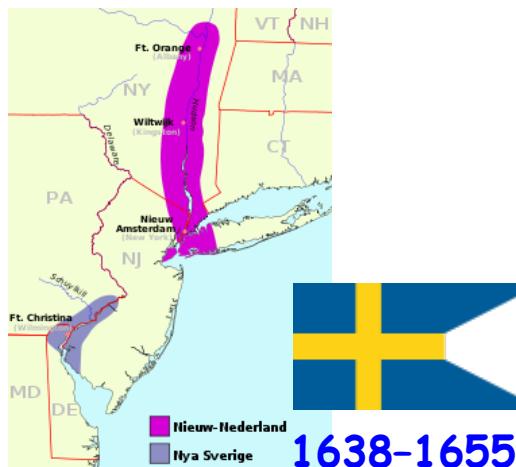


Anatomy of Spin-Orbit Torques in Topological-Insulator/Ferromagnet Heterostructures

Branislav K. Nikolić

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RIKEN Center for Emergent Matter Science, ASI, RIKEN, Wako 351-0198, Japan



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

The image shows a screenshot of a Wikipedia page for the Quantum Transport Theory Group (QTTG) at the University of Delaware. The page includes a navigation bar, a main content area with a welcome message and research highlights, and a sidebar with news and recent completed projects.

Main Page

Welcome to Wiki of the Quantum Transport Theory Group
Our group is a member of the Center for Spintronics and Biodection.

About QTTG

Our group conducts research on the frontier problems of quantum transport of electron charge and spin in a variety of nanostructures. The that we are currently pursuing include:
• nonequilibrium spintronics;
• topological-insulator spintronics;
• graphene-based nanoelectronics;
• nanoelectronic biosensors;
• nanoscale thermoelectrics;
• steady-state magnetotransport.

We are also working on the development of new theoretical and computational formalisms, often involving massively parallel codes, which are required to study quantum many-body systems far from equilibrium. The principal tools that we employ daily include nonequilibrium Green function theory, density functional theory, and dynamical mean field theory.

Our research is supported by the National Science Foundation and the U.S. Department of Energy.

Research Highlights

The image on the left depicts graphene nanoribbon which is converted into a two-dimensional metal-insulator-metal device. In such devices, the edge states are locally excited by spin-orbit coupling. We have predicted that the edge currents in this 2D TI will generate highly optimized Seebeck coefficient, while its nanoribbons will block phonon propagation, which together conspire to produce a thermoelectric figure of merit $ZT \approx 3$ at low temperatures $T \sim 40$ K.

News

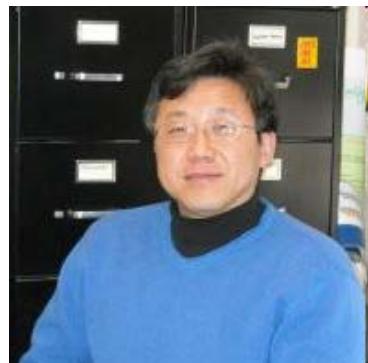
- Fall 2014 meeting schedule: Thursdays 10AM-12PM in A.J. Cannon room
- Recently Completed Projects
- First-principles vs. semi-empirical modeling of global and local electron transport for DNA sequencing
- Spin-to-charge conversion in lateral and vertical topological-insulator heterostructures
- Nonperturbative quantum physics from low-order perturbation theory
- Giant thermoelectric effect in graphene-based topological insulators will be signatures of electromagnon interaction in charge and spin currents via many-body perturbation theory approach.

QTG Motto

- The outcome of any serious research can only be to make the two que
- The essence of today think deeply instead of clearly. One must be at quite insane. (Nikola Tesla, 1924)
- Employing the computer for the study of a model has the feeling of an "empty" under study, analyze data, and come up with an intuitive plots results are not what we were expecting a priori, thus there is no conclusion is reached. (Boris Dugutis, 2012)
- Don't give me excuses, give me results! (Penguins of Madagascar)

Collaborators

Experiment



Prof. J. Q. Xiao



Prof. J.-P. Wang

Theory



Dr. Farzad Mahfouzi



Prof. N. Nagaosa



Prof. Nicholas Kiouassis

Computation



Dr. Po-Hao Chang



J. M. Marmolejo-
Tejada



Dr. Kurt Stokbro

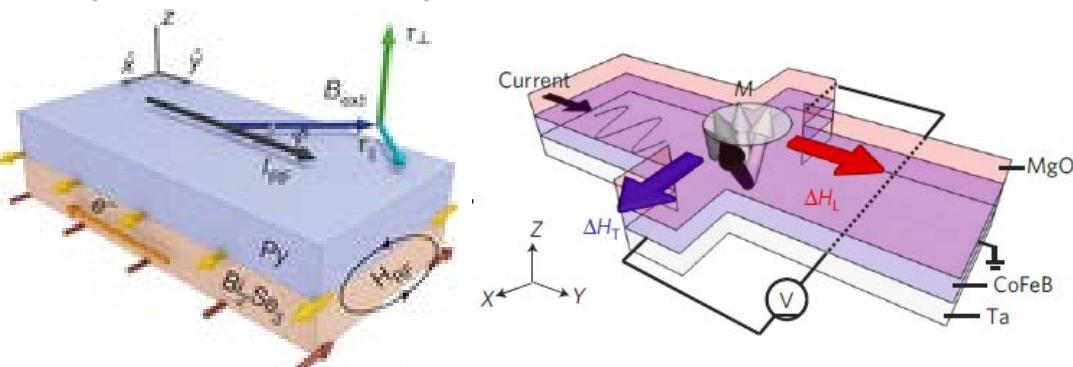
Experiments on SO Torque and Spin-to-Charge Conversion in Lateral TI/F Heterostructures

Ralph Lab, Nature 511, 449 (2014)

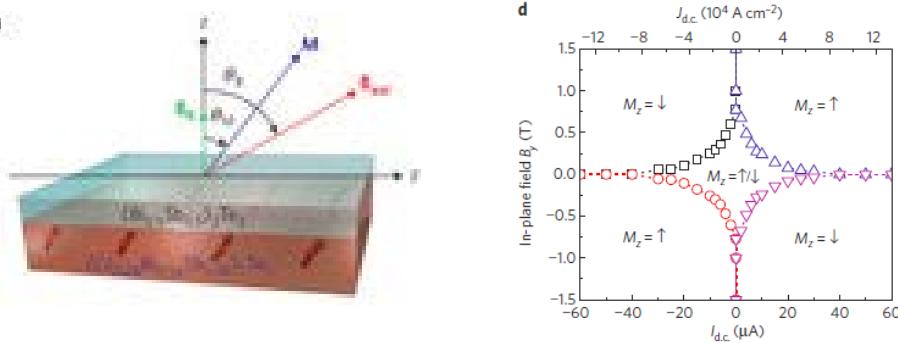
Table 1 | Comparison of room-temperature $\sigma_{s,\parallel}$ and $\theta_{s,\parallel}$ for Bi_2Se_3 with other materials

Parameter	Bi_2Se_3 (this work)	Pt (ref. 4)	$\beta\text{-Ta}$ (ref. 6)	Cu(Bi) (ref. 23)	$\beta\text{-W}$ (ref. 24)
θ_{\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

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

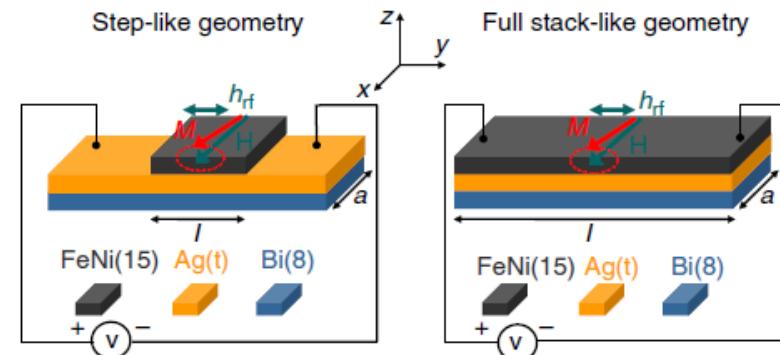


Wang Lab, Nature Mater. 13, 699 (2014): $\theta_{\parallel} \simeq 150 - 425$

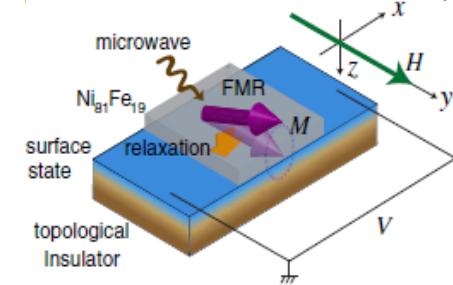


Yang Lab, PRL 114, 257202 (2015): $\theta_{\parallel} \simeq 0.047 \rightarrow 0.42$

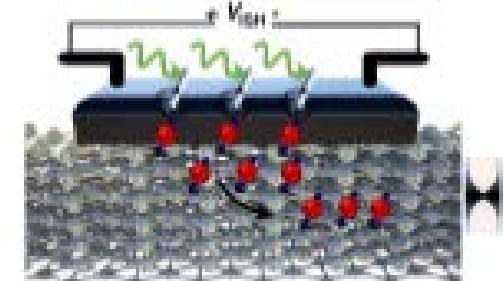
Fert & Vila, Nature Comm. 4, 2944 (2013)



Saitoh Lab, PRL 113, 196601 (2014)



