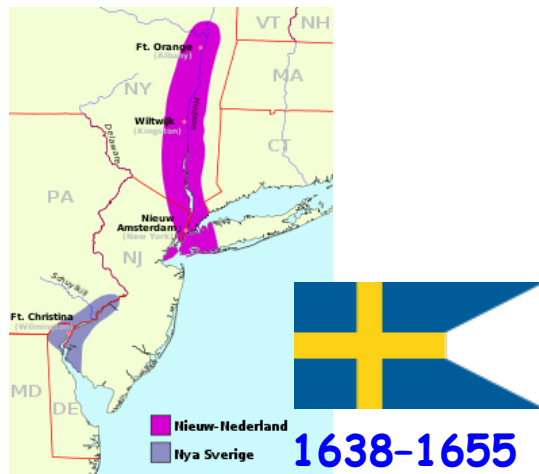


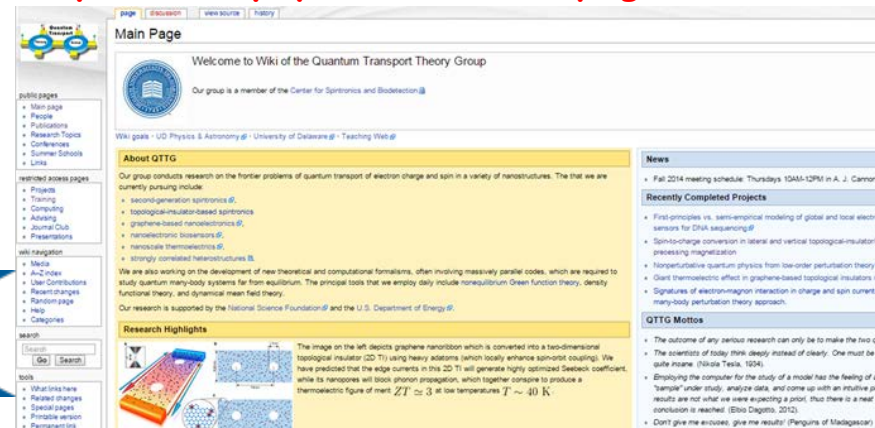
# Anatomy of Spin-Orbit Torques in Topological-Insulator/Ferromagnet Heterostructures

Branislav K. Nikolić

Department of Physics & Astronomy, University of Delaware, Newark, DE 19716, U.S.A.  
RIKEN Center for Emergent Matter Science, ASI, RIKEN, Wako 351-0198, Japan

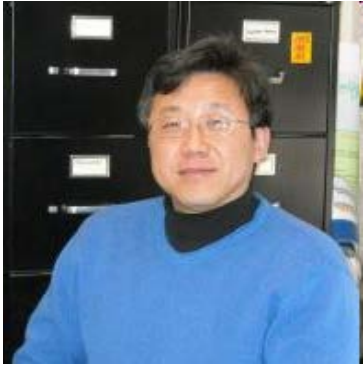


<https://wiki.physics.udel.edu/qttg>



# Collaborators

## Experiment



Prof. J. Q. Xiao



Prof. J.-P. Wang

## Theory



Dr. Farzad Mahfouzi

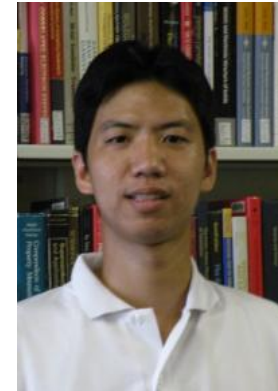


Prof. N. Nagaosa



Prof. Nicholas Kioussis

## Computation



Dr. Po-Hao Chang



J. M. Marmolejo-Tejada



Dr. Kurt Stokbro

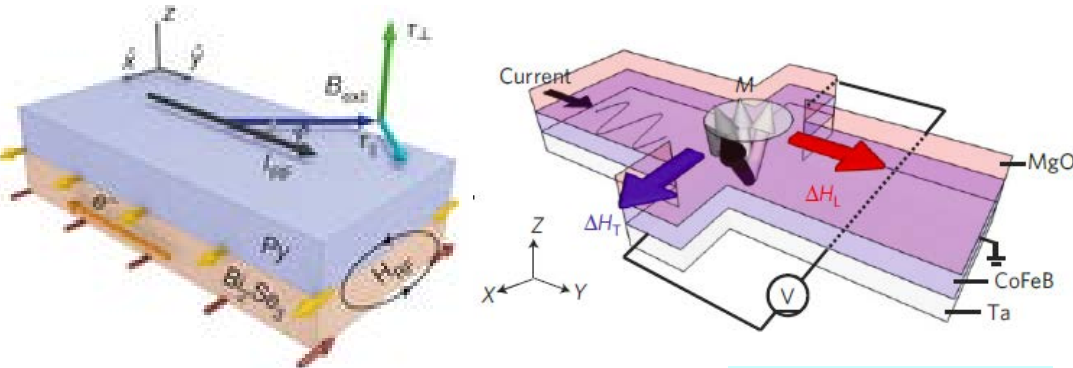
# Experiments on SO Torque and Spin-to-Charge Conversion in Lateral TI/F Heterostructures

Ralph Lab, Nature **511**, 449 (2014)

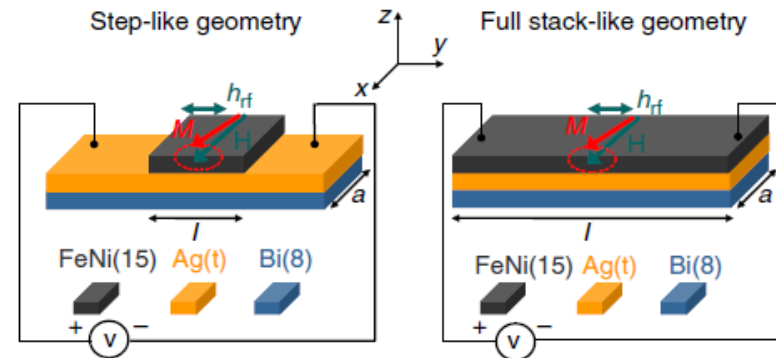
**Table 1 | Comparison of room-temperature  $\sigma_{s,\parallel}$  and  $\theta_{s,\parallel}$  for  $\text{Bi}_2\text{Se}_3$  with other materials**

Parameter	$\text{Bi}_2\text{Se}_3$ (this work)	Pt (ref. 4)	$\beta$ -Ta (ref. 6)	Cu(Bi) (ref. 23)	$\beta$ -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

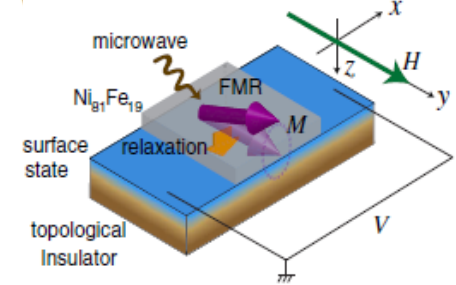
$\theta_{\parallel}$  is dimensionless and the units for  $\sigma_{S,\parallel}$  are  $10^5 \hbar / 2e \Omega^{-1} \text{m}^{-1}$ .



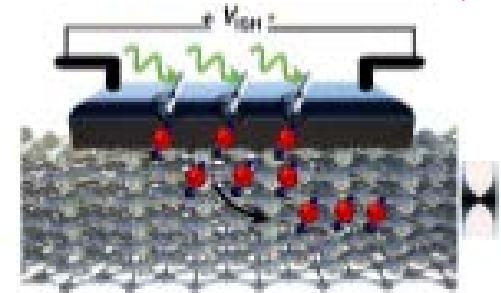
Fert & Vila, Nature Comm. **4**, 2944 (2013)



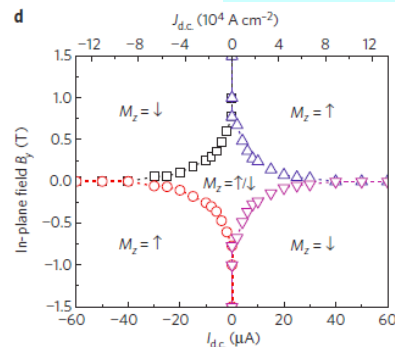
Saitoh Lab, PRL **113**, 196601 (2014)



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



Wang Lab, Nature Mater. **13**, 699 (2014):  $\theta_{\parallel} \approx 150 - 425$



Yang Lab, PRL **114**, 257202 (2015):  $\theta_{\parallel} \approx 0.047 \rightarrow 0.42$

