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Disorder Effects in Topological Systems

Sergey Y. Savrasov

Supported by NSF-DMR

Acknowledgment

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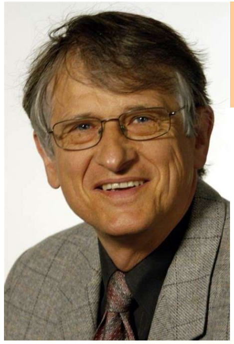
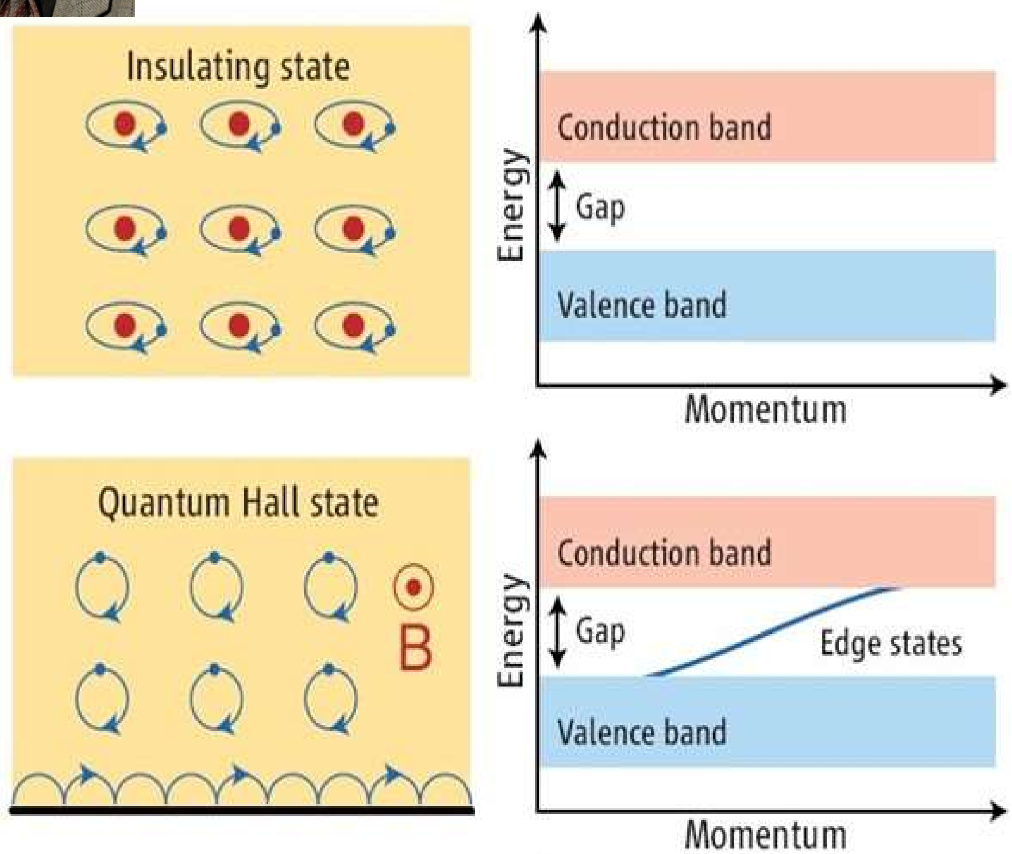
Nanjing University