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



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

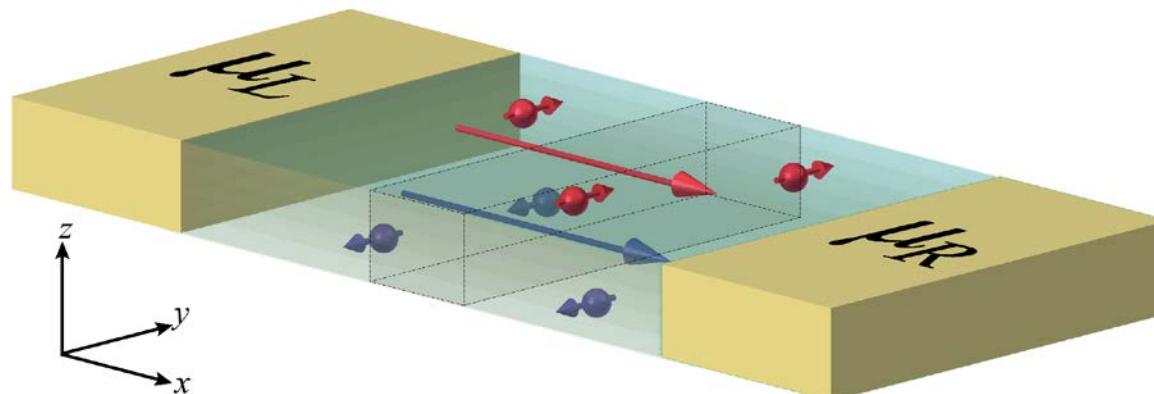
V.M. Edelstein

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

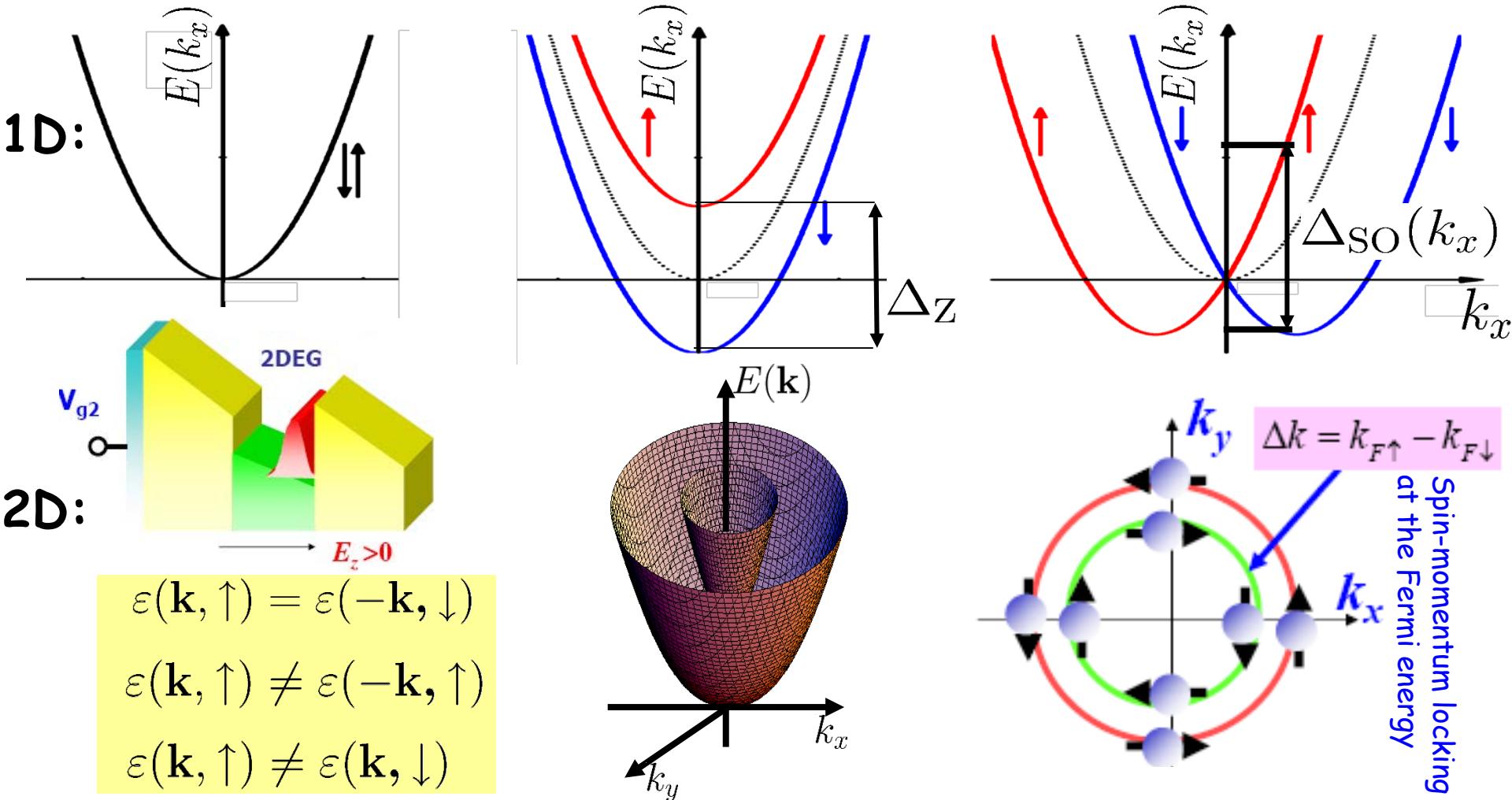
$$S_y = \beta E_x$$



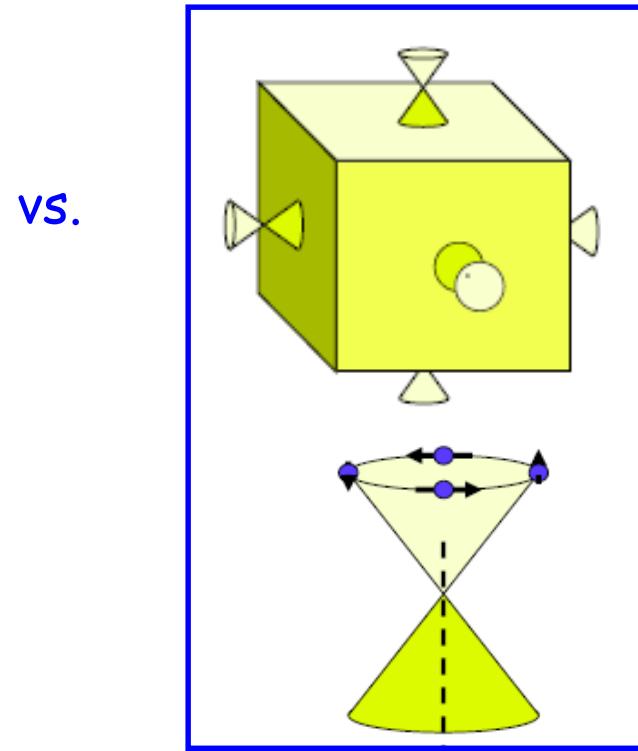
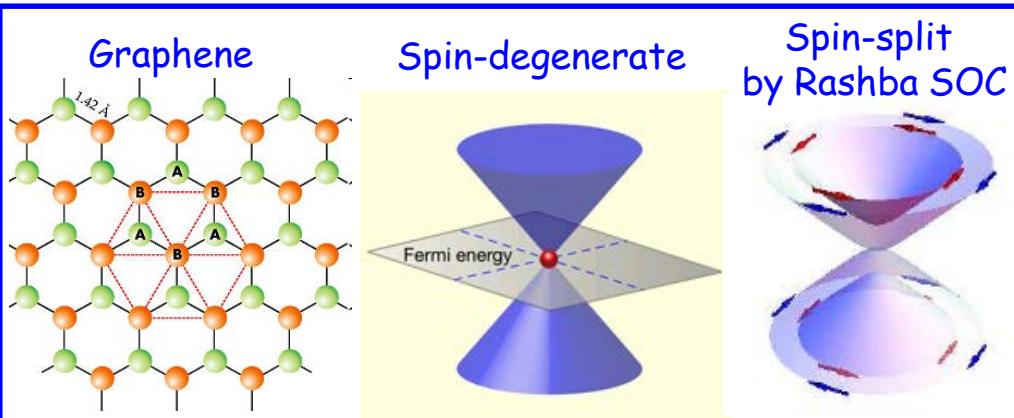
$$\frac{S_y^{\text{Rashba}}}{n} = \frac{e\tau E_x}{p_F} \frac{\alpha}{\hbar v_F} \text{ vs. } \frac{S_y^{\text{TI}}}{n} = \frac{e\tau E_x}{p_F}$$

Rashba SO Splitting of Energy Bands

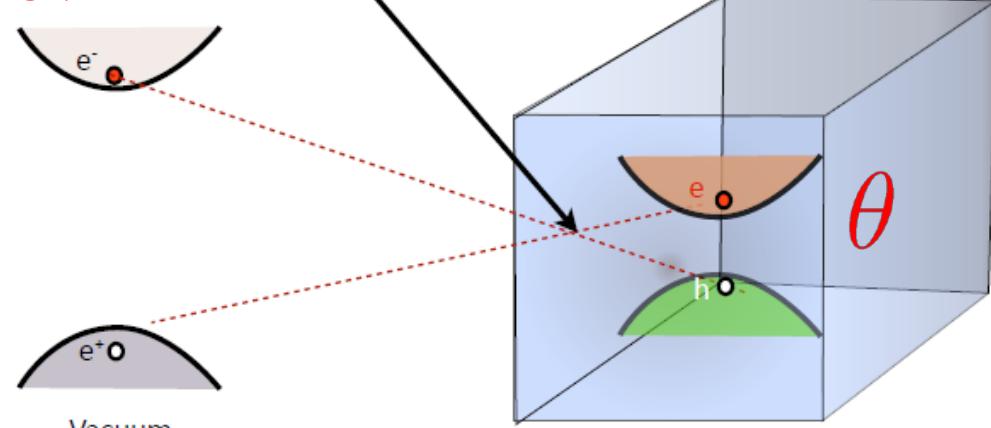
$$\hat{H}_{\text{SO}}^{\text{R}} = \frac{\alpha}{\hbar} (\hat{\sigma} \times \hat{\mathbf{p}}) \cdot \mathbf{e}_z \equiv -\frac{g\mu_B}{2} \hat{\sigma} \cdot \mathbf{B}_{\text{R}}(\hat{\mathbf{p}})$$