# Current-Driven Nonequilibrium Spin Density on the TI Surface as a Resource for Spintronics

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

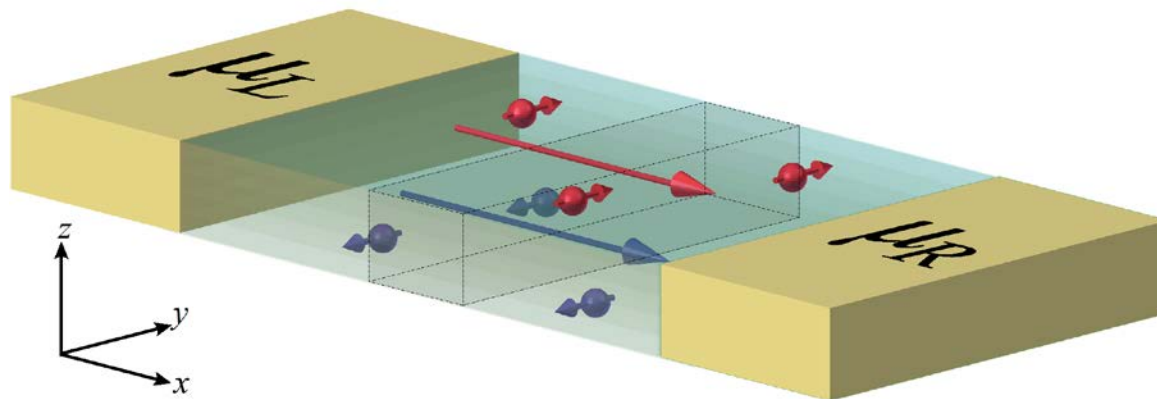
V.M. Edelstein

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

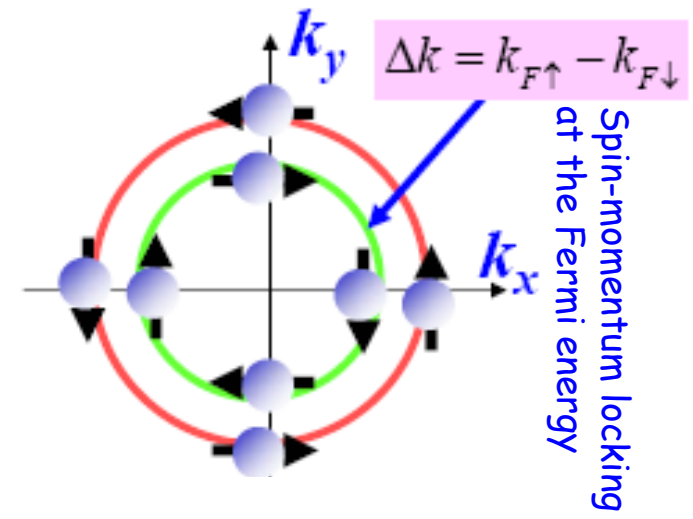
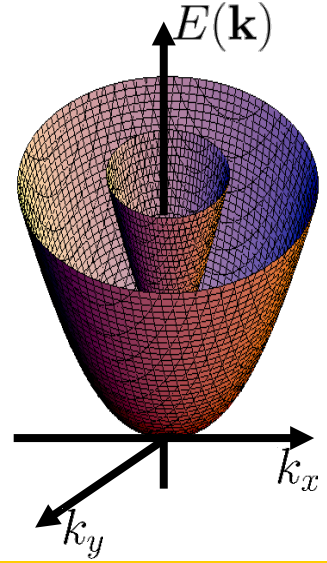
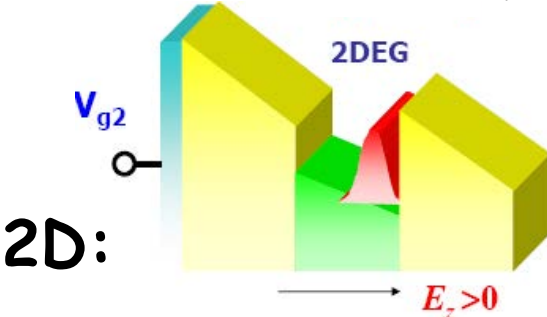
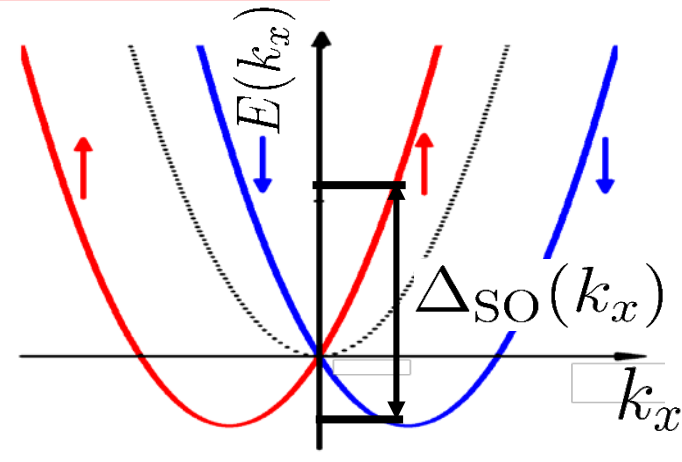
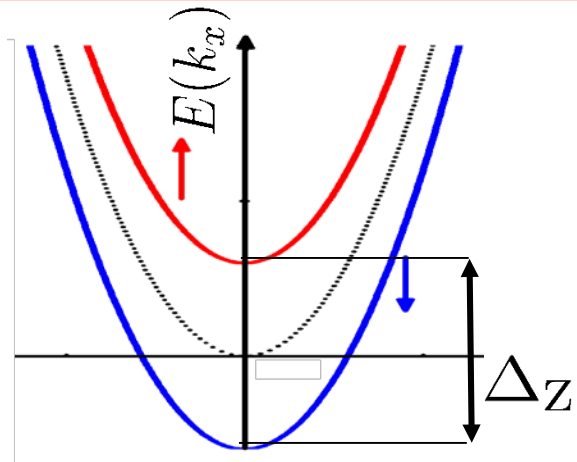
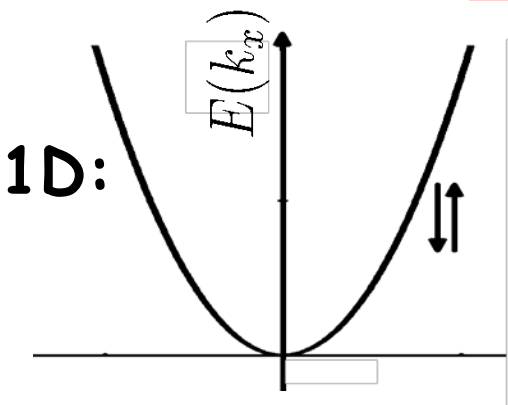
$$S_y = \beta E_x$$



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

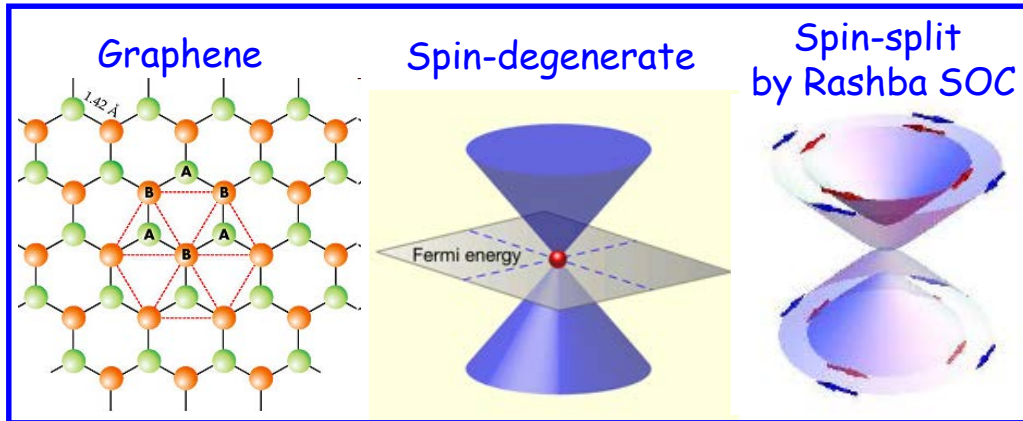
# Rashba SO Splitting of Energy Bands

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

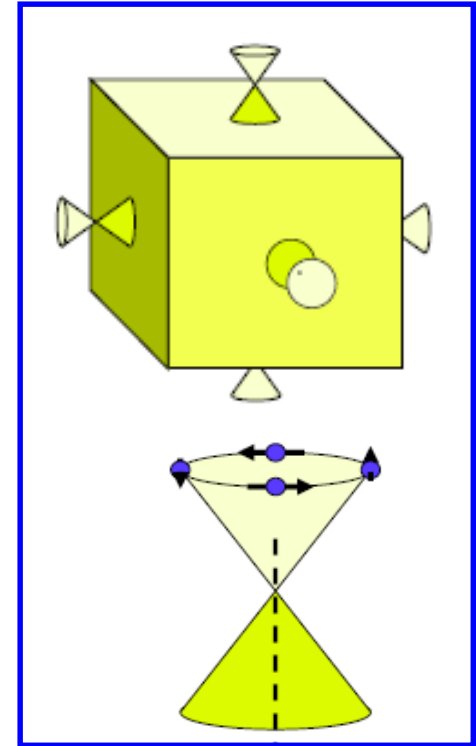


$$\begin{aligned} \varepsilon(\mathbf{k}, \uparrow) &= \varepsilon(-\mathbf{k}, \downarrow) \\ \varepsilon(\mathbf{k}, \uparrow) &\neq \varepsilon(-\mathbf{k}, \uparrow) \\ \varepsilon(\mathbf{k}, \uparrow) &\neq \varepsilon(\mathbf{k}, \downarrow) \end{aligned}$$

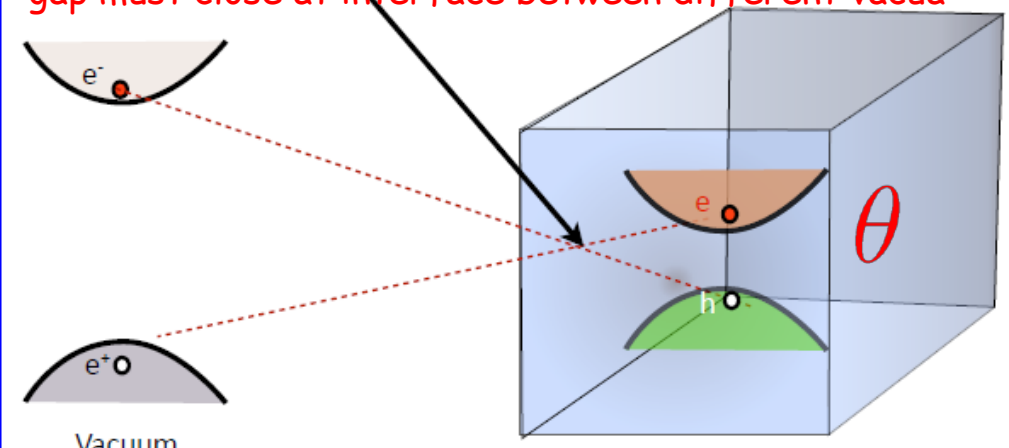
# Crash Course on 3D TIs



vs.