Xiangang Wan

Chiral Quantum Hall States

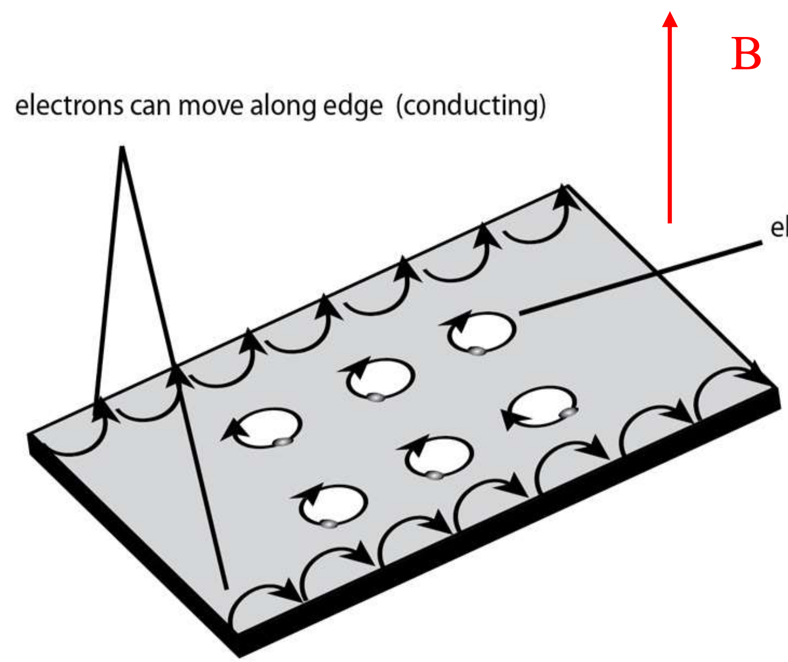


Klitzing, et.al. PRL (1980). *Nobel prize in Physics 1985*



Bulk insulating state
with zero conductivity

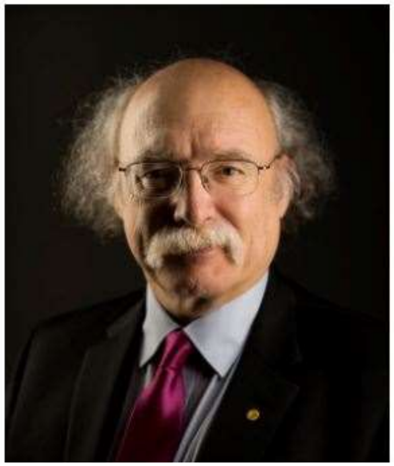
$$\sigma = 0$$



Both states of matter are differentiated by Chern number as a property of occupied Bloch functions of the bulk crystal.

The Nobel Prize in Physics 2016
David J. Thouless, F. Duncan M. Haldane, J. Michael Kosterlitz

F. Duncan M. Haldane - Facts



F. Duncan M. Haldane

Born: 14 September 1951, London, United Kingdom

Affiliation at the time of the award: Princeton University, Princeton, NJ, USA

Prize motivation: "for theoretical discoveries of topological phase transitions and topological phases of matter"

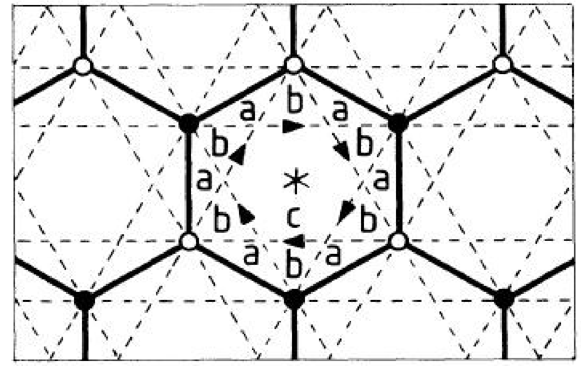


FIG. 1. The honeycomb-net model ("2D graphite") showing nearest-neighbor bonds (solid lines) and second-neighbor bonds (dashed lines). Open and solid points, respectively, mark the A and B sublattice sites. The Wigner-Seitz unit cell is conveniently centered on the point of sixfold rotation symmetry (marked "*") and is then bounded by the hexagon of nearest-neighbor bonds. Arrows on second-neighbor bonds mark the directions of positive phase hopping in the state with broken time-reversal invariance.

VOLUME 61, NUMBER 18 PHYSICAL REVIEW LETTERS 31 OCTOBER 1988

Model for a Quantum Hall Effect without Landau Levels: Condensed-Matter Realization of the "Parity Anomaly"

F. D. M. Haldane

Department of Physics, University of California, San Diego, La Jolla, California 92093

(Received 16 September 1987)

A two-dimensional condensed-matter lattice model is presented which exhibits a nonzero quantization of the Hall conductance σ^{xy} in the *absence* of an external magnetic field. Massless fermions *without spectral doubling* occur at critical values of the model parameters, and exhibit the so-called "parity anomaly" of (2+1)-dimensional field theories.

Two-dimensional massless electrons in an inverted contact

B. A. Volkov and O. A. Pankratov
P. N. Lebedev Physics Institute, Academy of Sciences of the USSR

(Submitted 20 June 1985)
Pis'ma Zh. Eksp. Teor. Fiz. **42**, No. 4, 145–148 (25 August 1985)

A new type of semiconductor structures based on the contact of two materials with mutually inverted bands is proposed. A qualitative feature of this contact is the presence of electron states which have a two-dimensional linear spectrum and which do not depend on the transition region. The properties of an inverted contact in an external magnetic field are determined.