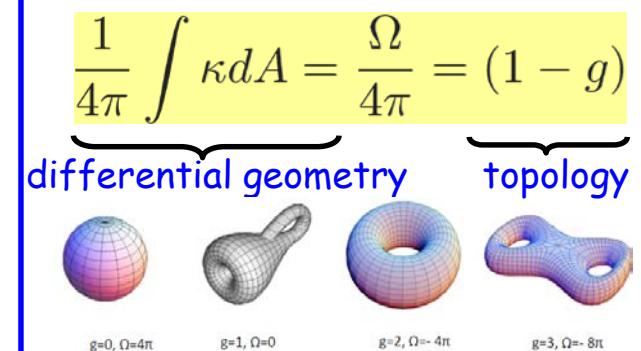
Crash Course on 3D TIs



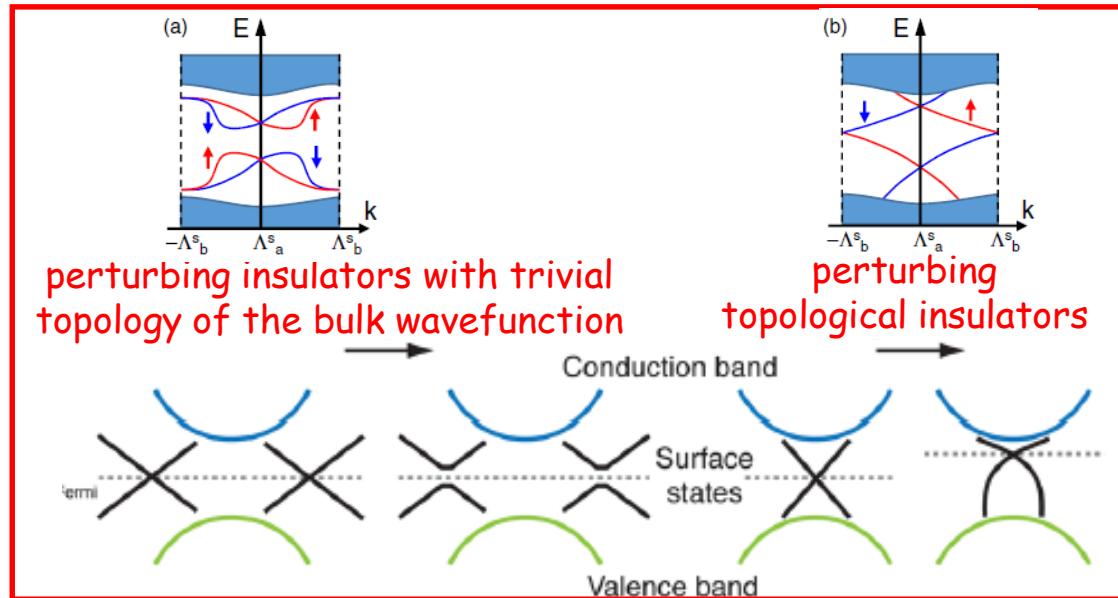
TIs are adiabatically disconnected from vacuum, so the gap must close at interface between different vacua



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

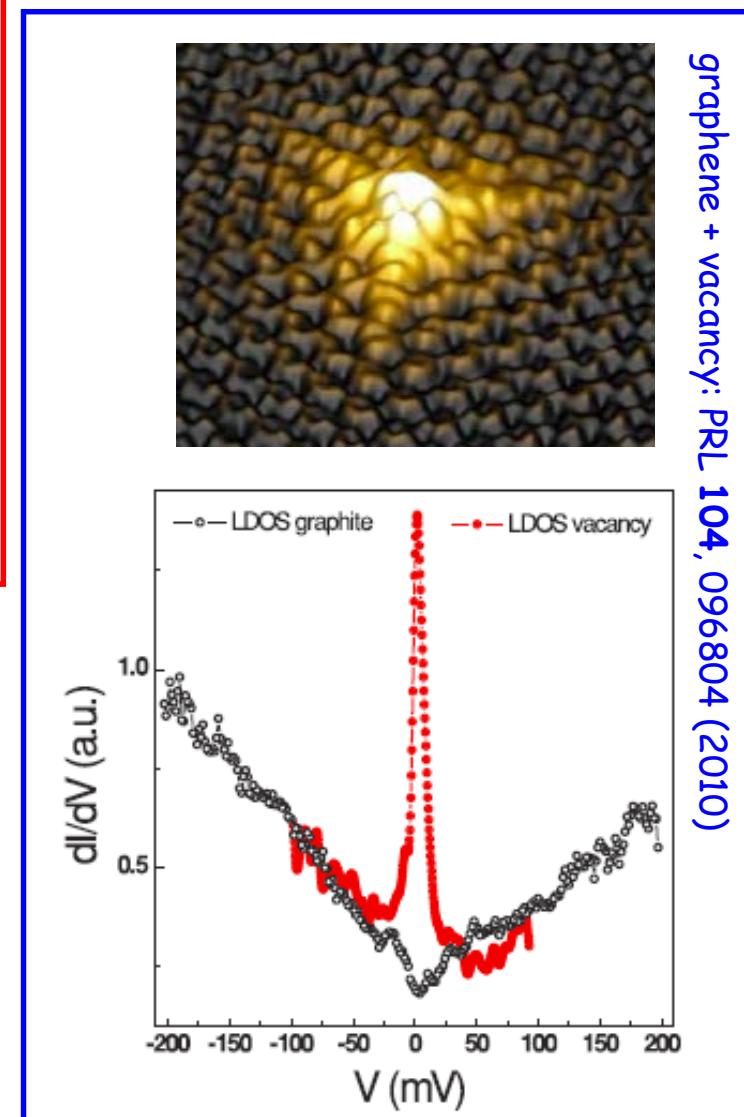
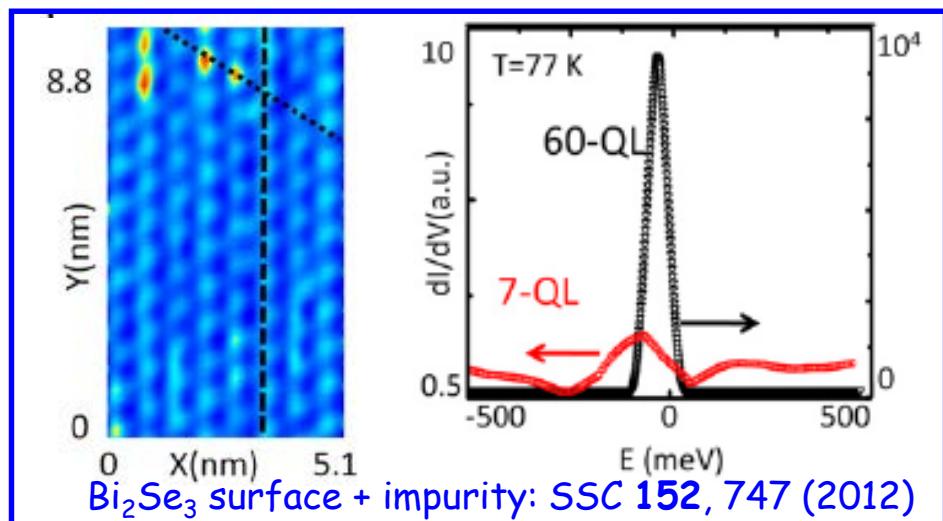


Physical Meaning of Topological Protection

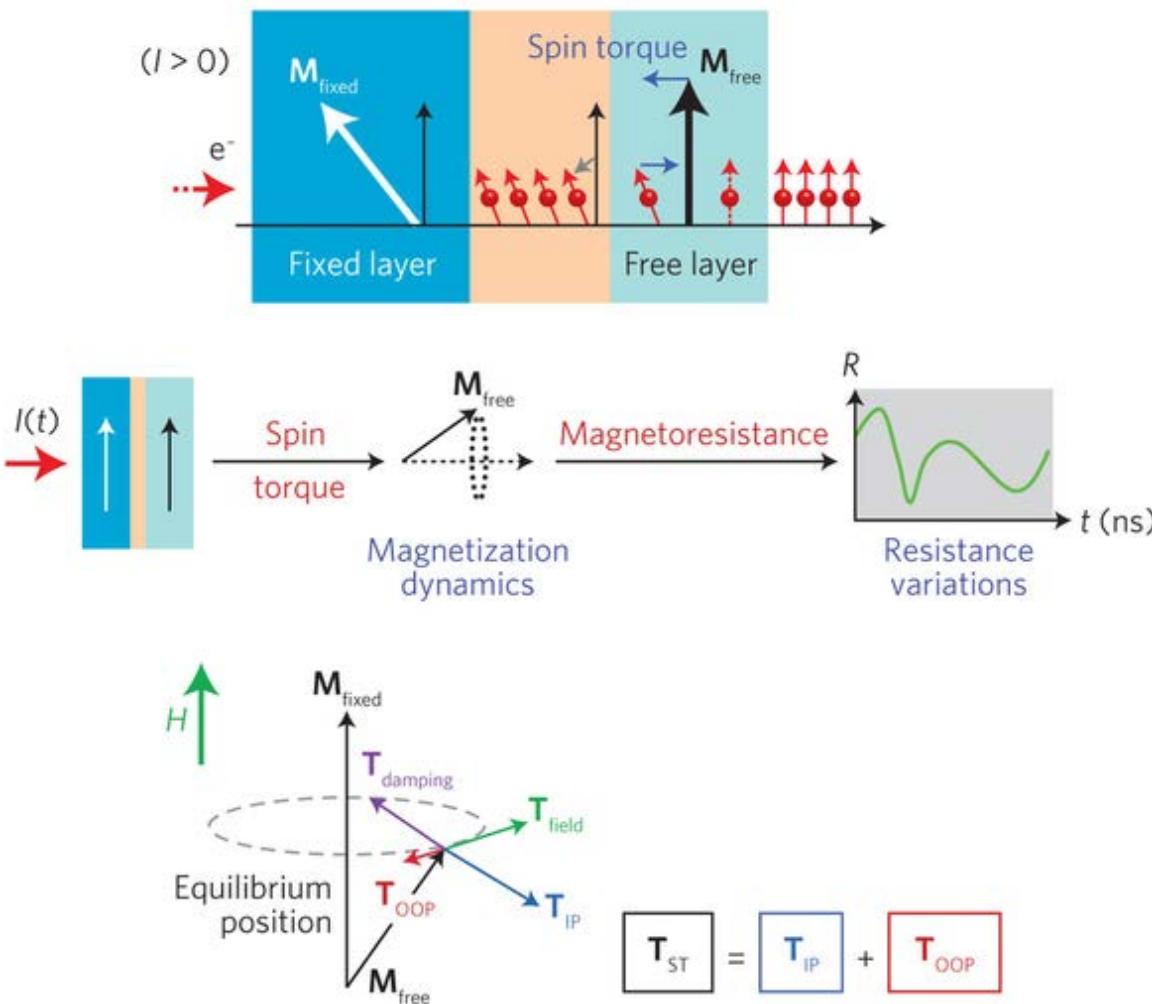


perturbing insulators with trivial topology of the bulk wavefunction

perturbing topological insulators



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^{a,*}, M.D. Stiles^b

REVIEW ARTICLES | INSIGHT

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

nature
materials

Current-induced torques in magnetic materials

Arne Brataas¹, Andrew D. Kent² and Hideo Ohno^{3,4}

nature
materials

PROGRESS ARTICLE

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

Spin-torque building blocks

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

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

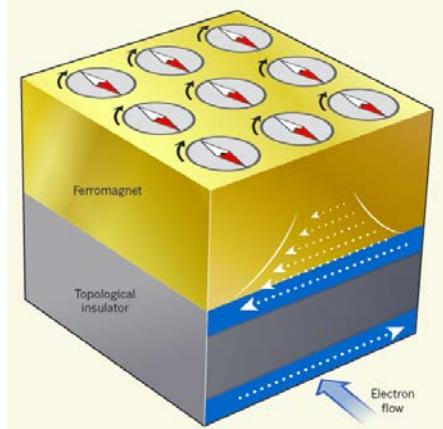
World Scientific
www.worldscientific.com