TIs are adiabatically disconnected from vacuum, so the gap must close at interface between different vacua

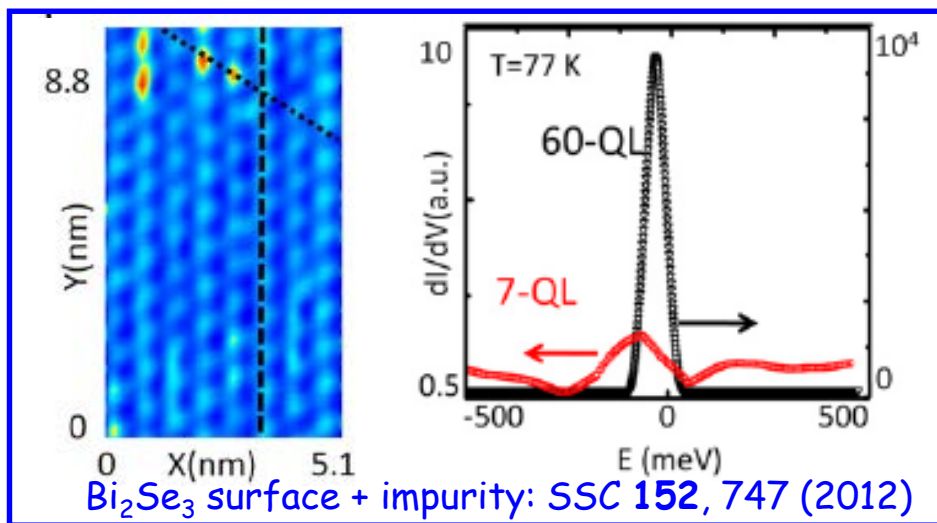
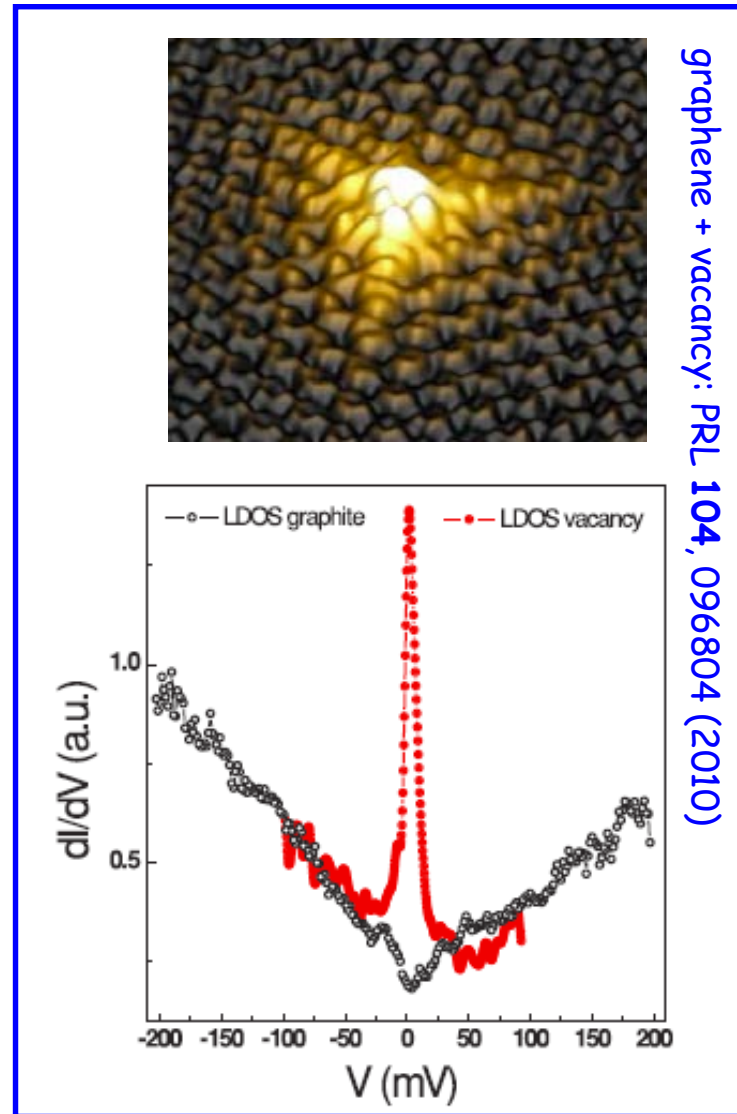
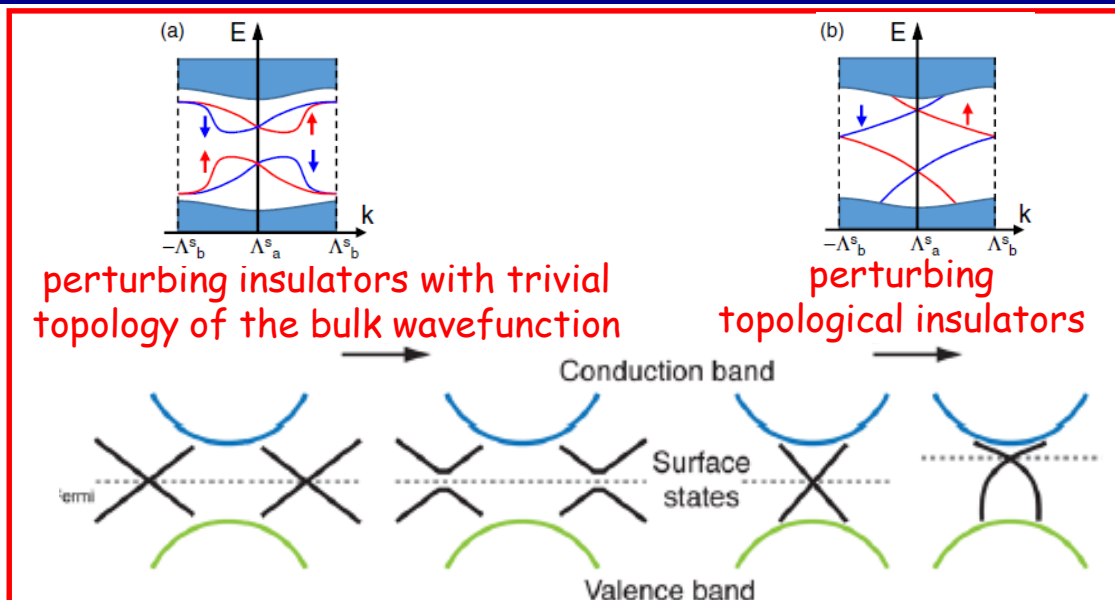


$$\theta = \frac{1}{4\pi} \int_{\text{BZ}} d^3k \epsilon^{ijk} \text{Tr} \left[ \mathcal{A}_i \partial_j \mathcal{A}_k - i \frac{2}{3} \mathcal{A}_i \mathcal{A}_j \mathcal{A}_k \right] = \pi$$

$$\underbrace{\frac{1}{4\pi} \int \kappa dA}_{\text{differential geometry}} = \underbrace{\frac{\Omega}{4\pi}}_{\text{topology}} = (1 - g)$$

g=0, Ω=4π      g=1, Ω=0      g=2, Ω=-4π      g=3, Ω=-8π

# Physical Meaning of Topological Protection



# Crash Course on Spin-Transfer Torque

Learn more about STT from:

Journal of Magnetism and Magnetic Materials 320 (2008) 1190–1216

Current Perspectives

Spin transfer torques

D.C. Ralph<sup>a,\*</sup>, M.D. Stiles<sup>b</sup>

REVIEW ARTICLES | INSIGHT

PUBLISHED ONLINE: 23 APRIL 2012 | DOI: 10.1038/NMAT3311

nature  
materials

Current-induced torques in magnetic materials

Arne Brataas<sup>†</sup>, Andrew D. Kent<sup>‡</sup> and Hideo Ohno<sup>§,4</sup>

nature  
materials

PROGRESS ARTICLE

PUBLISHED ONLINE: 17 DECEMBER 2013 | DOI: 10.1038/NMAT3823

Spin-torque building blocks

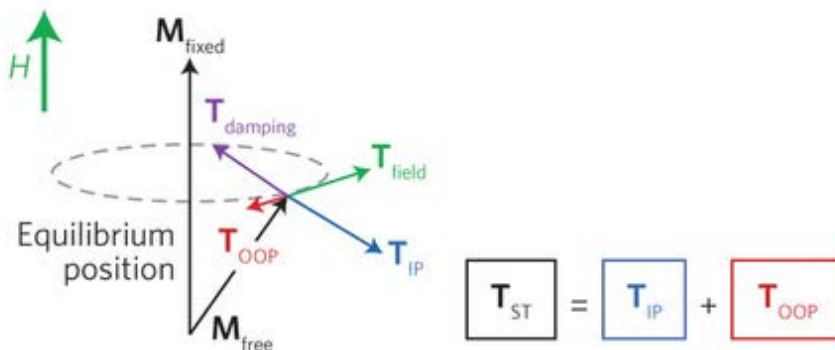
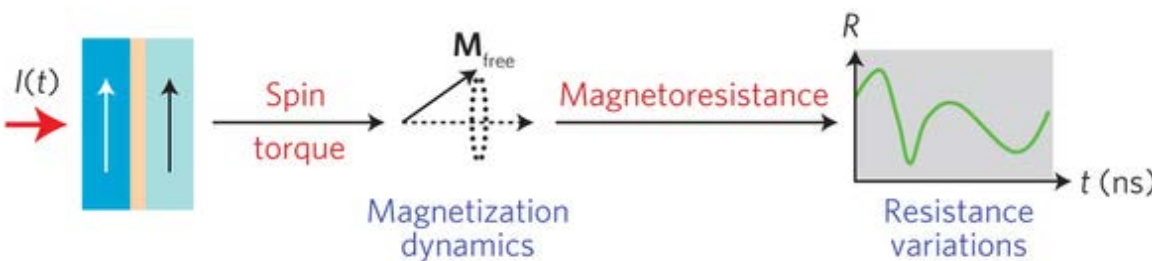
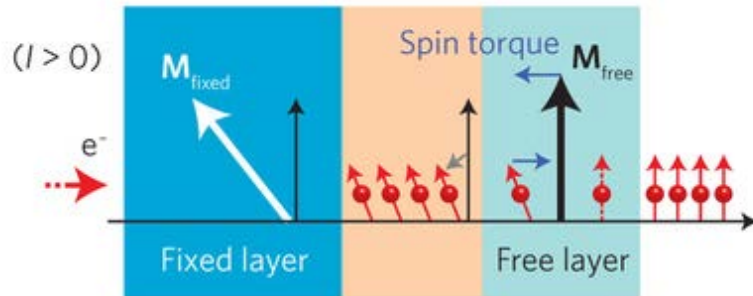
N. Locatelli, V. Cros and J. Grollier<sup>\*</sup>

SPIN  
Vol. 3, No. 2 (2013) 1330002 (17 pages)  
© World Scientific Publishing Company  
DOI: 10.1142/S2010324713300028

