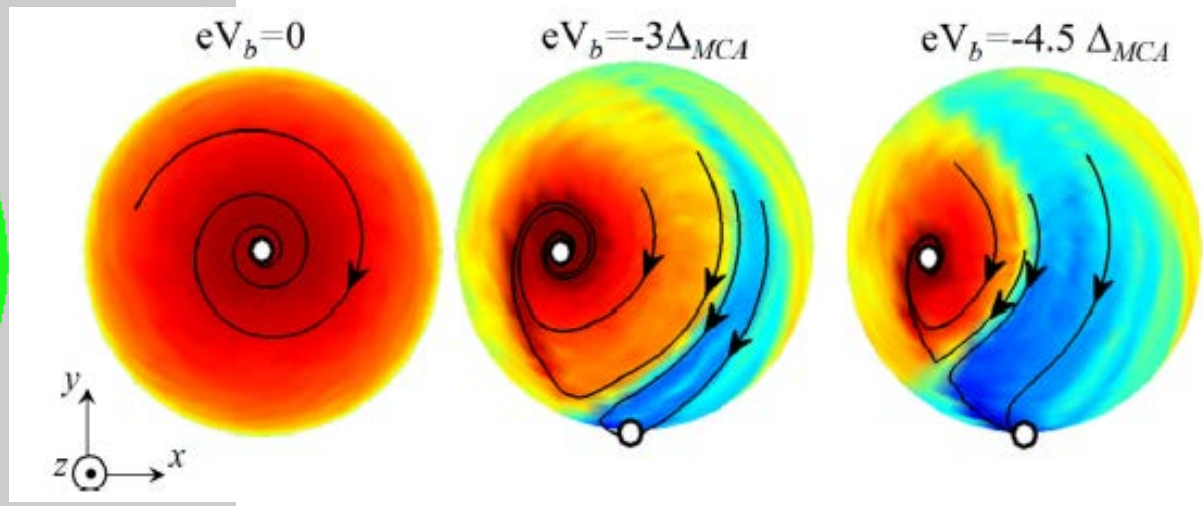
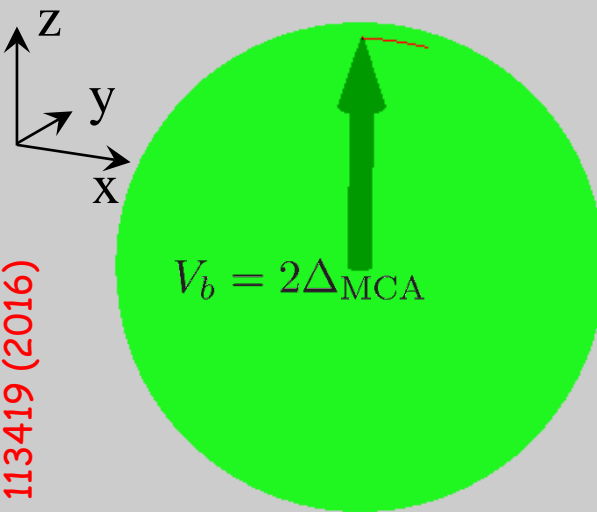
PRB 95, 113419 (2016)



PRB 89, 195418 (2014)



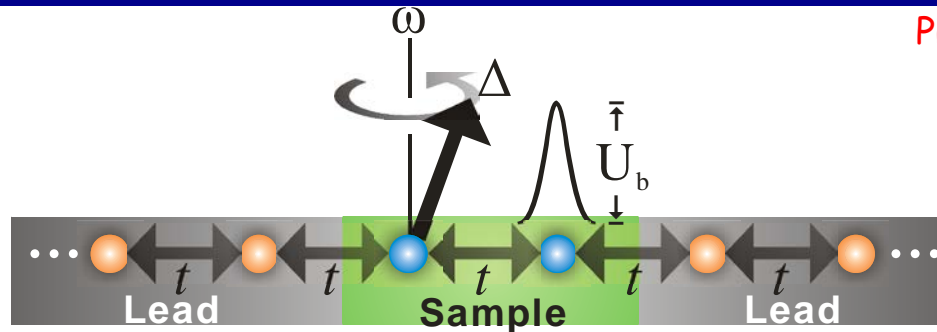
# LLG Simulations of Magnetization Reversal and Switching Phase Diagram for TI/FI Bilayer