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

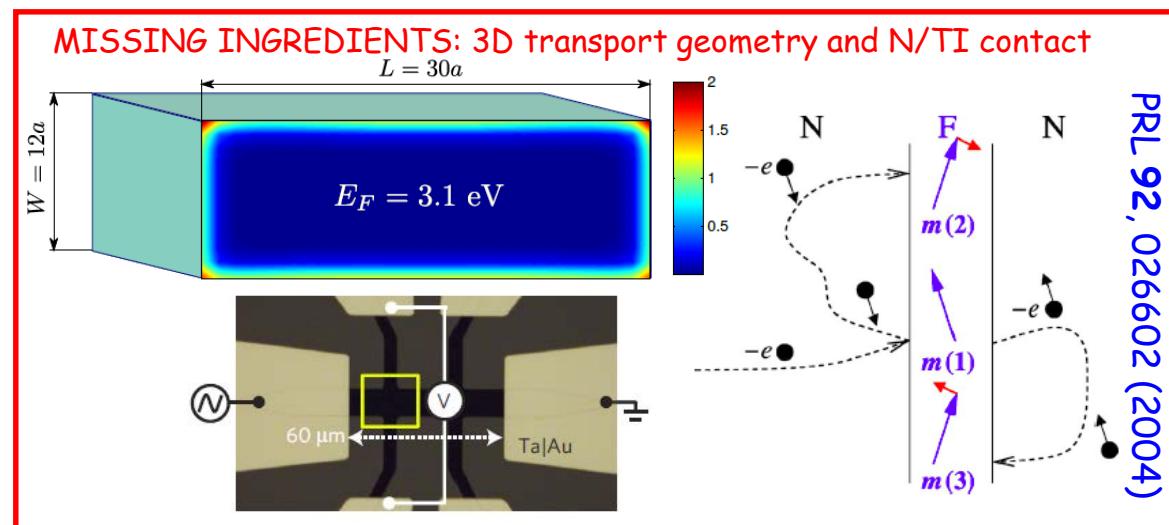
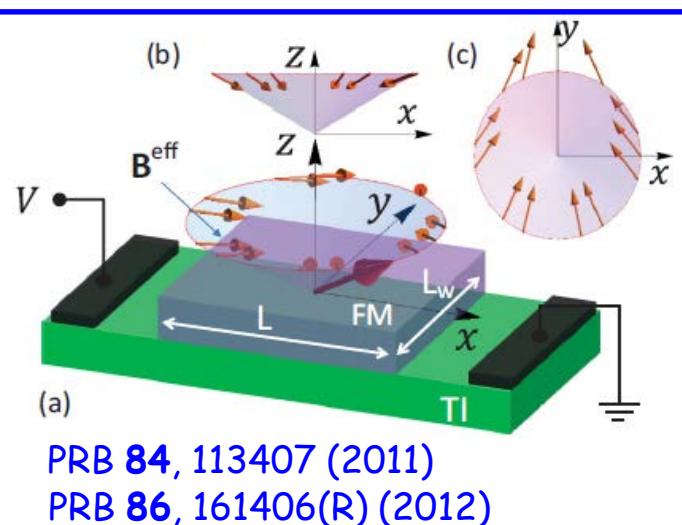
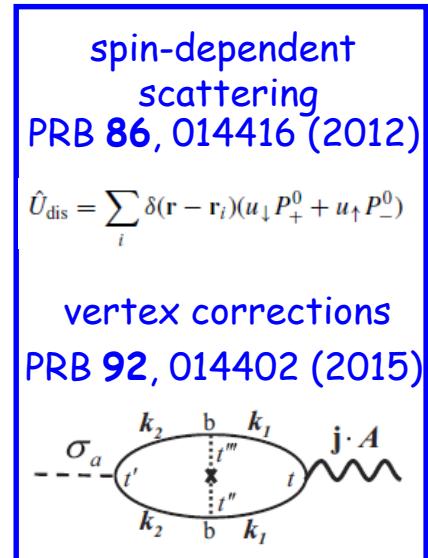
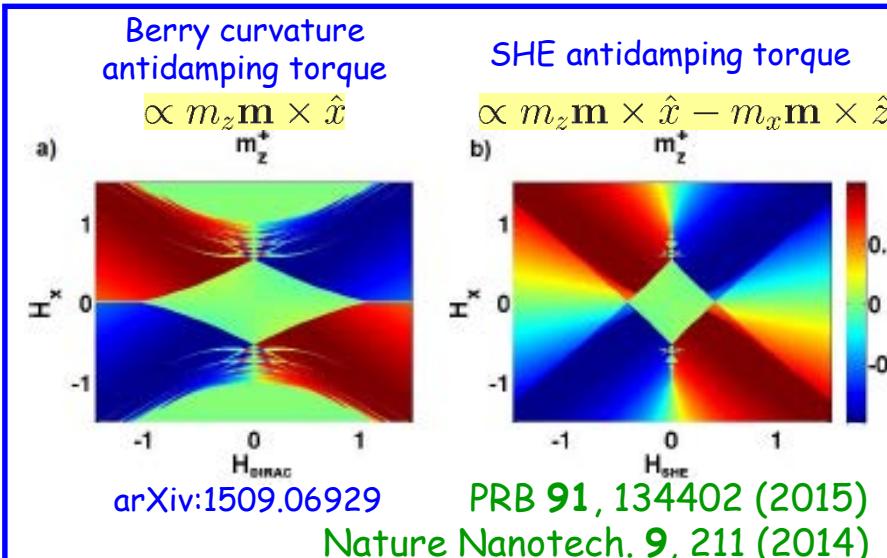
FARZAD MAHFUZI and BRANISLAV K. NIKOLIĆ*

Anatomy of SOT

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



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



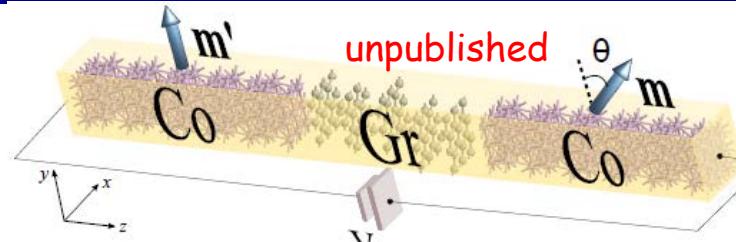
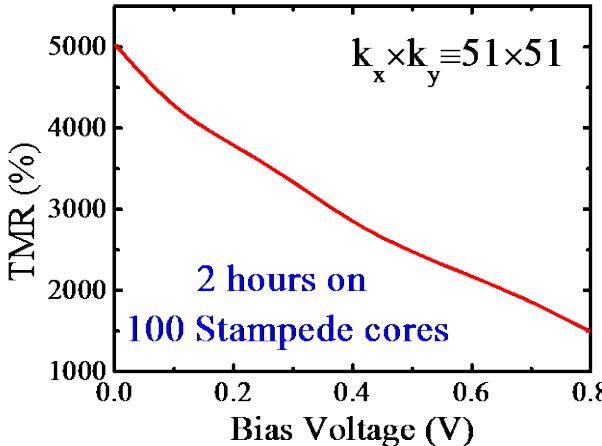
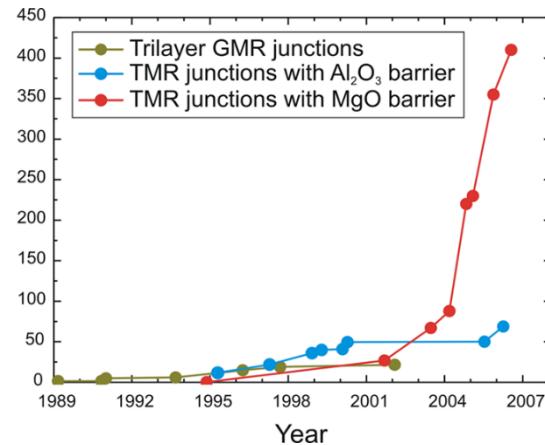
What Can Computation Do for Topological Spintronics: Find Optimal Materials Combinations

PHYSICAL REVIEW B, VOLUME 63, 054416

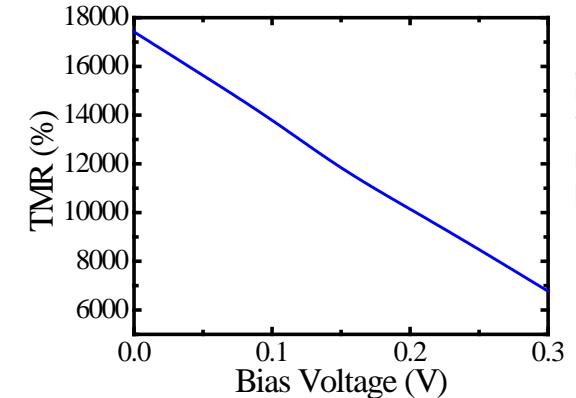
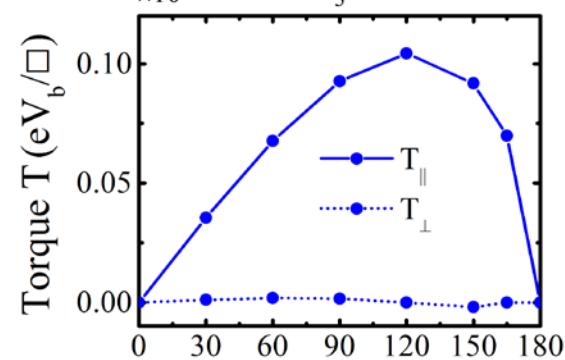
Spin-dependent tunneling conductance of Fe/MgO/Fe sandwiches