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www.worldscientific.com

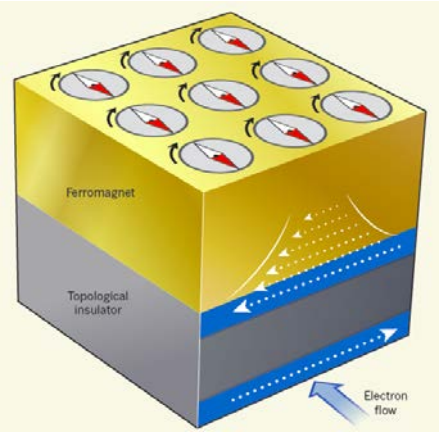
HOW TO CONSTRUCT THE PROPER  
GAUGE-INVARIANT DENSITY MATRIX  
IN STEADY-STATE NONEQUILIBRIUM:  
APPLICATIONS TO SPIN-TRANSFER  
AND SPIN-ORBIT TORQUES

FARZAD MAHFOUZI and BRANISLAV K. NIKOLIĆ<sup>\*</sup>





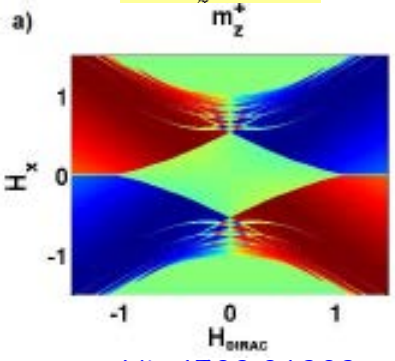
# What Can Theory Do for Topological Spintronics: Understand, Control and Design Antidamping SOT



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

Berry curvature antidamping torque

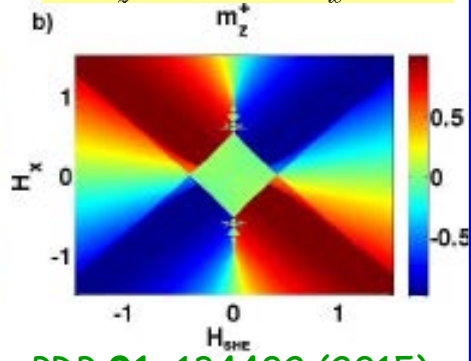
$$\propto m_z \mathbf{m} \times \hat{x} / m_z^+$$



arXiv:1509.06929

SHE antidamping torque

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



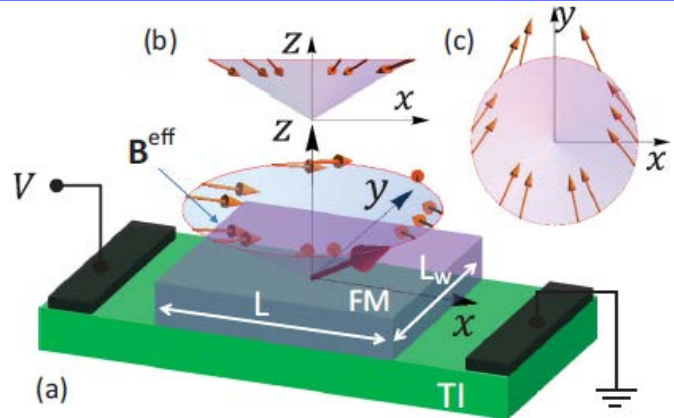
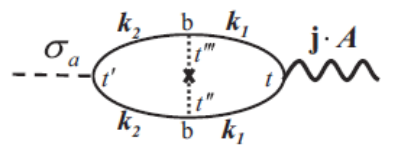
PRB **91**, 134402 (2015)

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

spin-dependent scattering  
PRB **86**, 014416 (2012)

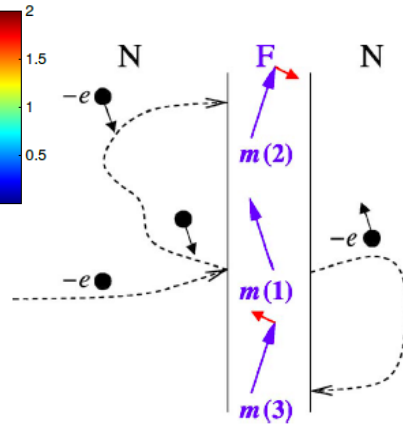
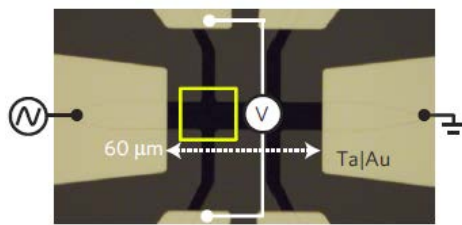
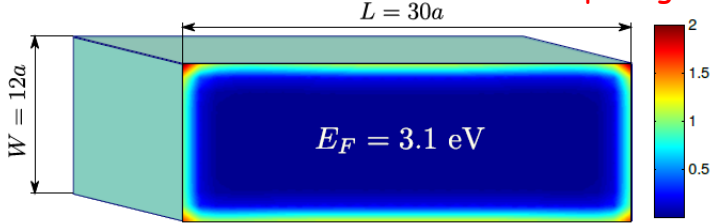
$$\hat{U}_{\text{dis}} = \sum_i \delta(\mathbf{r} - \mathbf{r}_i) (u_{\downarrow} P_{+}^0 + u_{\uparrow} P_{-}^0)$$

vertex corrections  
PRB **92**, 014402 (2015)



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

MISSING INGREDIENTS: 3D transport geometry and N/TI contact



PRL **92**, 026602 (2004)

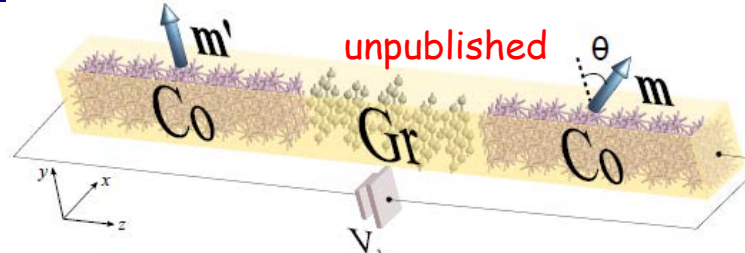
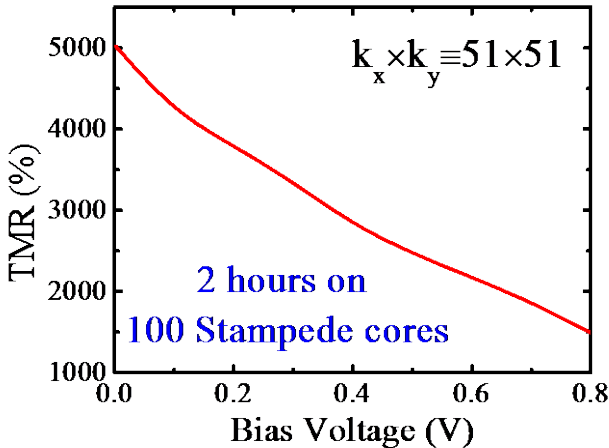
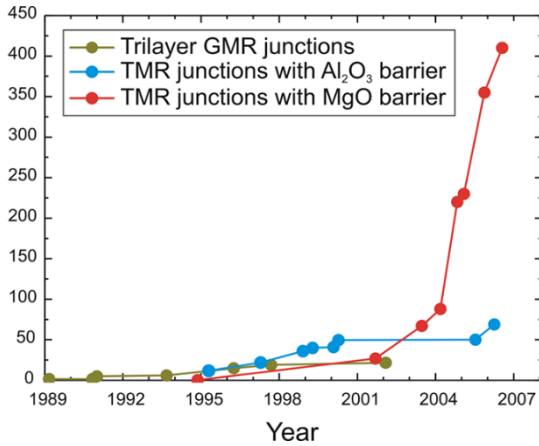
# What Can Computation Do for Topological Spintronics: Find Optimal Materials Combinations

PHYSICAL REVIEW B, VOLUME 63, 054416

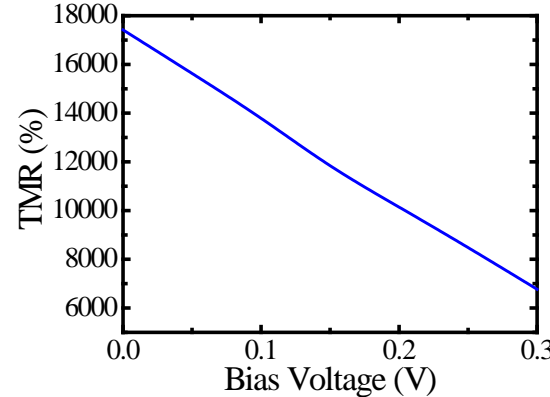
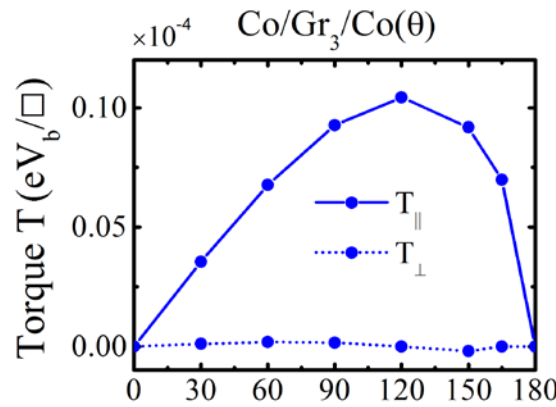
Spin-dependent tunneling conductance of Fe|MgO|Fe sandwiches

W. H. Butler, X.-G. Zhang, and T. C. Schulthess  
Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6114

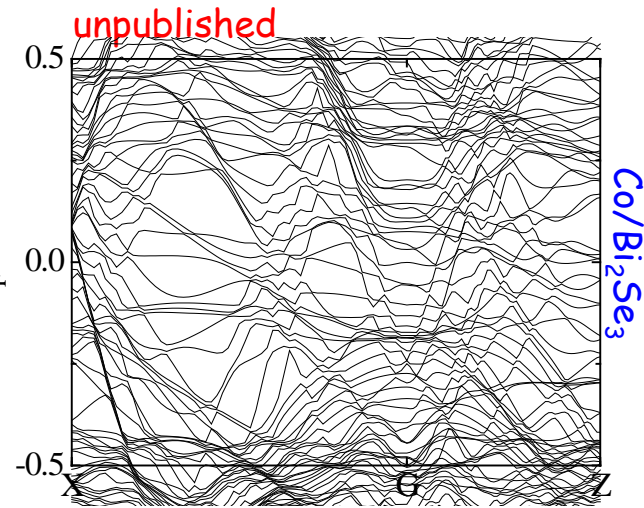
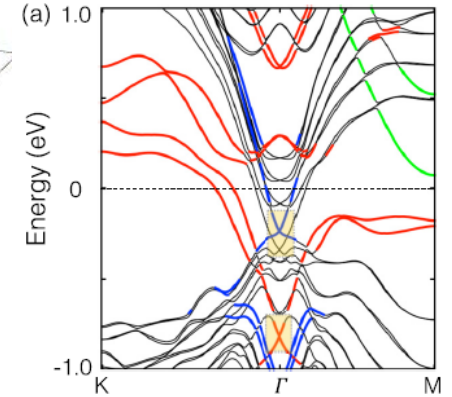
J. M. MacLaren  
Department of Physics, Tulane University, New Orleans, Louisiana 70018