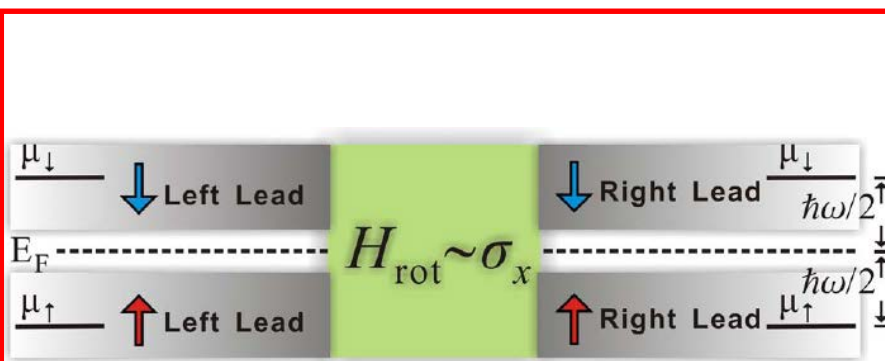
# Exact Rotating Frame Approach to Spin Pumping in the Absence of Spin Flips

PRB 79, 054424 (2009)



$$\hat{H}_{\text{lab}}(t) = \sum_{\mathbf{r}, \sigma, \sigma'} \left( \varepsilon_{\mathbf{r}} \delta_{\sigma\sigma'} - \frac{\Delta_{\mathbf{r}}}{2} \mathbf{m}_{\mathbf{r}}(t) \cdot \hat{\boldsymbol{\sigma}}^{\sigma\sigma'} \right) \hat{c}_{\mathbf{r}\sigma}^{\dagger} \hat{c}_{\mathbf{r}\sigma'} - \gamma \sum_{\langle \mathbf{r}\mathbf{r}' \rangle \sigma} \hat{c}_{\mathbf{r}\sigma}^{\dagger} \hat{c}_{\mathbf{r}'\sigma}$$

$$\hat{H}_{\text{rot}} = \hat{U} \hat{H}_{\text{lab}}(t) \hat{U}^{\dagger} - i\hbar \hat{U} \frac{\partial}{\partial t} \hat{U}^{\dagger} = \hat{H}_{\text{lab}}(0) - \frac{\hbar\omega}{2} \hat{\sigma}_z$$