In a two-band approximation the energy spectrum of such a contact is described by a Dirac equation with a band gap which depends on the z coordinate:

$$\begin{pmatrix} -\epsilon & i\epsilon_g/2 + \boldsymbol{\sigma}\mathbf{p} \\ -i\epsilon_g/2 + \vec{\sigma}\mathbf{p} & -\epsilon \end{pmatrix} \begin{pmatrix} \chi_- \\ \chi_+ \end{pmatrix} = 0, \qquad (1)$$

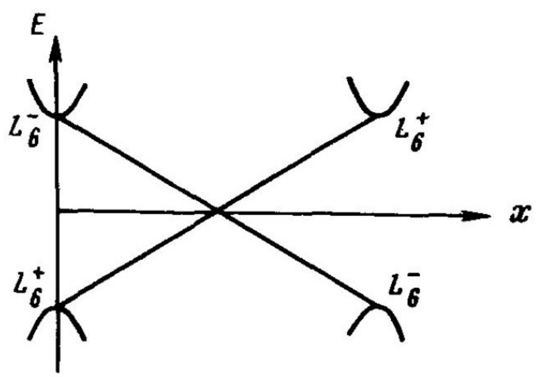
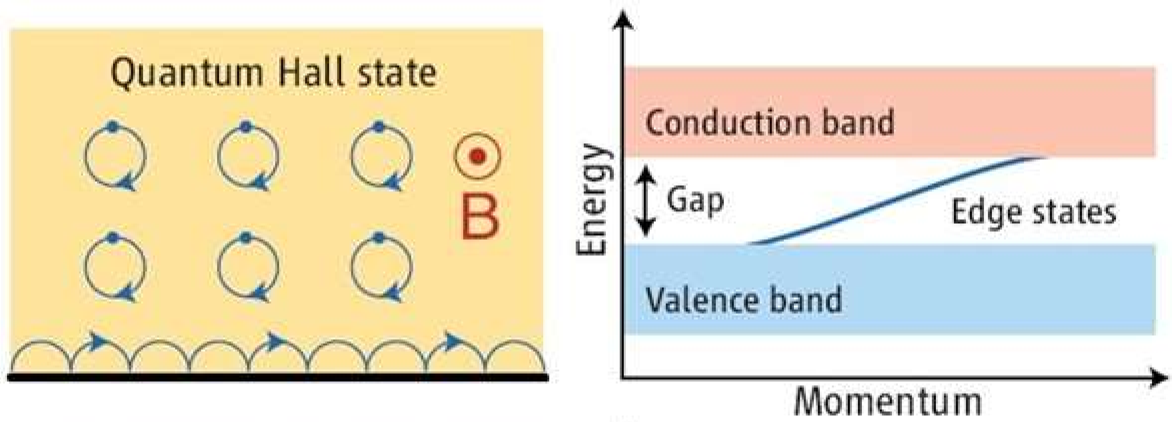


FIG. 1. Inversion of the $L_6^{\pm}$ bands in $Pb_{1-x}Sn_xTe(Se)$ involving a change in the composition.

Topological Quantum Materials



Quantum Hall state permits conduction in one dimension along sample boundary

Topological Insulators in Three Dimensional Solids

ARTICLES
PUBLISHED ONLINE: 10 MAY 2009 | DOI: 10.1038/NPHYS1270
nature physics

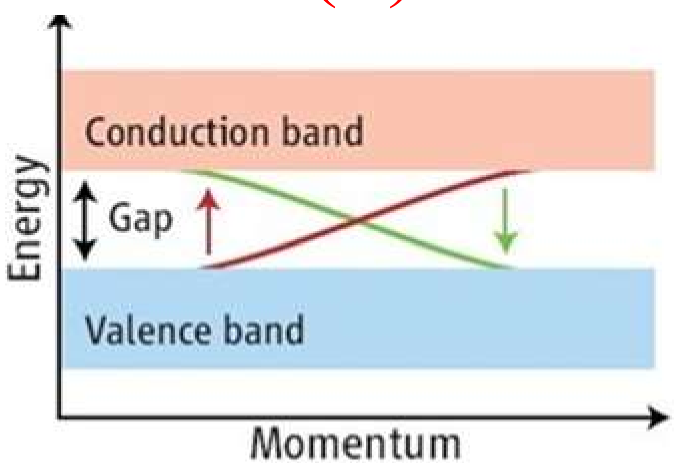
Topological insulators in Bi_2Se_3, Bi_2Te_3 and Sb_2Te_3 with a single Dirac cone on the surface