STT-MRAM cell with high TMR and low RA



PRB 90, 115103 (2014)



# Spin Density and STT from NEGF Formalism

## □ Fundamental quantities of NEGF formalism:

density of available quantum states:

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

how are those states occupied:

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

## □ NEGF for steady-state transport:

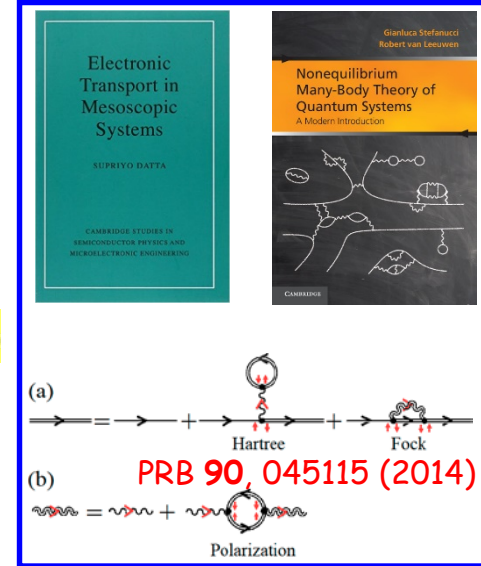
$$G^r(t, t') \rightarrow G^r(t - t') \xrightarrow{\text{FT}} G^r(E)$$

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

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

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

Learn more about NEGF from:



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

SPIN 3, 1330002 (2013)

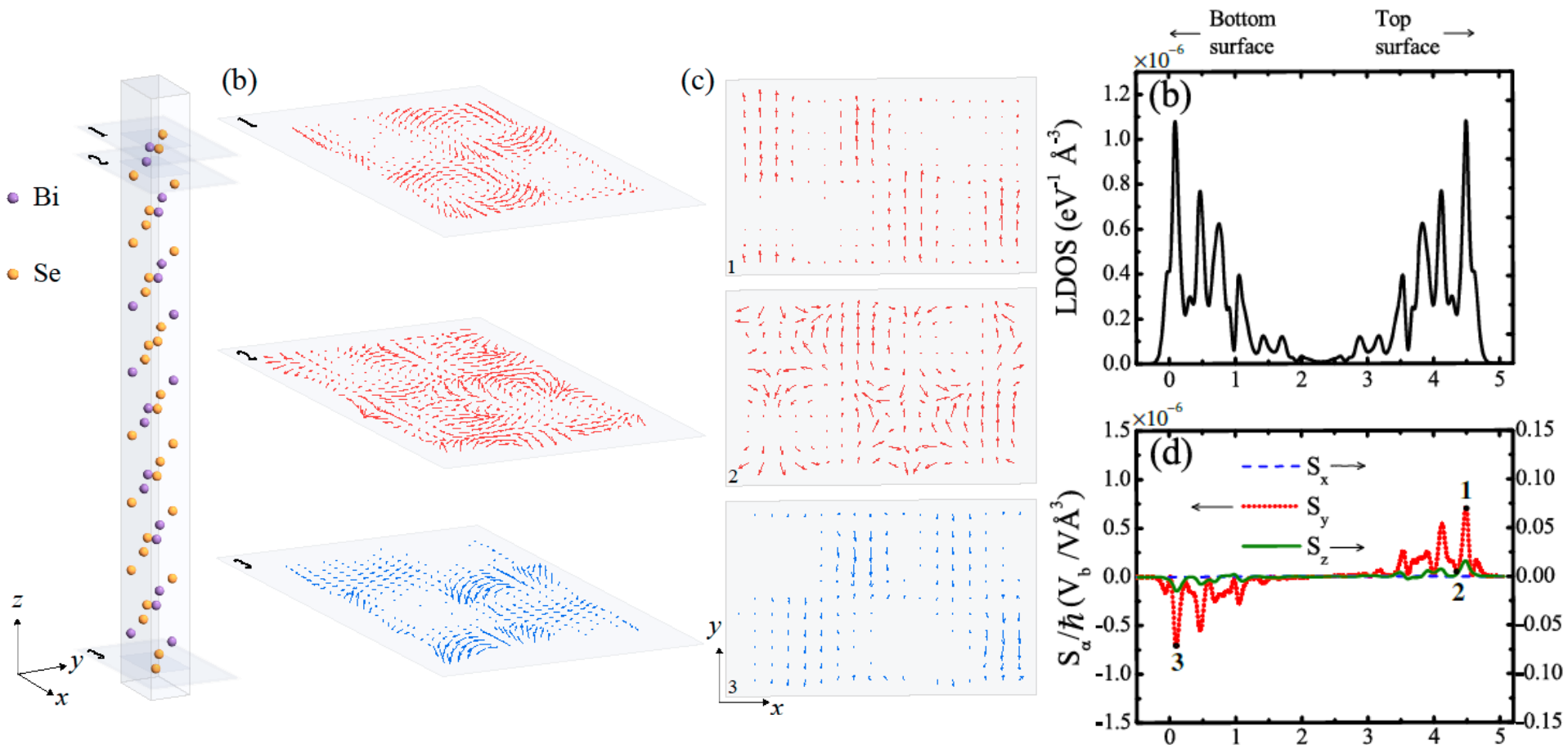
$$\hat{H} = -\frac{\hbar^2 \nabla^2}{2m} + V_H(\mathbf{r}) + V_{\text{XC}}(\mathbf{r}) + V_{\text{ext}}(\mathbf{r}) - \boldsymbol{\sigma} \cdot \mathbf{B}_{\text{XC}}(\mathbf{r}) \Rightarrow \hat{\mathbf{T}} = \frac{d\hat{\mathbf{S}}}{dt} = \frac{1}{2i} [\hat{\boldsymbol{\sigma}}, \hat{H}]$$

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

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)



# Adiabatic Expansion of NEGFs in Derivatives of Slow Magnetization

$$\mathbf{G}(E, t) \simeq \mathbf{G}_t + i(\partial\mathbf{G}_t/\partial E)(\partial\mathbf{U}_t/\partial t)\mathbf{G}_t$$

$$\mathbf{G}^<(t, t) \simeq \int \frac{dE}{2\pi} [\mathbf{G}(E, t) - \mathbf{G}^\dagger(E, t)] f + i \sum_{\alpha=L,R} f' e V_\alpha \mathbf{G}_t \Gamma_\alpha \mathbf{G}_t^\dagger + i f' \mathbf{G}_t \frac{\partial\mathbf{U}_t}{\partial t} \mathbf{G}_t^\dagger$$

$$\rho(t) = \frac{1}{i} \mathbf{G}^<(t, t)$$

$$T^{\alpha\beta}(E) = \text{Tr} \left[ \Gamma_\alpha \mathbf{G}_t \Gamma_\beta \mathbf{G}_t^\dagger \right] \text{charge current}$$

$$T^{\alpha i}(E) = \text{Tr} \left[ \mathbf{1}_m \sigma_i \mathbf{G}_t^\dagger \Gamma_\alpha \mathbf{G}_t \right] \text{spin torque}$$

$$T^{i\alpha}(E) = \text{Tr} \left[ \mathbf{1}_m \sigma_i \mathbf{G}_t \Gamma_\alpha \mathbf{G}_t^\dagger \right] \text{charge pumping}$$