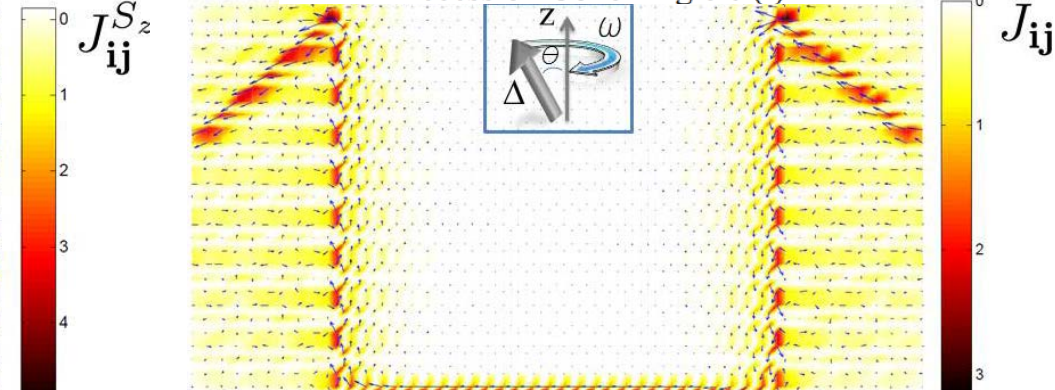
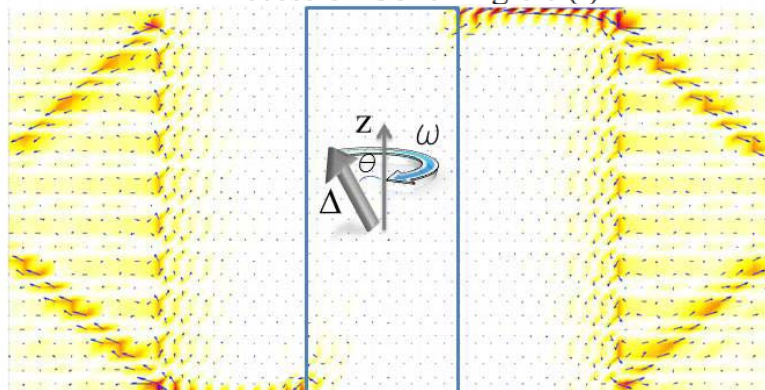
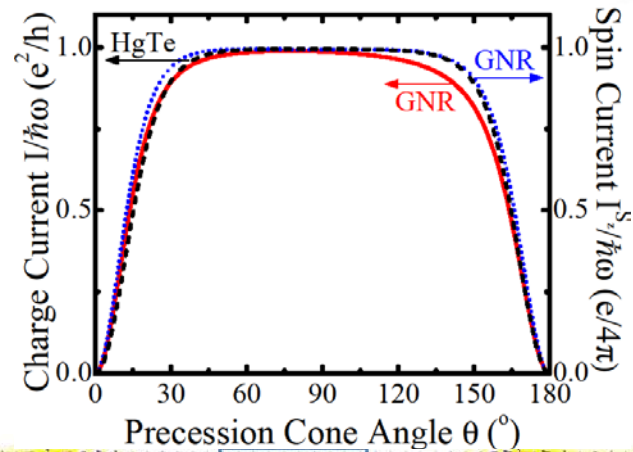
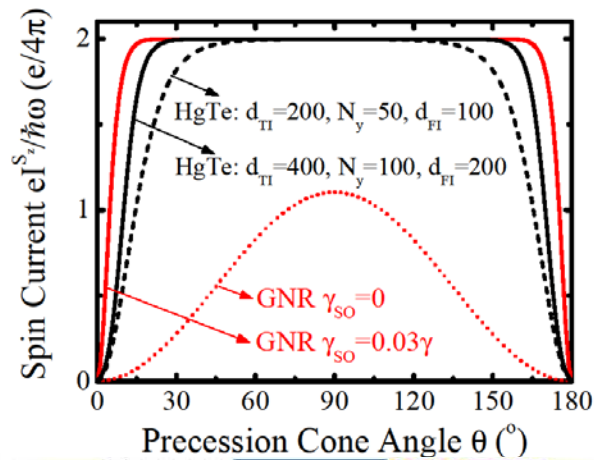
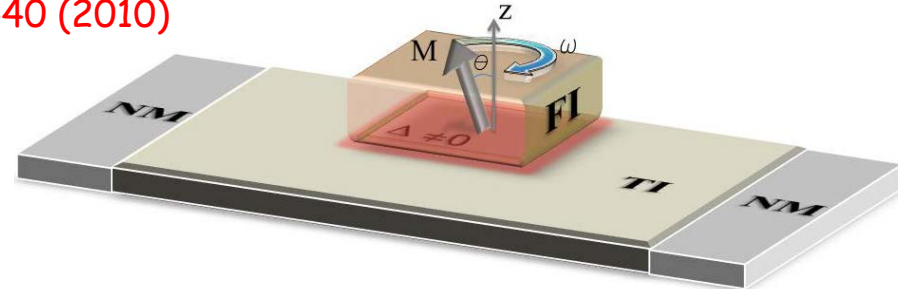
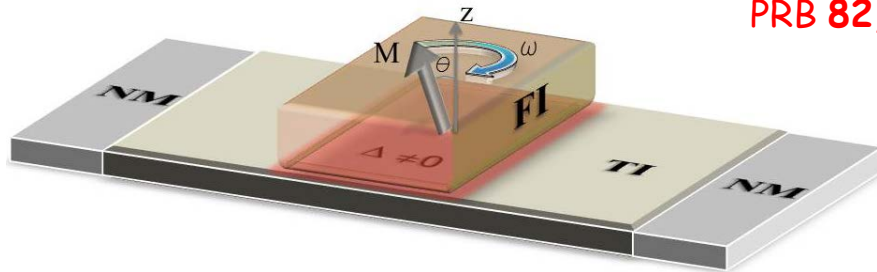
$$I_L^S = \frac{e\omega}{2\pi} \int_{\text{BZ}} d\mathbf{k}_{\parallel} (T_{LR}^{\uparrow\downarrow} + T_{RL}^{\uparrow\downarrow} + 2T_{LL}^{\uparrow\downarrow})$$