Haijun Zhang[1], Chao-Xing Liu[2], Xiao-Liang Qi[3], Xi Dai[1], Zhong Fang[1] and Shou-Cheng Zhang[3]*

Dirac cones dispersion with Fermi surface as a circle. Spins are perpendicular to momentum

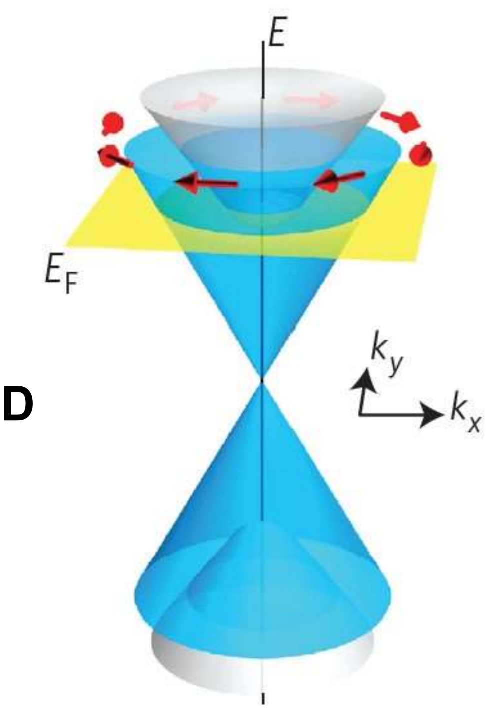
Edge states in 2D become surface states in 3D
The electron energy is a "relativistic" linear function of momentum