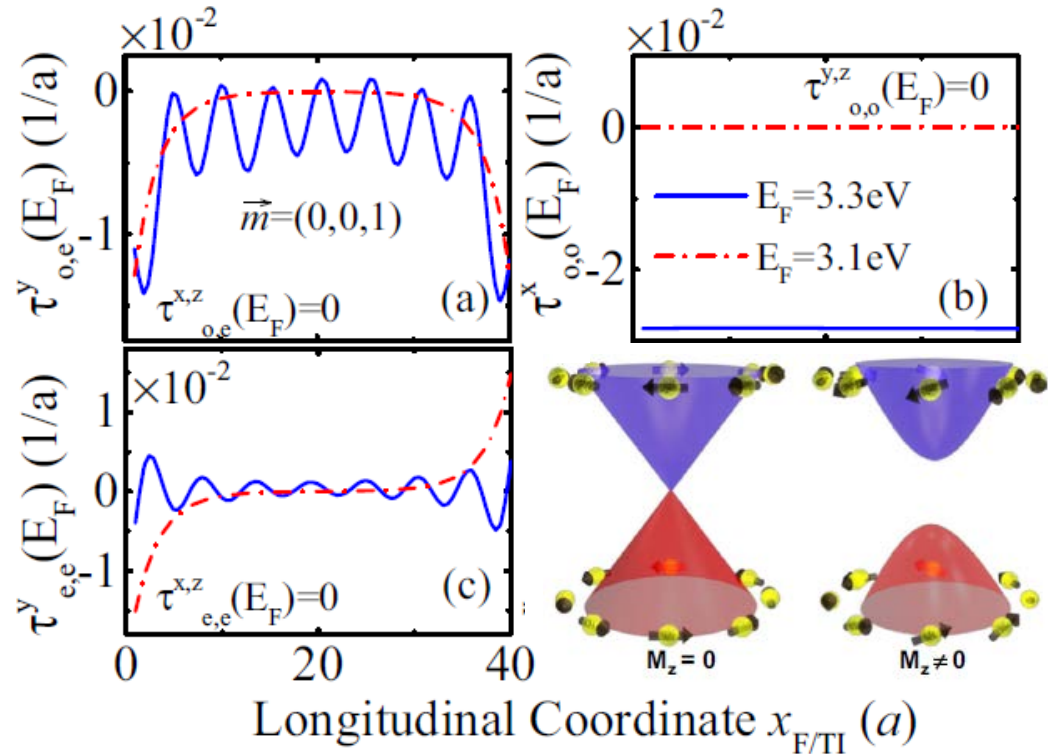
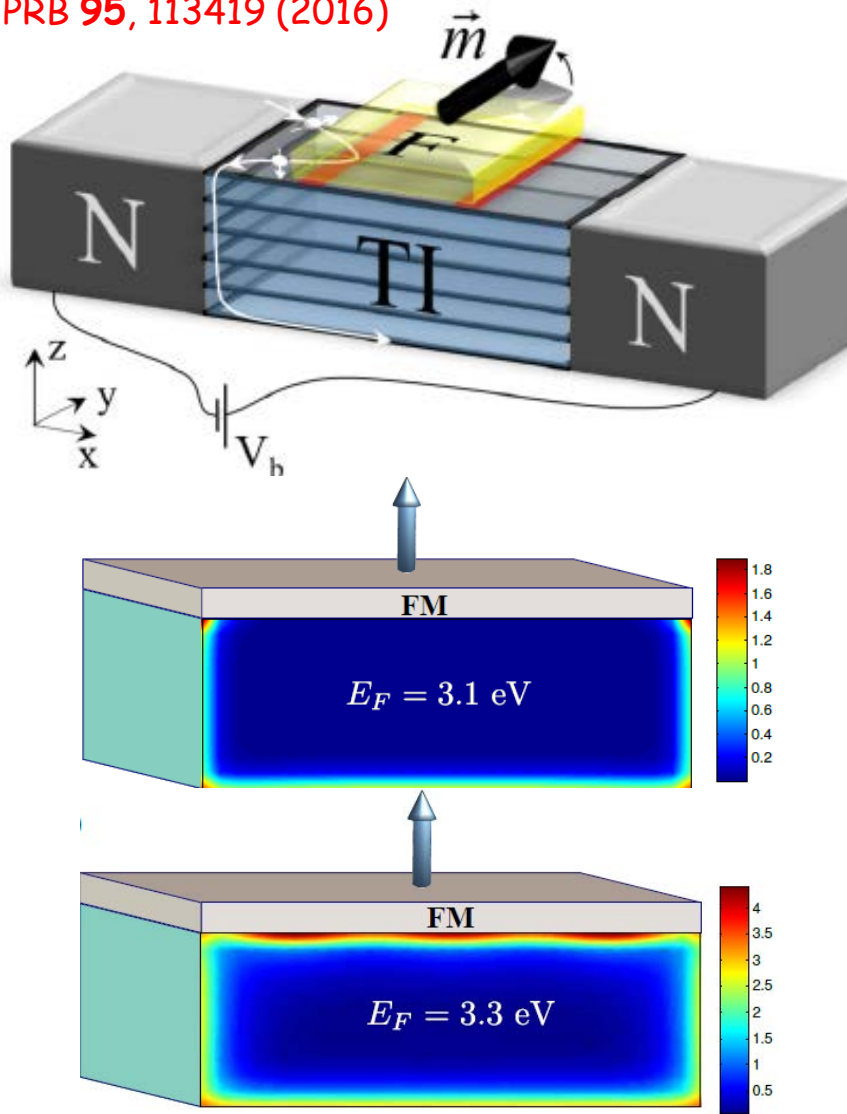
$$T^{ij}(E) = \text{Tr} \left[ \mathbf{1}_m \sigma_i (\mathbf{G}_t^\dagger - \mathbf{G}_t) \mathbf{1}_m \sigma_j (\mathbf{G}_t - \mathbf{G}_t^\dagger) \right] \text{Gilbert damping}$$

$$\rho \begin{cases} \rho_{oo} = \int dE (f_L - f_R) [\mathbf{G} \Gamma_L \mathbf{G}^\dagger - \mathbf{G}^\dagger \Gamma_L \mathbf{G} - \mathbf{G} \Gamma_R \mathbf{G}^\dagger + \mathbf{G}^\dagger \Gamma_R \mathbf{G}] / 8\pi & \text{gives field-like torque} \\ + \\ \rho_{oe} = \int dE (f_L - f_R) [\mathbf{G} \Gamma_L \mathbf{G}^\dagger + \mathbf{G}^\dagger \Gamma_L \mathbf{G} - \mathbf{G} \Gamma_R \mathbf{G}^\dagger - \mathbf{G}^\dagger \Gamma_R \mathbf{G}] / 8\pi & \text{gives antidamping torque} \\ + \\ \rho_{ee} = \int dE (f_L + f_R) [-\text{Im} \mathbf{G}] / 2\pi \\ + \\ \rho_{eo} \equiv 0 \end{cases}$$

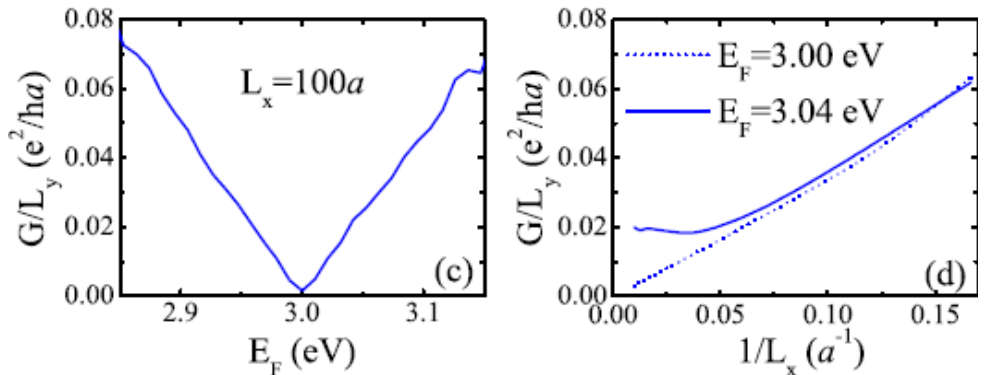
PRB 95, 113419 (2016)

# Spatial Profile of Antidamping SO Torque and the Role of Evanescent Wavefunctions

PRB 95, 113419 (2016)

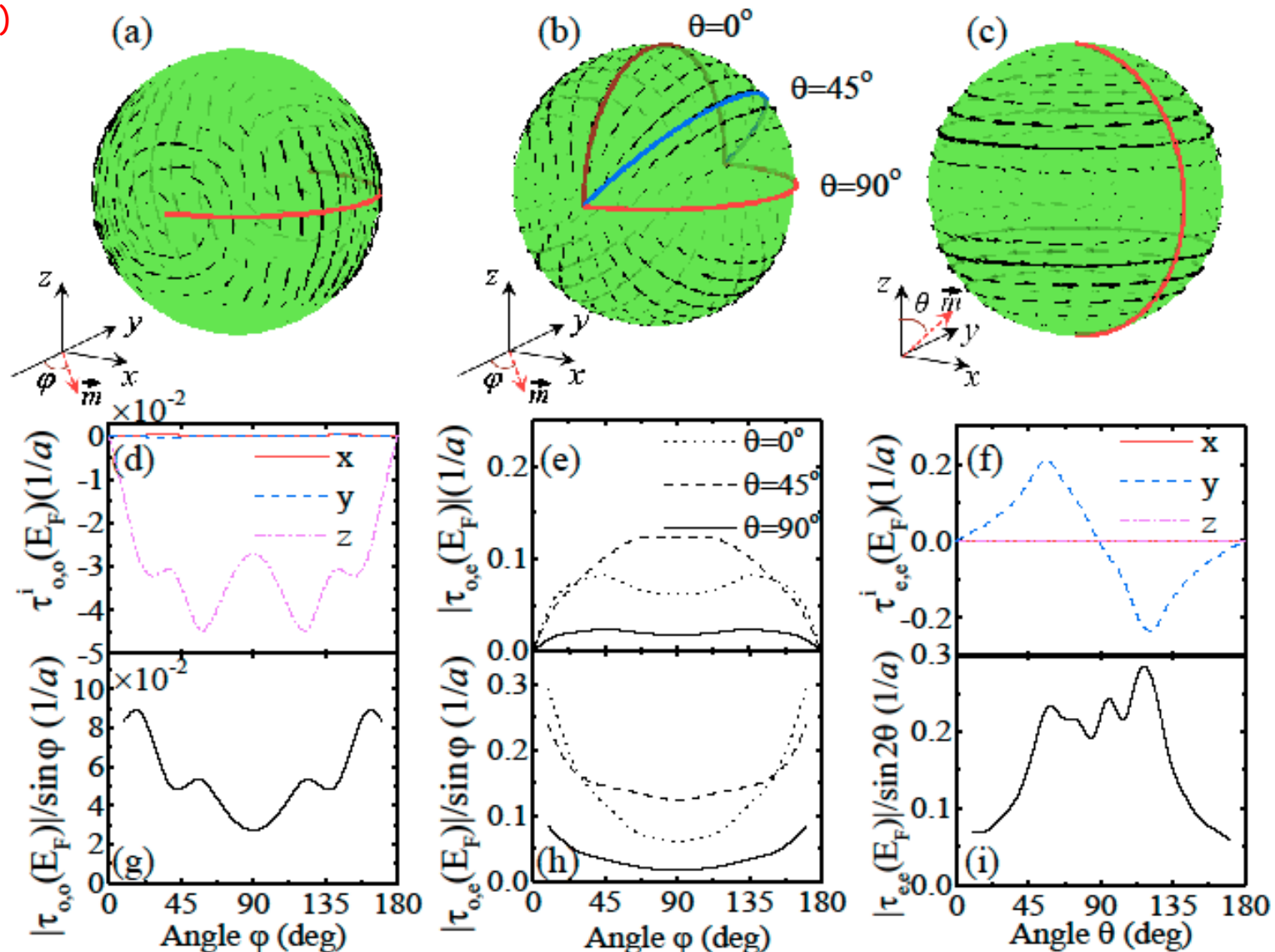


PRB 89, 195418 (2014)