$$I = \frac{e\omega}{2\pi} \int_{\text{BZ}} d\mathbf{k}_{\parallel} (T_{RL}^{\uparrow\downarrow} - T_{LR}^{\uparrow\downarrow})$$

$$V_{\text{pump}} = IG(\theta)^{-1}$$

# Quantized Spin and Charge Pumping Due to Spin-Momentum Locking in 2D TIs

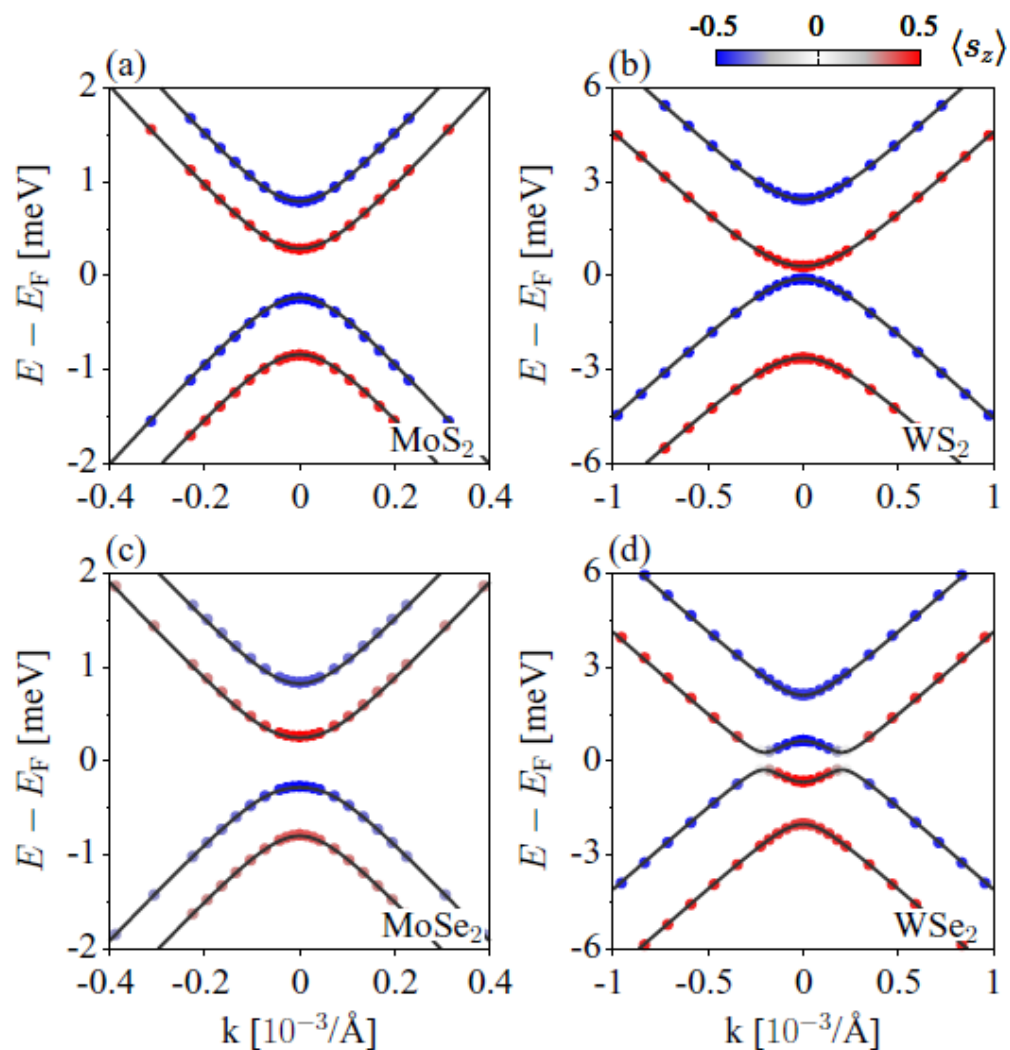
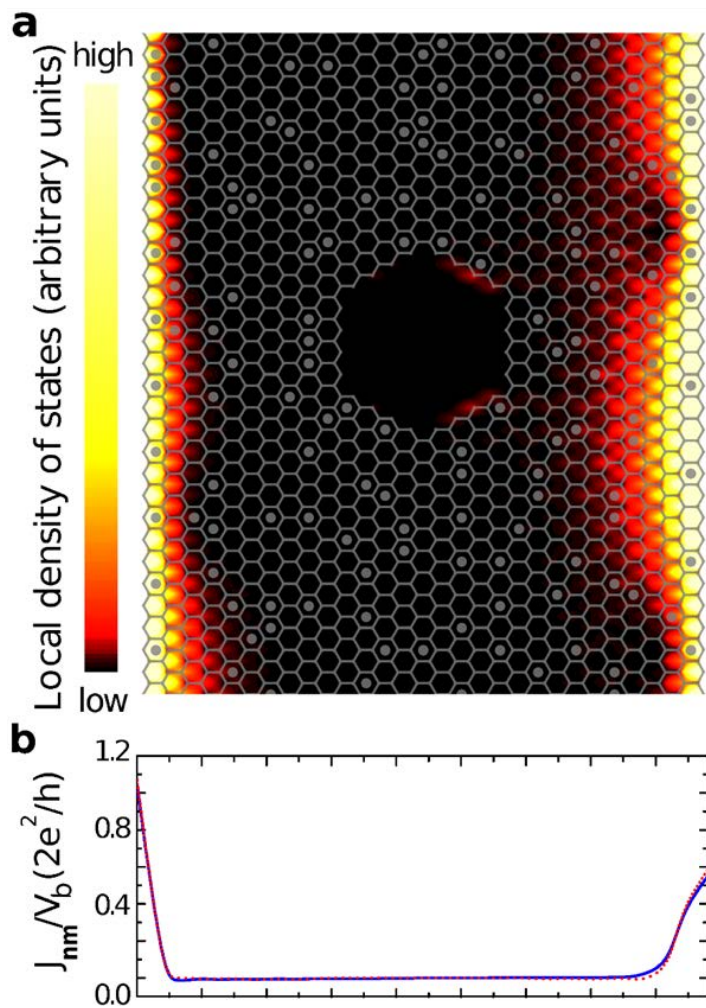
PRB **82**, 195440 (2010)