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

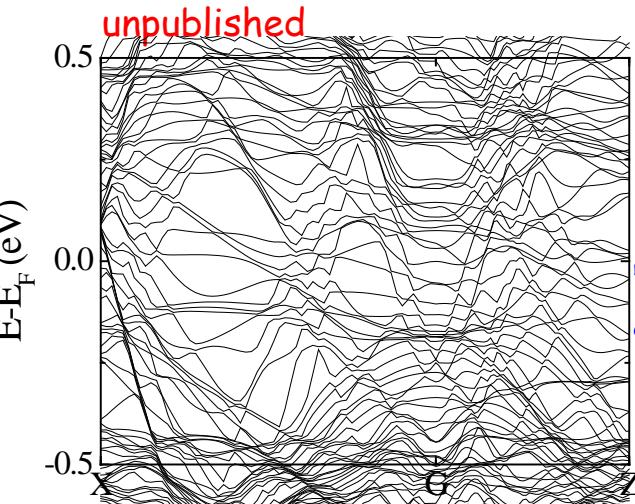
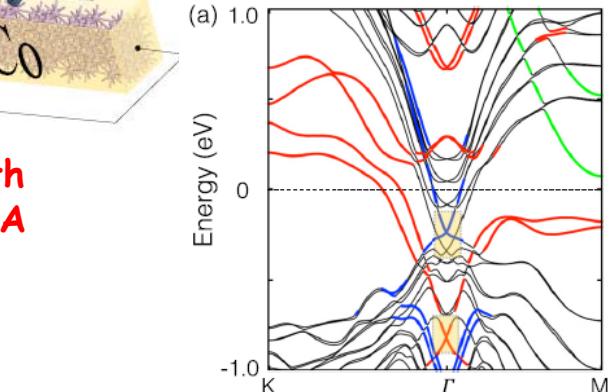
J. M. MacLaren
Department of Physics, Tulane University, New Orleans, Louisiana 70018



STT-MRAM cell with high TMR and low RA
 $\text{Co}/\text{Gr}_3/\text{Co}(\theta)$



PRB 90, 115103 (2014)



EuS/Bi₂Se₃

Co/Bi₂Se₃

Spin Density and STT from NEGF Formalism

❑ Fundamental quantities of NEGF formalism:

density of available quantum states:

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

how are those states occupied:

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

❑ NEGF for steady-state transport:

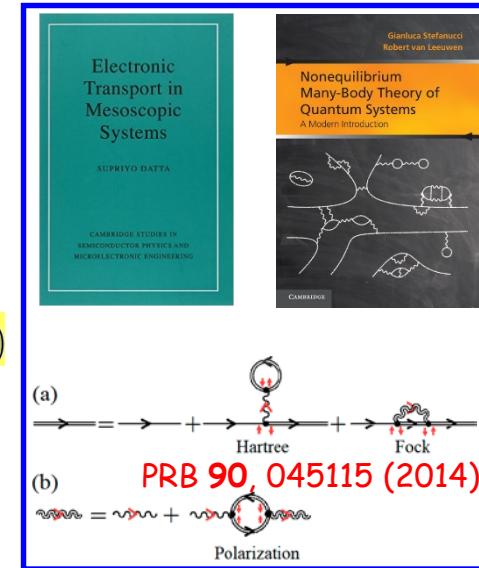
$$G^r(t, t') \rightarrow G^r(t - t') \xrightarrow{\text{FT}} G^r(E)$$

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

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

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

Learn more about NEGF from:



❑ NEGF-based expression for spin-transfer torque:

SPIN 3, 1330002 (2013)

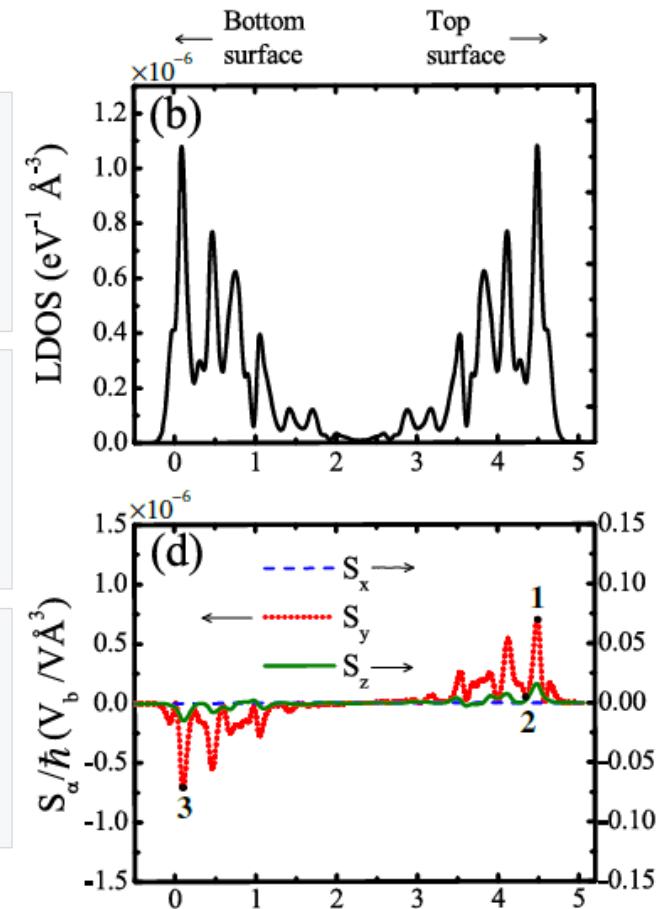
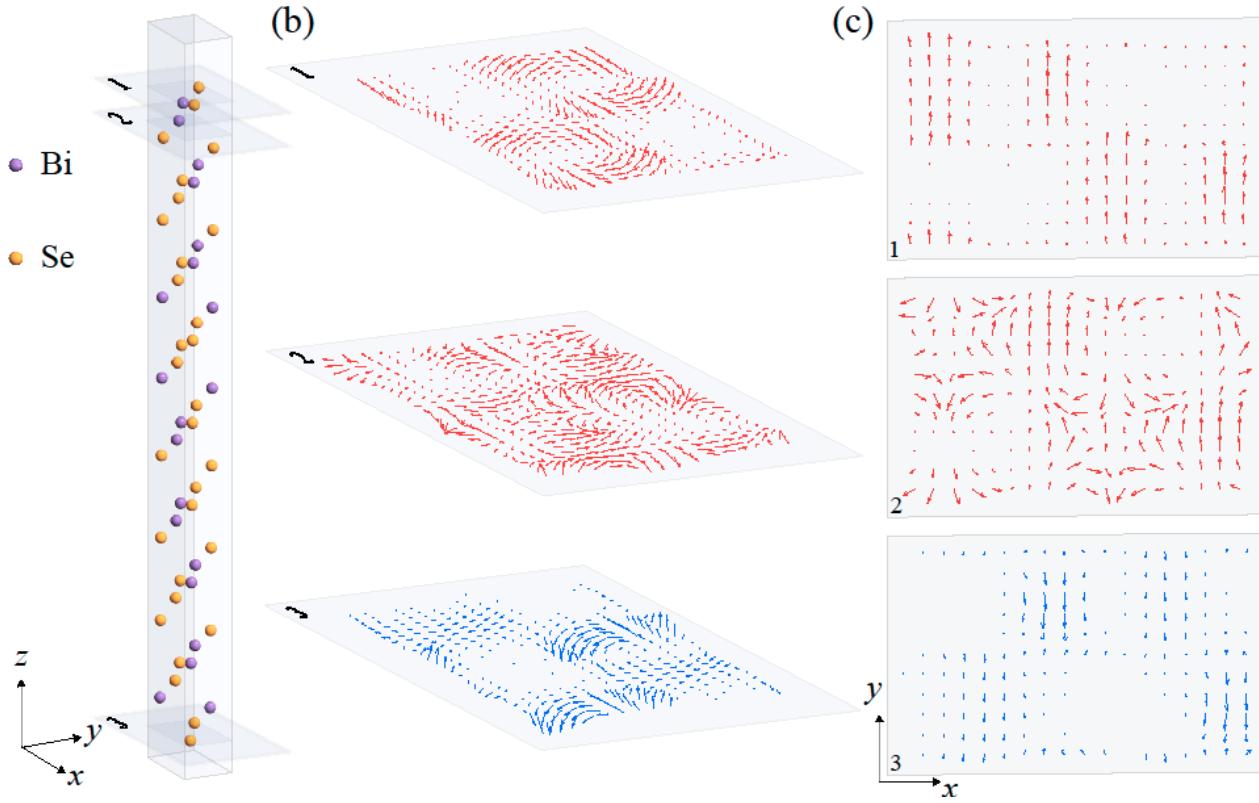
$$\hat{H} = -\frac{\hbar^2 \nabla^2}{2m} + V_H(\mathbf{r}) + V_{XC}(\mathbf{r}) + V_{\text{ext}}(\mathbf{r}) - \boldsymbol{\sigma} \cdot \mathbf{B}_{XC}(\mathbf{r}) \Rightarrow \hat{\mathbf{T}} = \frac{d\hat{\mathbf{S}}}{dt} = \frac{1}{2i} [\hat{\boldsymbol{\sigma}}, \hat{H}]$$

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

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 Bi_2Se_3

PRB 92, 20406(R) (2015)



Adiabatic Expansion of NEGFs in Derivatives of Slow Magnetization

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

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

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

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

$$T^{\alpha i}(E) = \text{Tr} \left[\mathbf{1}_m \boldsymbol{\sigma}_i \mathbf{G}_t^\dagger \mathbf{\Gamma}_\alpha \mathbf{G}_t \right] \text{spin torque}$$

$$T^{i\alpha}(E) = \text{Tr} \left[\mathbf{1}_m \boldsymbol{\sigma}_i \mathbf{G}_t \mathbf{\Gamma}_\alpha \mathbf{G}_t^\dagger \right] \text{charge pumping}$$