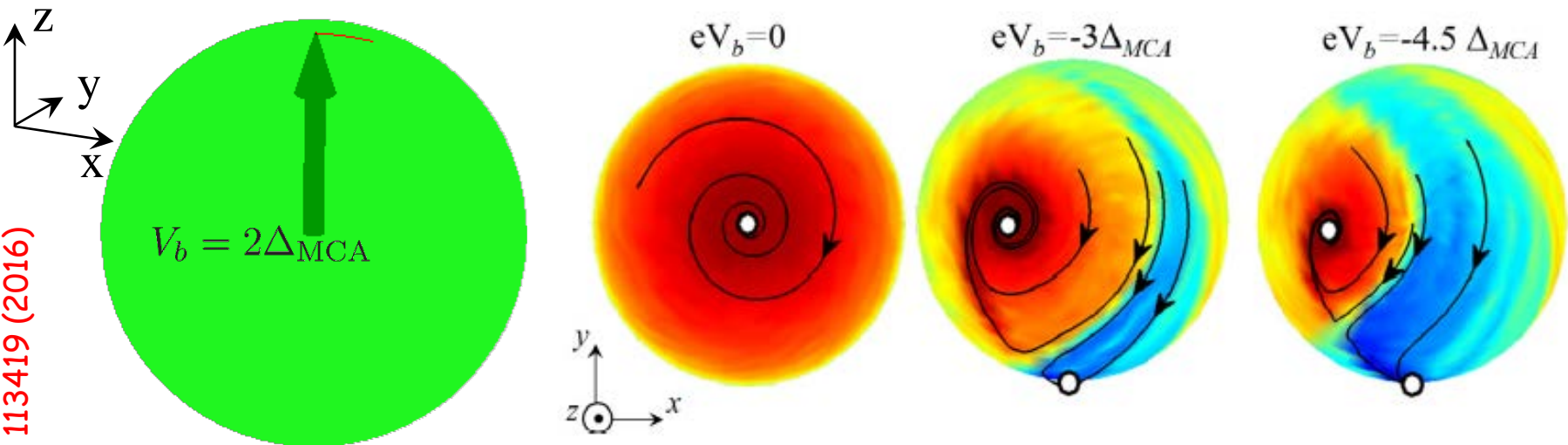


# Angular Dependence of SO Torque in Lateral TI/F Heterostructures

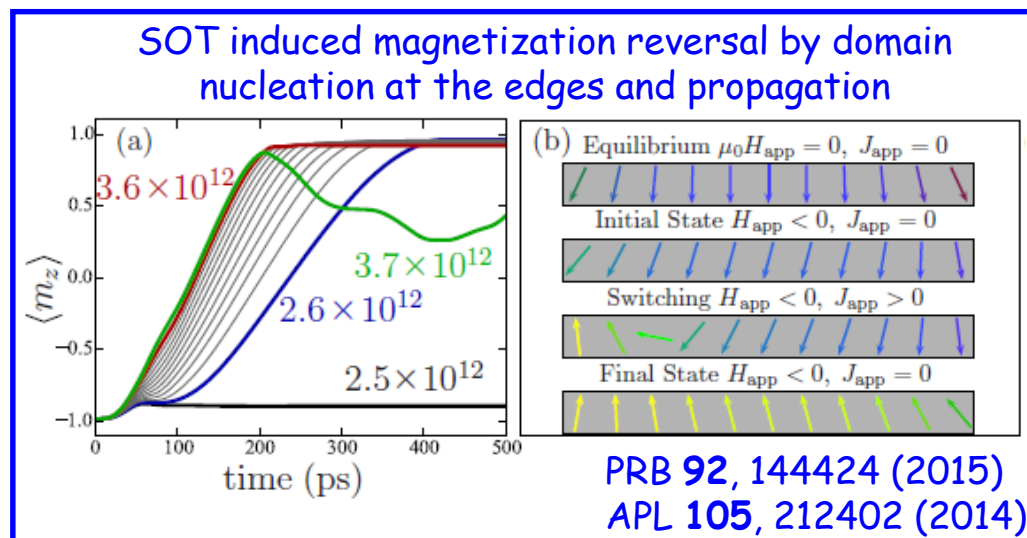
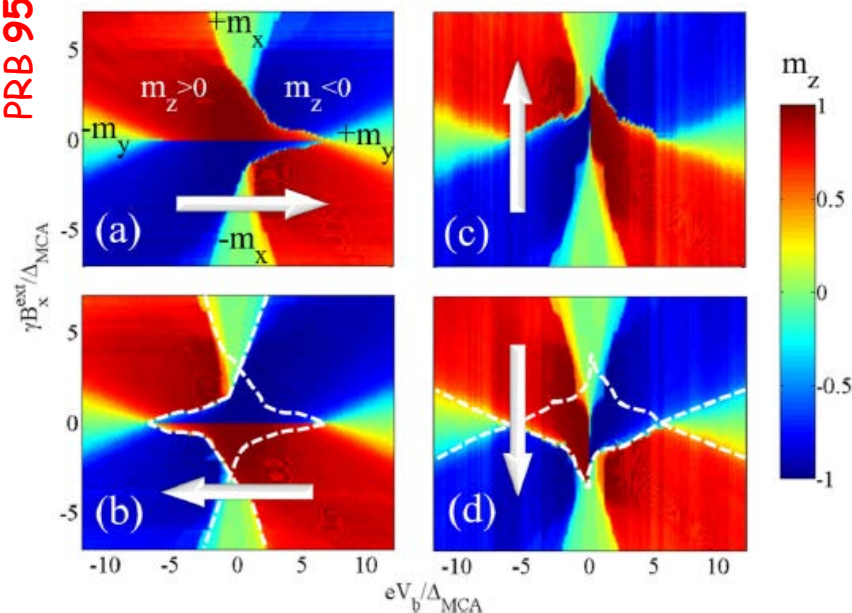
PRB 95, 113419 (2016)



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

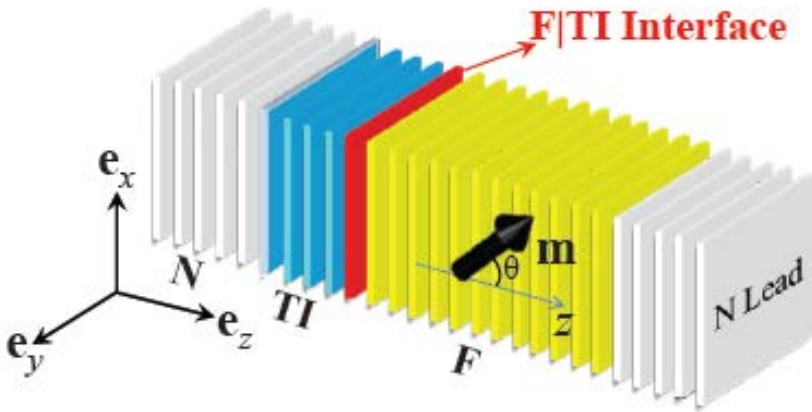


PRB 95, 113419 (2016)

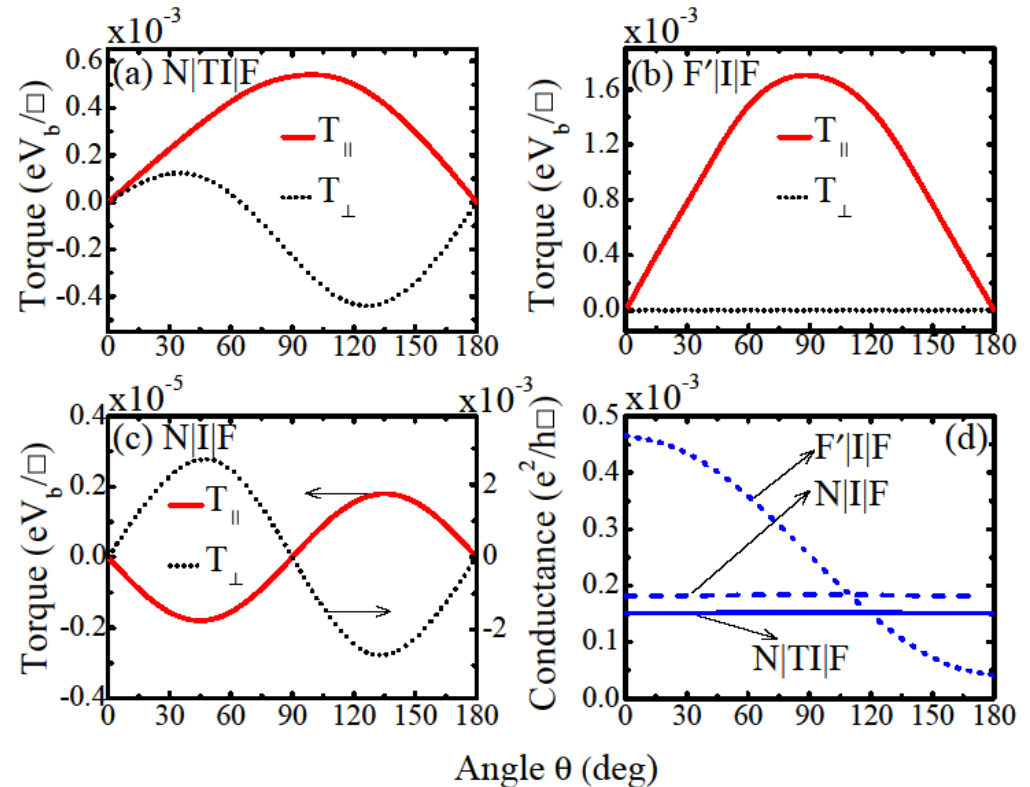
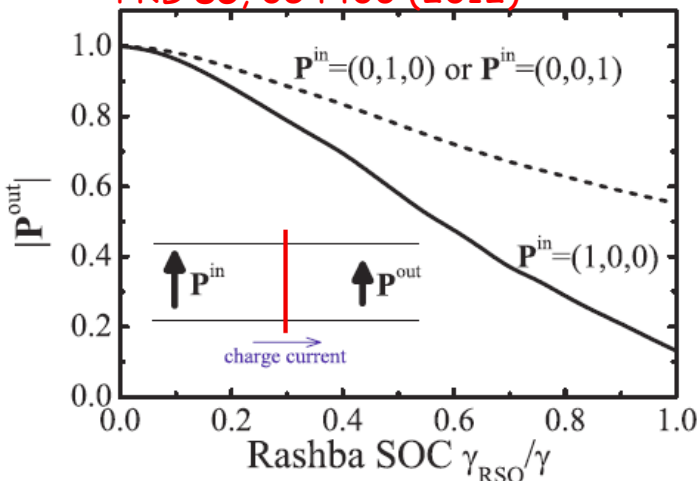




# SO Torque in Vertical TI/F Heterostructures



PRB 85, 054406 (2012)



$$\mathbf{T} = \mathbf{T}_{\parallel} + \mathbf{T}_{\perp} = \tau_{\parallel} \mathbf{m} \times (\mathbf{m} \times \mathbf{e}_z) + \tau_{\perp} \mathbf{m} \times \mathbf{e}_z$$