# How to Create 2D TI with Exposed Surface

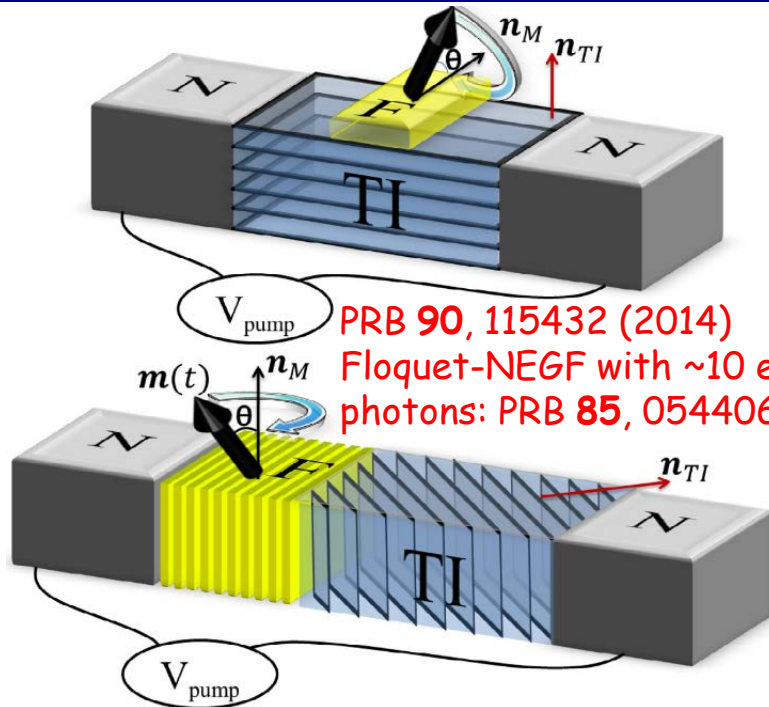
Nano Lett. 14, 3779 (2014)