$$E(k) = vk$$



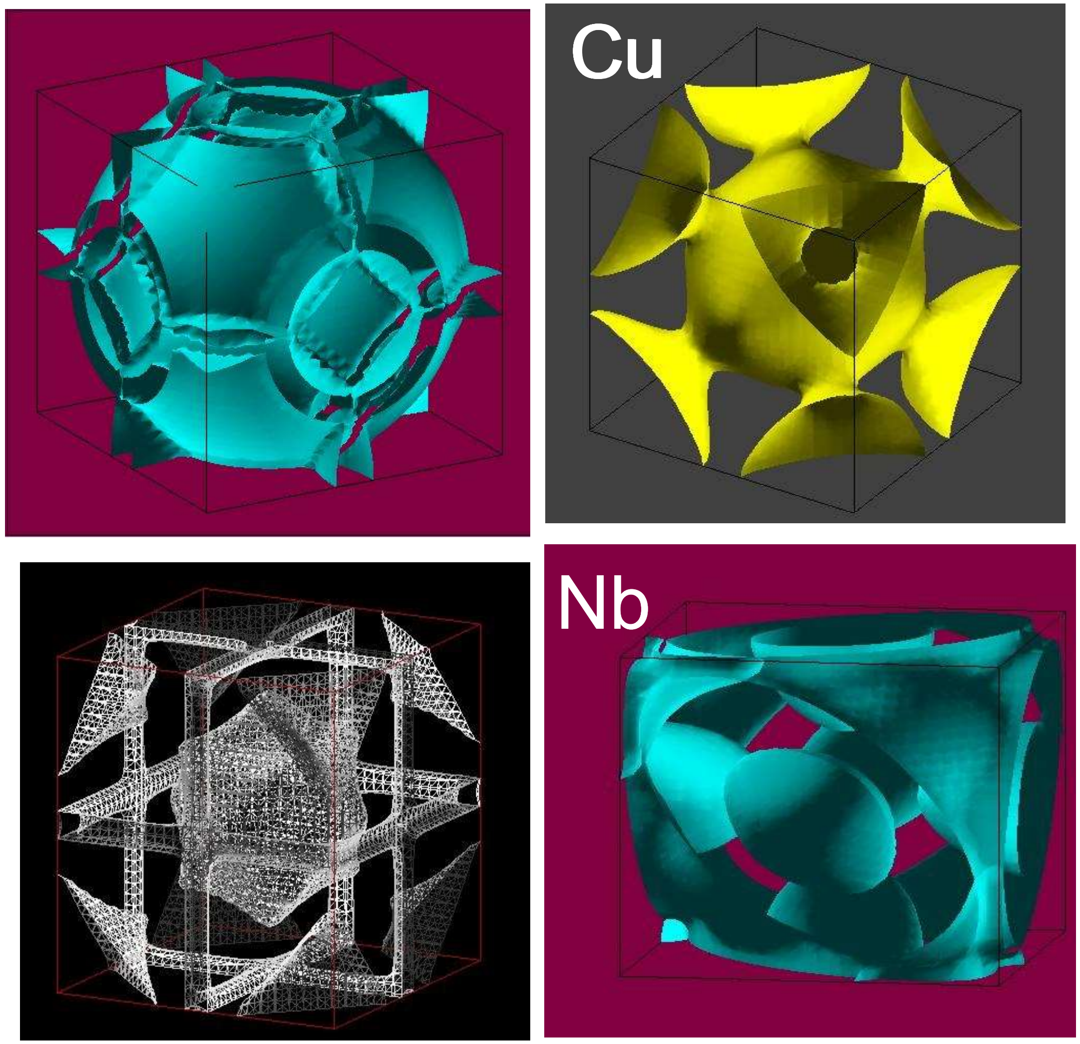
2D

3D



TRANSPORT

Fermi surfaces of regular metals are complex. No guiding principles to design good conductors



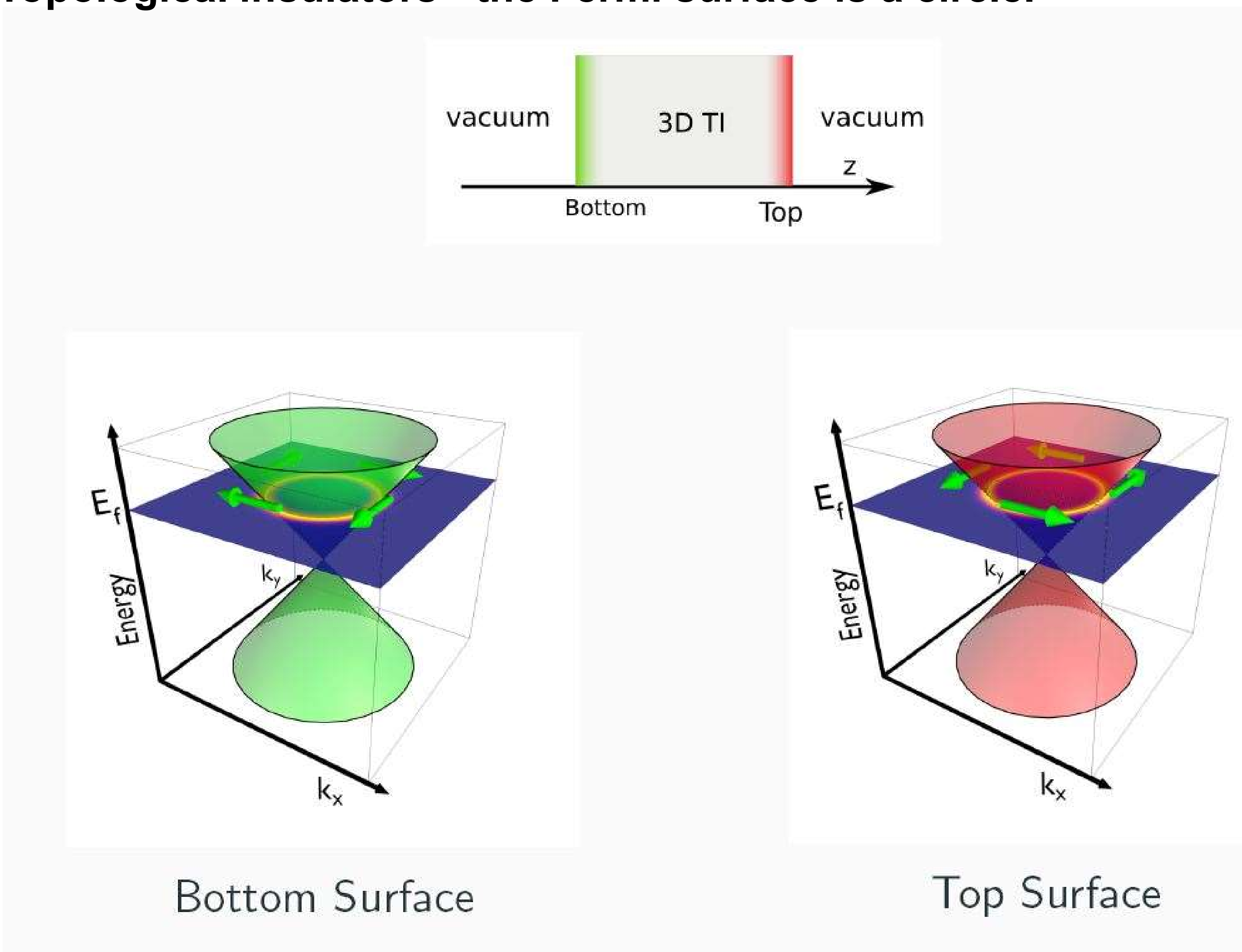
$$\frac{1}{\tau(\varepsilon_{\mathbf{k}})} = \sum_{\mathbf{k}'} (1 - \cos\,\theta_{\mathbf{k}\mathbf{k}'}) W_{\mathbf{k}\mathbf{k}'} \frac{1 - f(\varepsilon')}{1 - f(\varepsilon)},$$