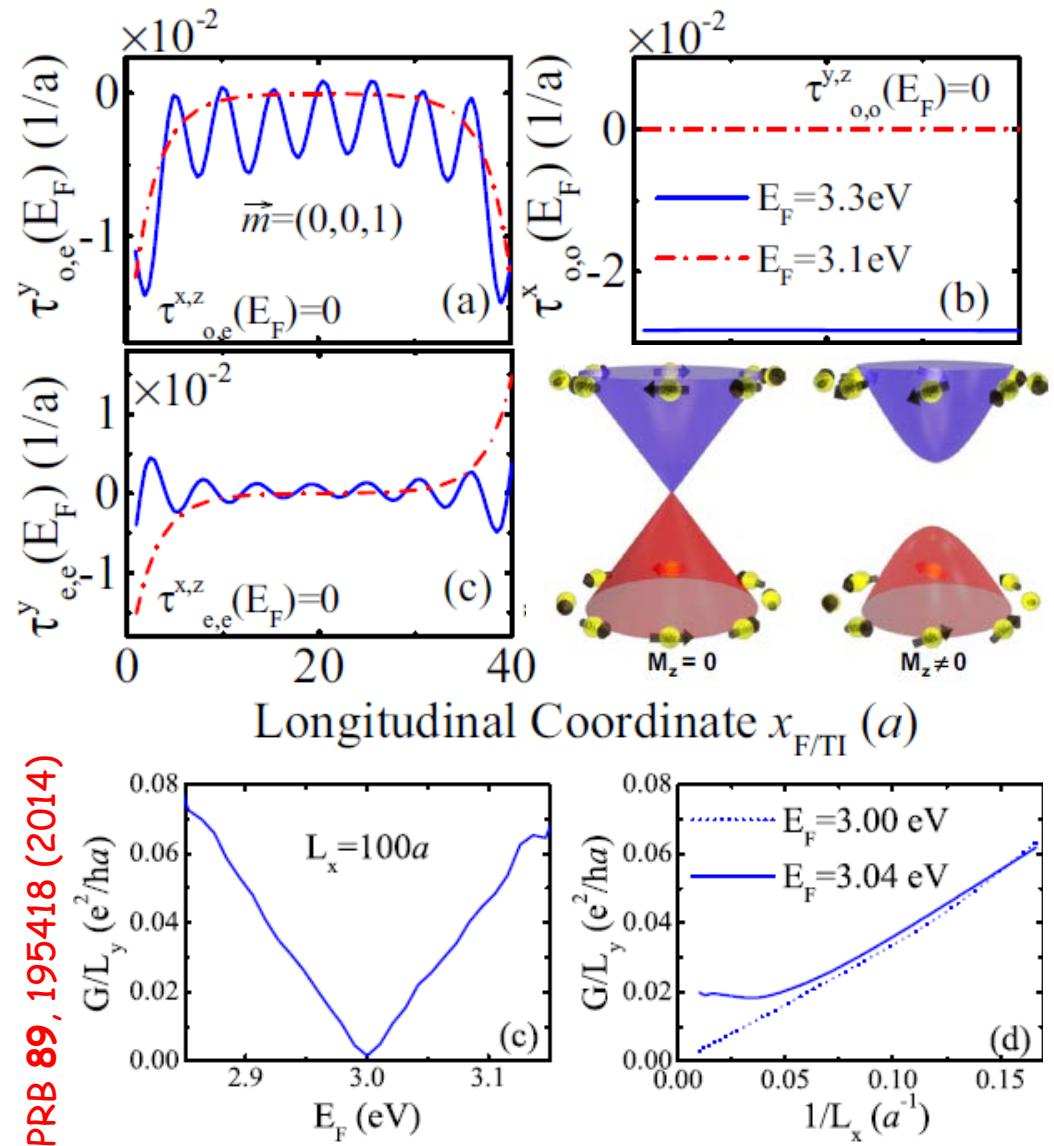
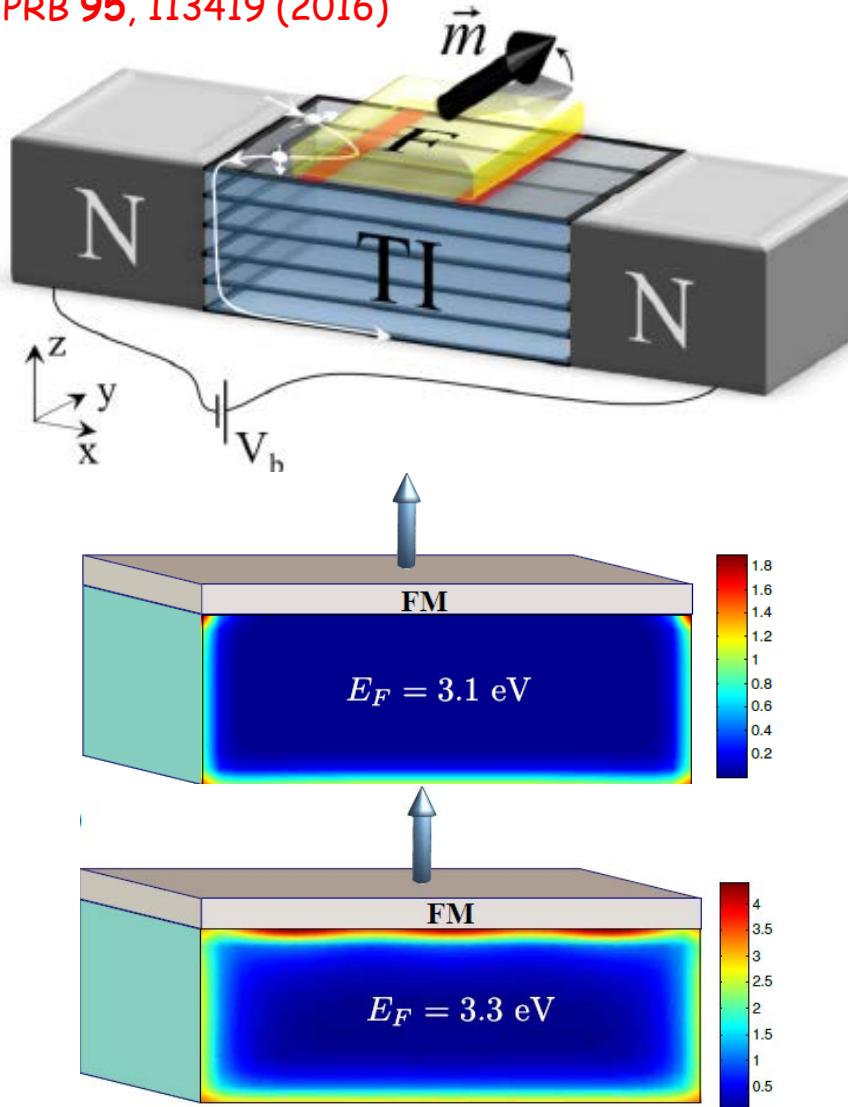
$$T^{ij}(E) = \text{Tr} \left[\mathbf{1}_m \boldsymbol{\sigma}_i (\mathbf{G}_t^\dagger - \mathbf{G}_t) \mathbf{1}_m \boldsymbol{\sigma}_j (\mathbf{G}_t - \mathbf{G}_t^\dagger) \right] \text{Gilbert damping}$$

$$\rho \left\{ \begin{array}{l} \rho_{oo} = \int dE (f_L - f_R) [\mathbf{G} \mathbf{\Gamma}_L \mathbf{G}^\dagger - \mathbf{G}^\dagger \mathbf{\Gamma}_L \mathbf{G} - \mathbf{G} \mathbf{\Gamma}_R \mathbf{G}^\dagger + \mathbf{G}^\dagger \mathbf{\Gamma}_R \mathbf{G}] / 8\pi \quad \text{gives field-like torque} \\ + \\ \rho_{oe} = \int dE (f_L - f_R) [\mathbf{G} \mathbf{\Gamma}_L \mathbf{G}^\dagger + \mathbf{G}^\dagger \mathbf{\Gamma}_L \mathbf{G} - \mathbf{G} \mathbf{\Gamma}_R \mathbf{G}^\dagger - \mathbf{G}^\dagger \mathbf{\Gamma}_R \mathbf{G}] / 8\pi \quad \text{gives antidamping torque} \\ + \\ \rho_{ee} = \int dE (f_L + f_R) [-\text{Im} \mathbf{G}] / 2\pi \\ + \\ \rho_{eo} \equiv 0 \end{array} \right.$$

PRB 95, 113419 (2016)

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

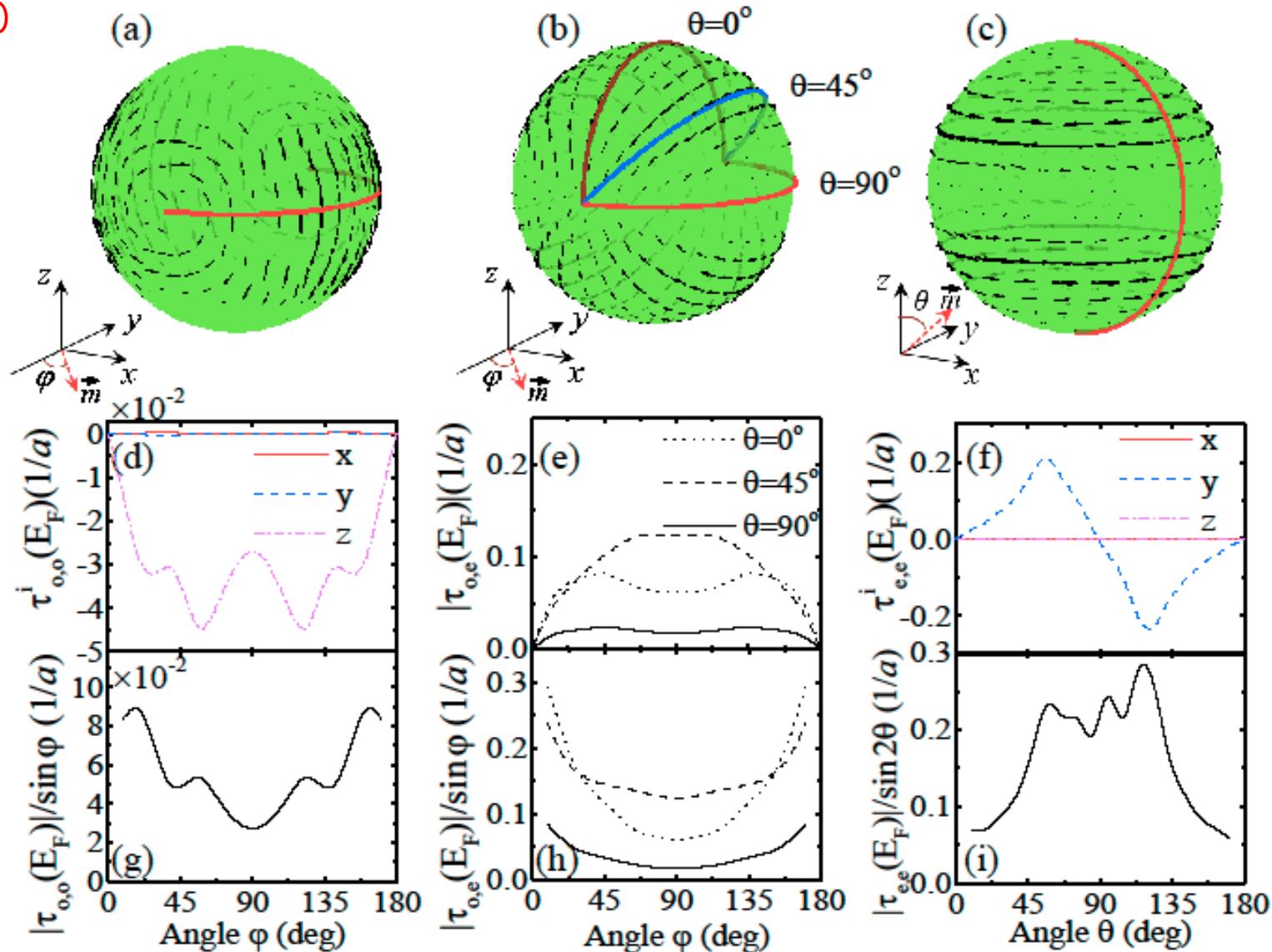
PRB 95, 113419 (2016)