PRB 93, 155104 (2016)



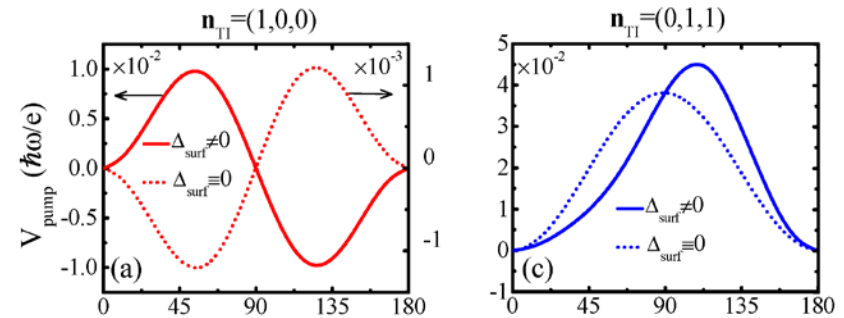
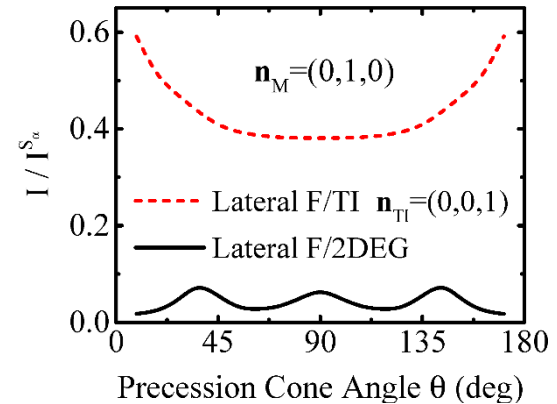


# Spin Pumping-to-Charge Conversion in TI/FM Heterostructures

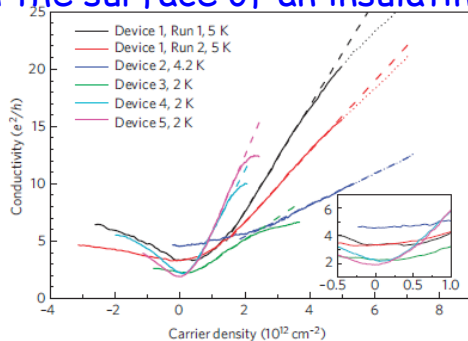


PRB 90, 115432 (2014)

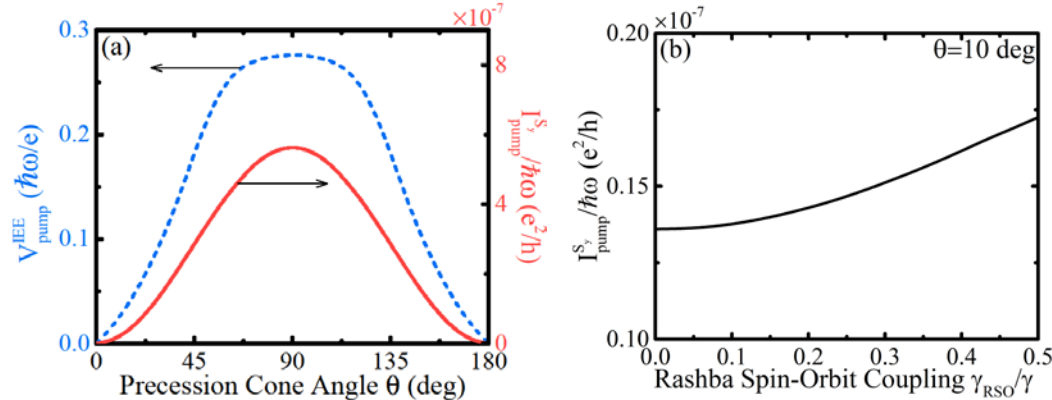
Floquet-NEGF with  $\sim 10$  exchanged photons: PRB 85, 054406 (2012)