In transport (such as electrical conductance) backscattering ($\theta_{kk'}=\pi$) dominates

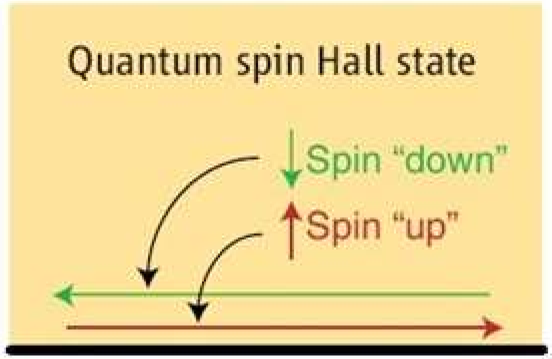
Fermi surfaces in topological quantum materials are simple!

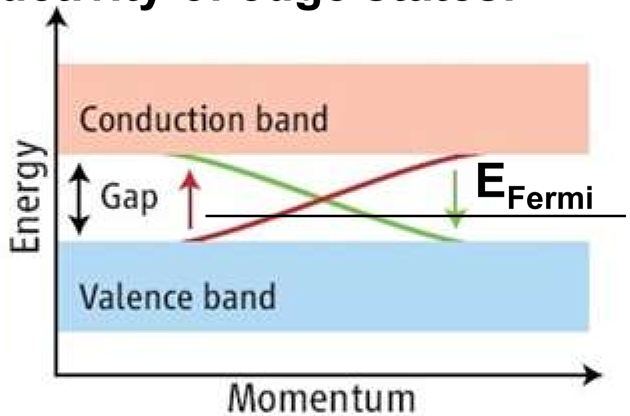
2D Topological insulators - the Fermi surface is a couple of points.

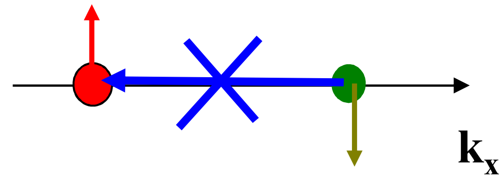
3D Topological insulators - the Fermi surface is a circle.



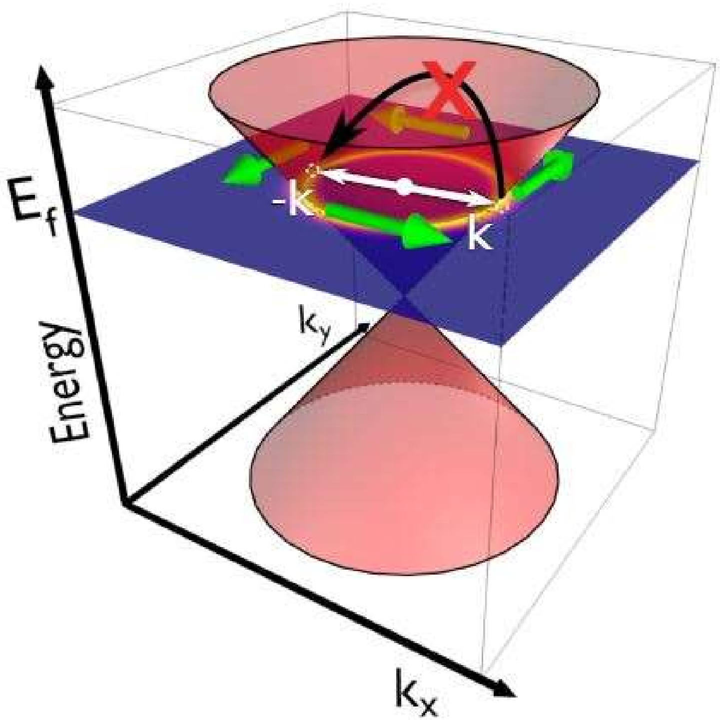
The backscattering in 2D topological insulators is completely suppressed - Disorder tolerant conductivity of edge states!