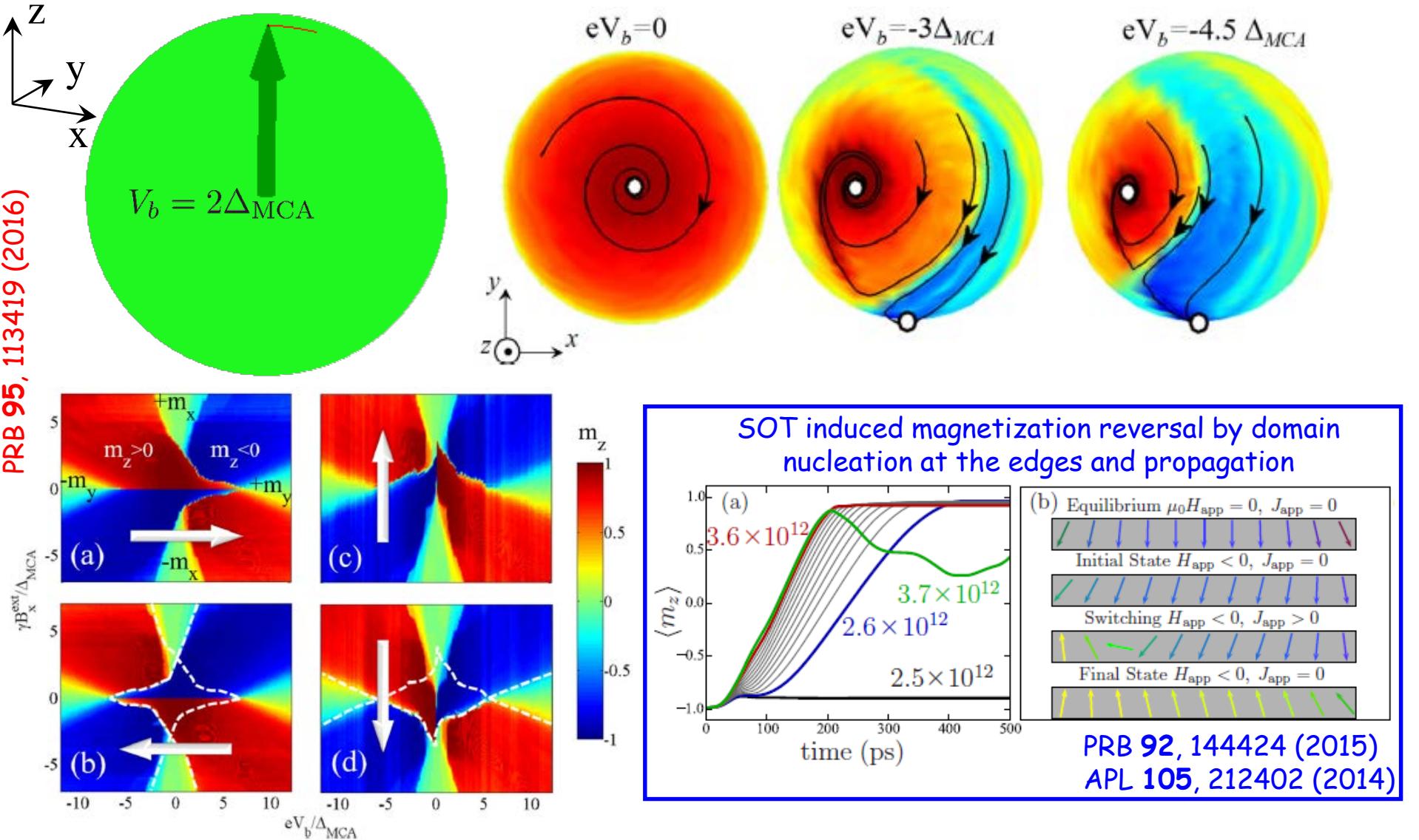
PRB 89, 195418 (2014)

Angular Dependence of SO Torque in Lateral TI/F Heterostructures

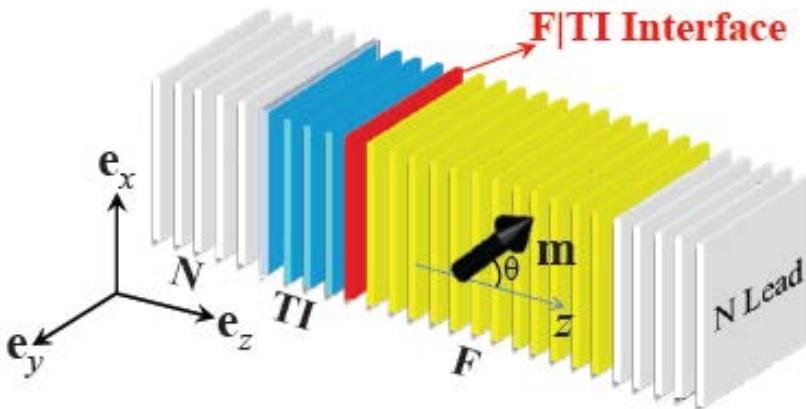
PRB 95, 113419 (2016)



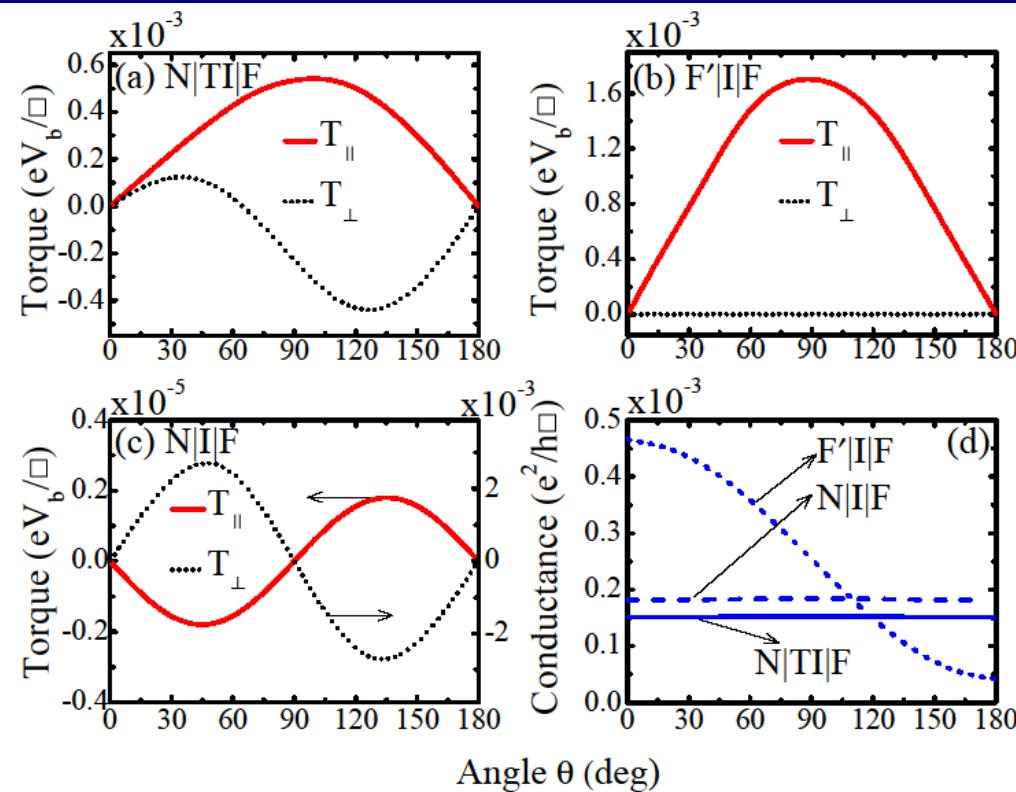
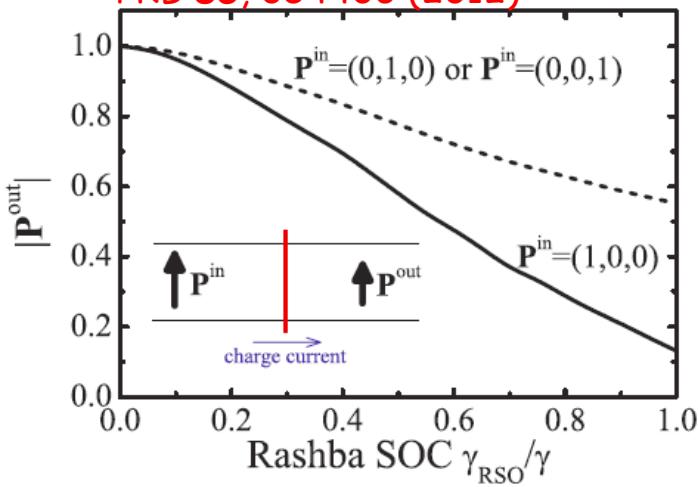
LLG Simulations of Magnetization Reversal and Switching Phase Diagram for TI/F Bilayer