Ambipolar electronic transport on the surface of an insulating bulk



Nano Lett. 15, 7126 (2015)

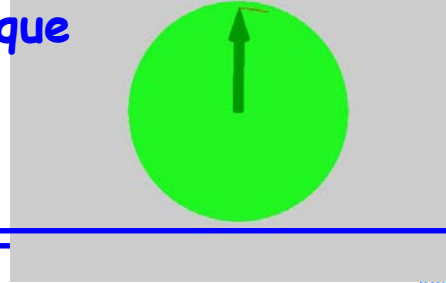
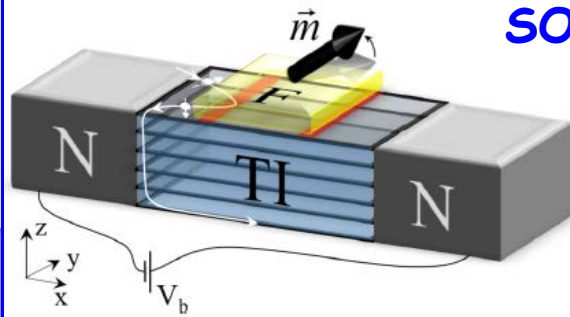


Topological proximity effect



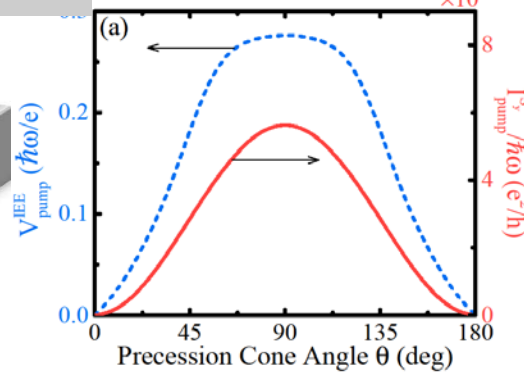
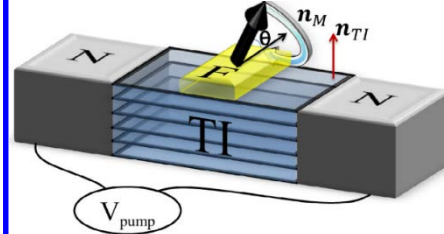
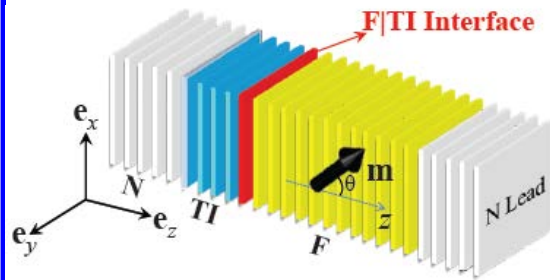
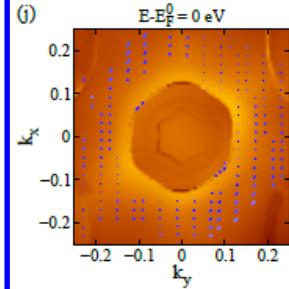
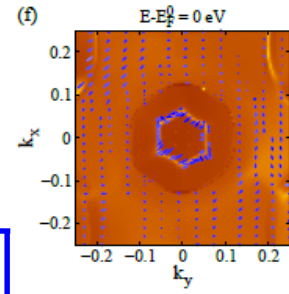
# Conclusions and Open Questions in Pictures

## SO torque



## Open questions:

- computationally efficient *ab initio* calculations of SOT in arbitrary geometry



## Spin-to-charge conversion