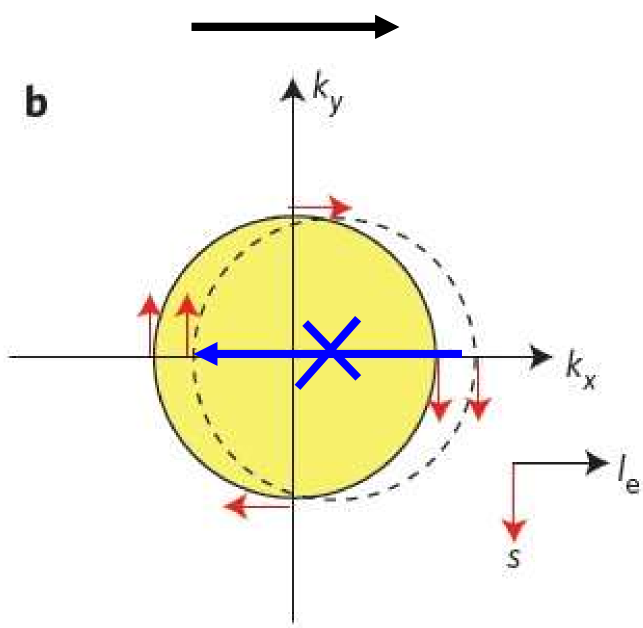




The 180 degrees backscattering in 3D topological insulators is also suppressed!

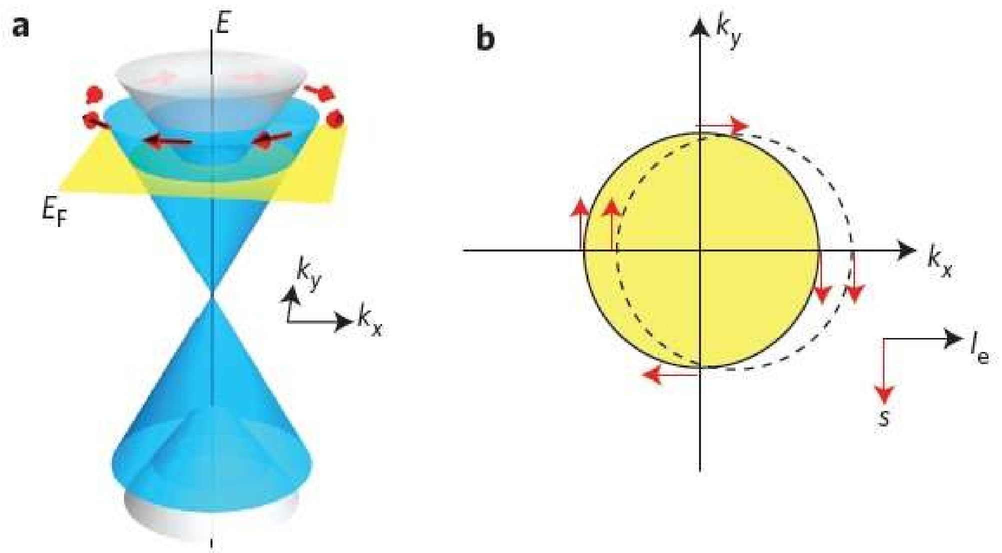


$j_x=\sigma_{xx}E_x$



Spin Polarized Currents in 3D Topological Insulators

Spins in TIs can carry information for novel spintronic devices.