SO Torque in Vertical TI/F Heterostructures



PRB 85, 054406 (2012)

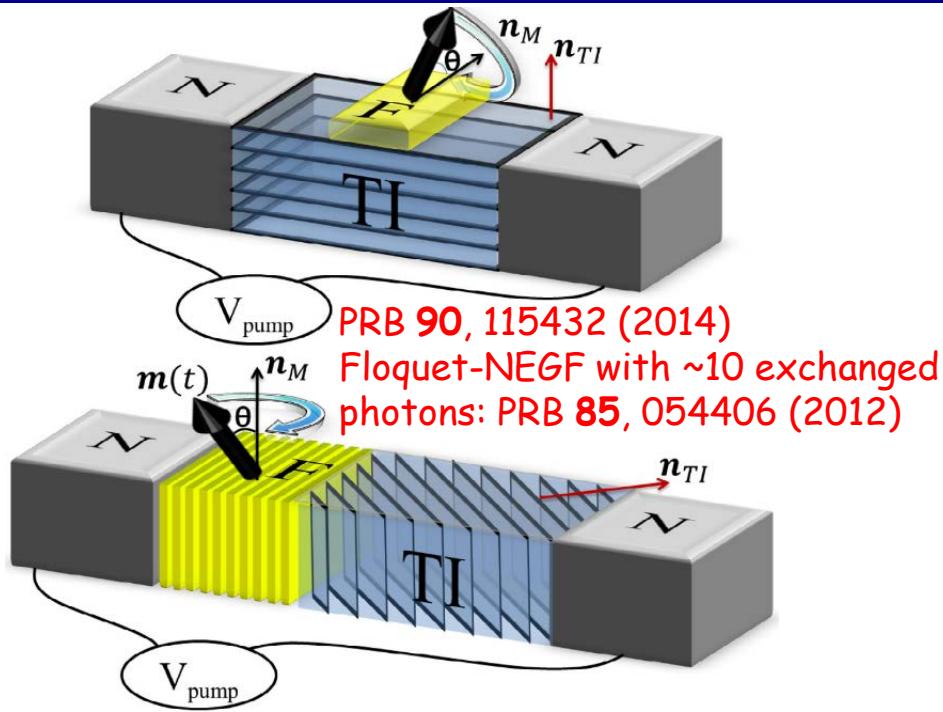


$$\mathbf{T} = \mathbf{T}_{\parallel} + \mathbf{T}_{\perp} = \tau_{\parallel} \mathbf{m} \times (\mathbf{m} \times \mathbf{e}_z) + \tau_{\perp} \mathbf{m} \times \mathbf{e}_z$$

PRB 71, 195328 (2005)

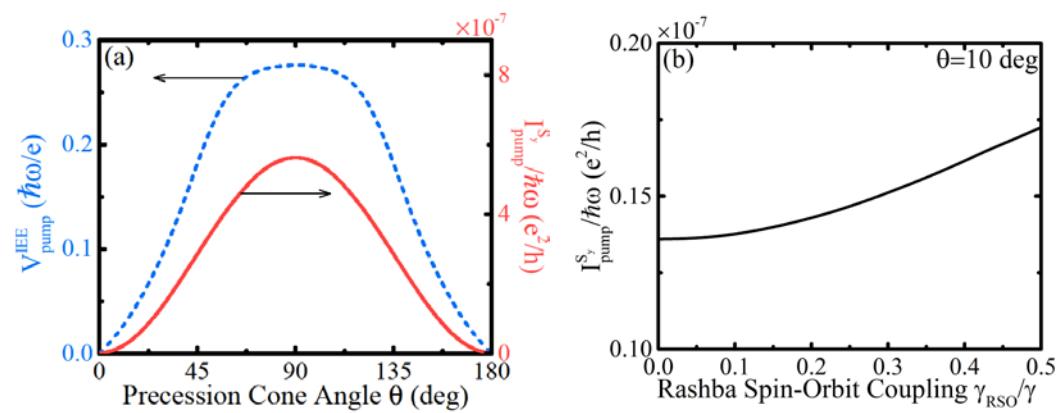
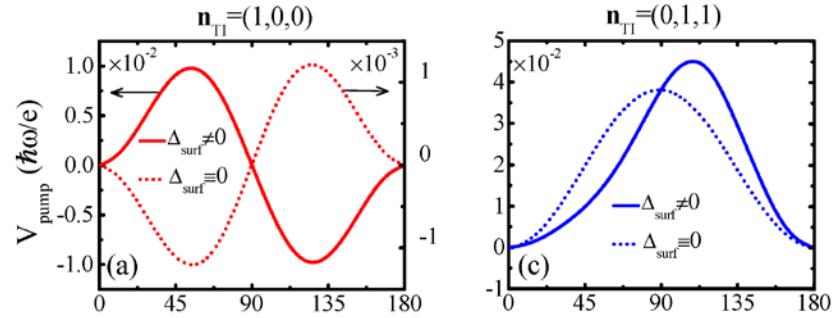
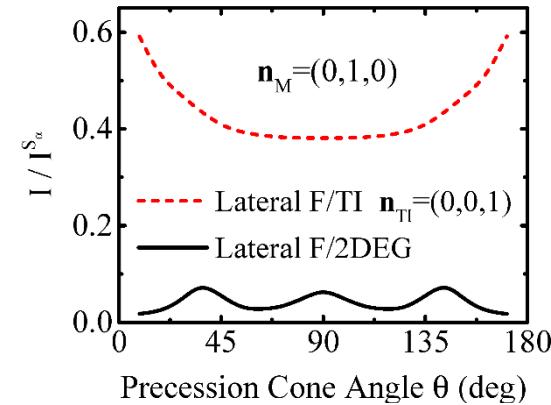
$$\begin{aligned} \hat{\rho}^{\text{out}} &= \frac{1}{2}(1 + \mathbf{P}^{\text{out}} \cdot \boldsymbol{\sigma}) \\ \hat{\rho}^{\text{out}} &= \frac{e^2/h}{n_{\uparrow}(G^{\uparrow\uparrow} + G^{\downarrow\uparrow}) + n_{\downarrow}(G^{\uparrow\downarrow} + G^{\downarrow\downarrow})} \sum_{n',n=1}^M \left(\begin{array}{cc} |\mathbf{t}_{n'n,\uparrow\uparrow}|^2 + |\mathbf{t}_{n'n,\uparrow\downarrow}|^2 & \mathbf{t}_{n'n,\uparrow\uparrow}\mathbf{t}_{n'n,\downarrow\uparrow}^* + \mathbf{t}_{n'n,\uparrow\downarrow}\mathbf{t}_{n'n,\downarrow\downarrow}^* \\ \mathbf{t}_{n'n,\uparrow\uparrow}^*\mathbf{t}_{n'n,\downarrow\uparrow} + \mathbf{t}_{n'n,\uparrow\downarrow}^*\mathbf{t}_{n'n,\downarrow\downarrow} & |\mathbf{t}_{n'n,\uparrow\downarrow}|^2 + |\mathbf{t}_{n'n,\downarrow\downarrow}|^2 \end{array} \right) \end{aligned}$$

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



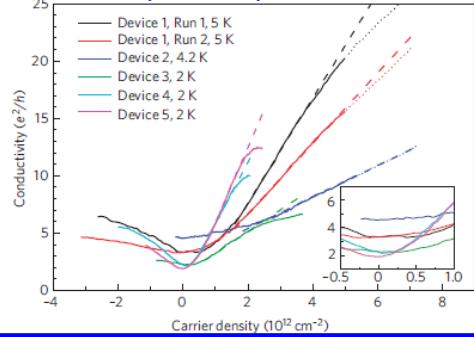
PRB 90, 115432 (2014)

Floquet-NEGF with ~10 exchanged photons: PRB 85, 054406 (2012)



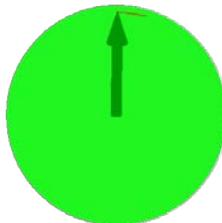
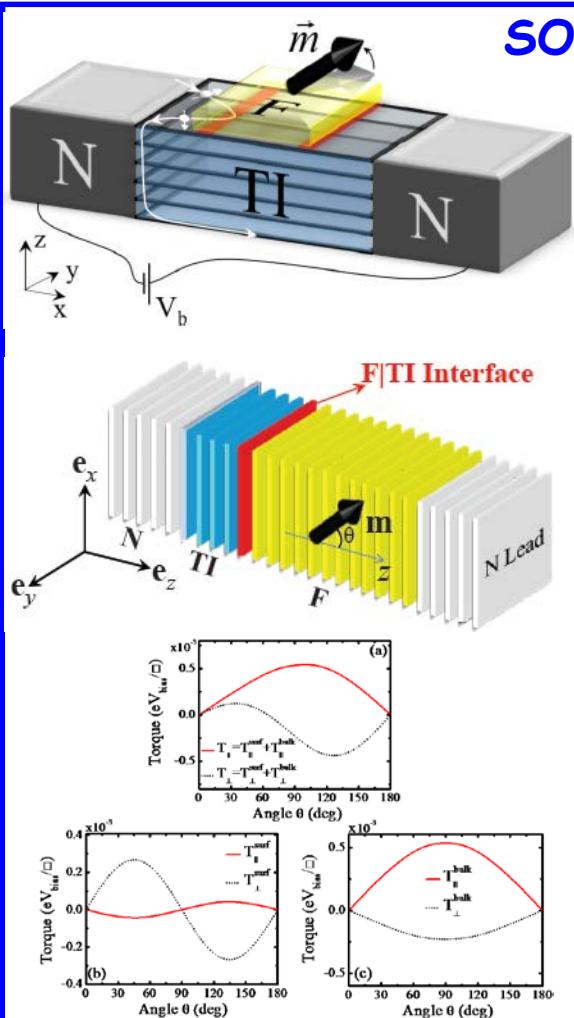
Nature Phys. 8, 459 (2012)

Ambipolar electronic transport on the surface of an insulating bulk



Nano Lett. 15, 7126 (2015)

Conclusions and Open Questions in Pictures



Open questions:

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