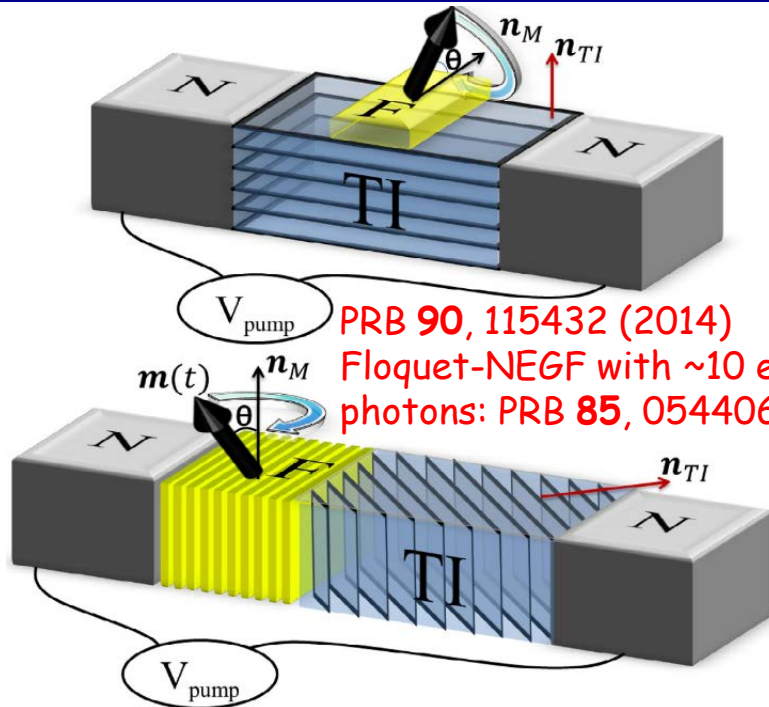
PRB 71, 195328 (2005)

$$\hat{\rho}^{\text{out}} = \frac{1}{2}(1 + \mathbf{P}^{\text{out}} \cdot \boldsymbol{\sigma})$$

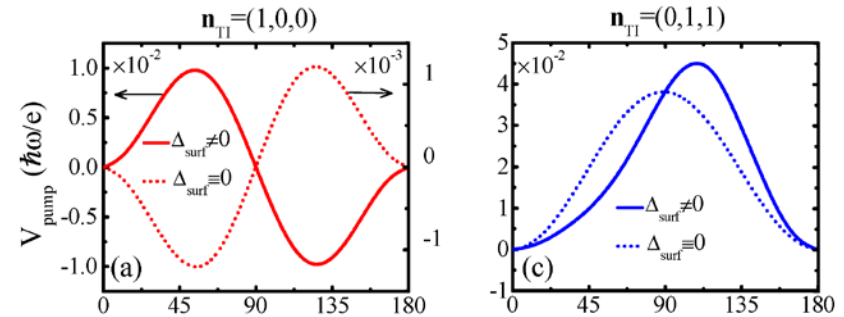
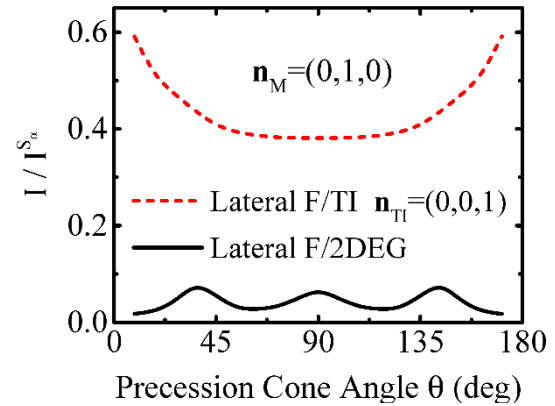
$$\hat{\rho}^{\text{out}} = \frac{e^2/h}{n_{\uparrow}(G^{\uparrow\uparrow} + G^{\downarrow\uparrow}) + n_{\downarrow}(G^{\uparrow\downarrow} + G^{\downarrow\downarrow})} \sum_{n',n=1}^M \begin{pmatrix} |\mathbf{t}_{n'n,\uparrow\uparrow}|^2 + |\mathbf{t}_{n'n,\uparrow\downarrow}|^2 & \mathbf{t}_{n'n,\uparrow\uparrow} \mathbf{t}_{n'n,\downarrow\uparrow}^* + \mathbf{t}_{n'n,\uparrow\downarrow} \mathbf{t}_{n'n,\downarrow\downarrow}^* \\ \mathbf{t}_{n'n,\uparrow\uparrow}^* \mathbf{t}_{n'n,\downarrow\uparrow} + \mathbf{t}_{n'n,\uparrow\downarrow}^* \mathbf{t}_{n'n,\downarrow\downarrow} & |\mathbf{t}_{n'n,\downarrow\uparrow}|^2 + |\mathbf{t}_{n'n,\downarrow\downarrow}|^2 \end{pmatrix}$$

PRL 109, 166602 (2012)

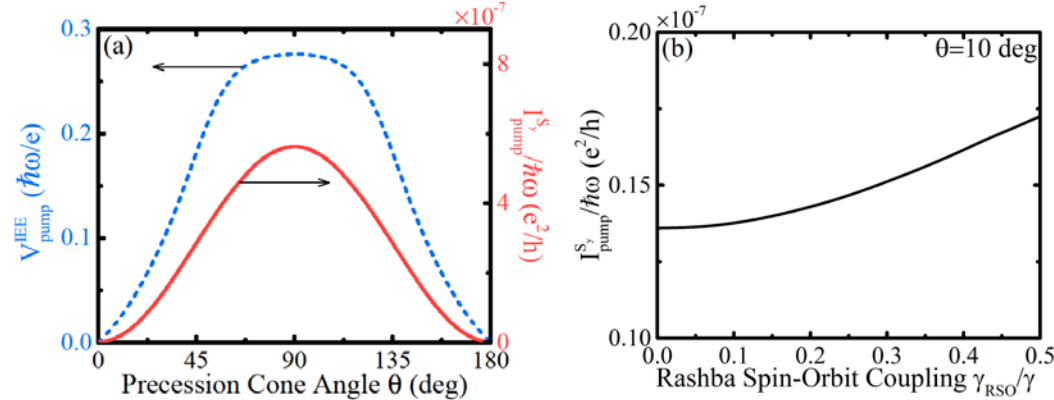
# Spin Pumping-to-Charge Conversion in Lateral and Vertical TI/F Heterostructures



PRB 90, 115432 (2014)  
 Floquet-NEGF with  $\sim 10$  exchanged photons: PRB 85, 054406 (2012)

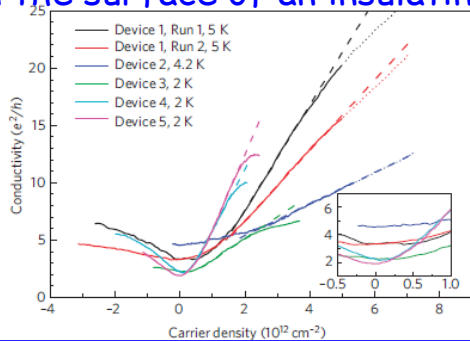


Nano Lett. 15, 7126 (2015)



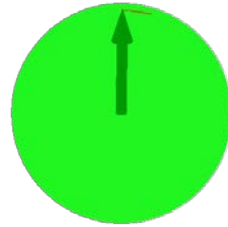
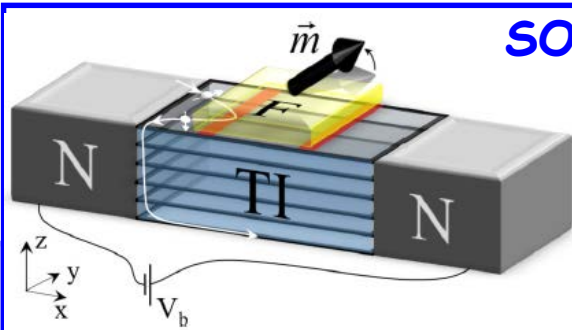
Nature Phys. 8, 459 (2012)

Ambipolar electronic transport on the surface of an insulating bulk



# Conclusions and Open Questions in Pictures

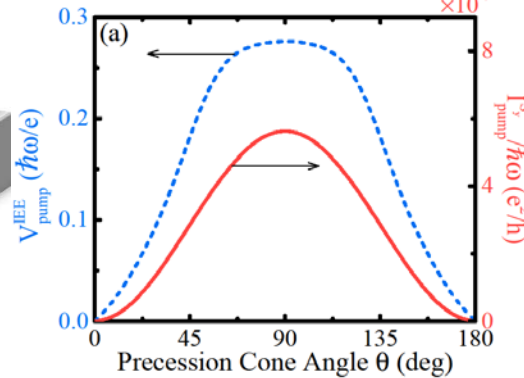
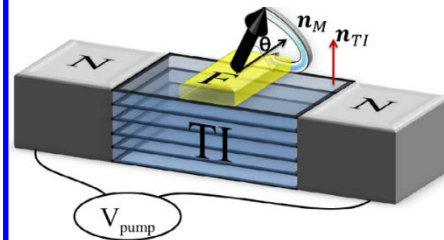
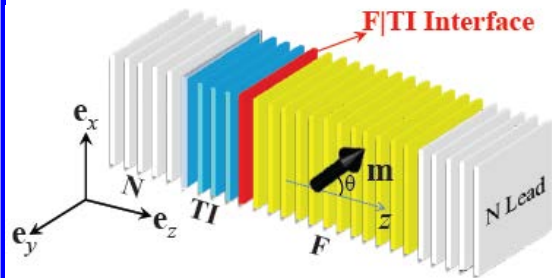
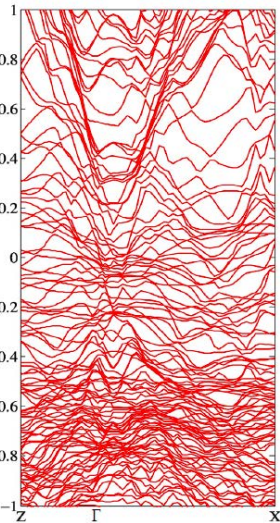
## SO torque



## Open questions:

- hybridization between TI and F states
- SO torque from first principles

(b) Bi<sub>2</sub>Se<sub>3</sub>/Ni



## Spin-to-charge conversion