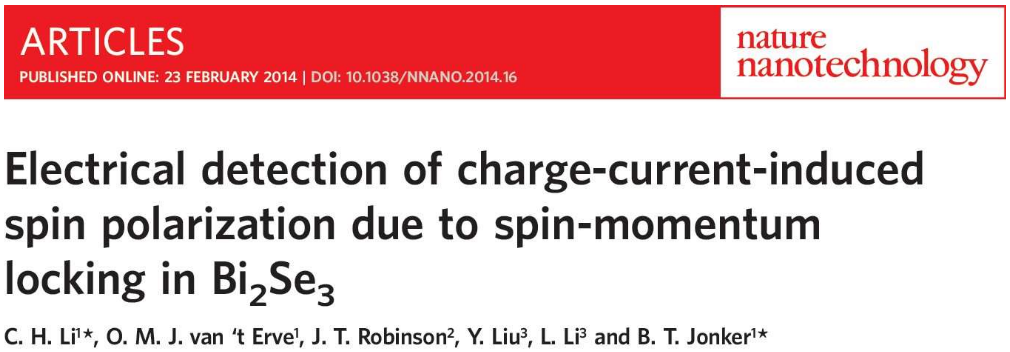


Charge current along "x" induces spin current with polarization along "-y"

- So far discussion on single-surface phenomenon
- Charge current
- → Fermi surface shift

  → Spin accumulation

Topological nature of band structures is ignored!



ARTICLES
PUBLISHED ONLINE: 23 FEBRUARY 2014 | DOI: 10.1038/NNANO.2014.16
nature nanotechnology

Electrical detection of charge-current-induced spin polarization due to spin-momentum locking in Bi_2Se_3

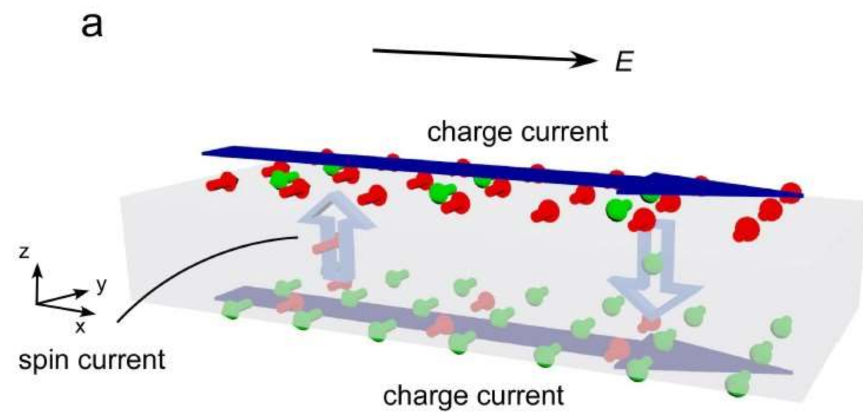
C. H. Li[1]*, O. M. J. van 't Erve[1], J. T. Robinson[2], Y. Liu[3], L. Li[3] and B. T. Jonker[1]*

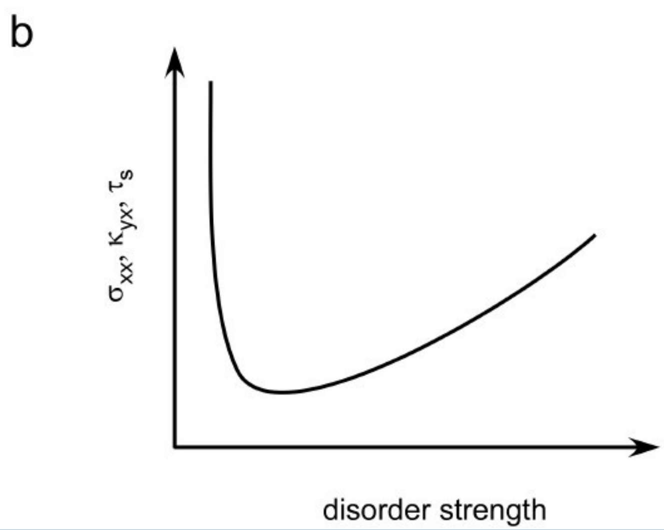
Spin Dynamics in 3D TIs

OUR PICTURE : An electric field driving charge current at the surface also induces a transverse spin current in the bulk.

Opposite spins accumulate on top and bottom surfaces, leading to charge current

However, spin is not conserved, and relaxes quickly





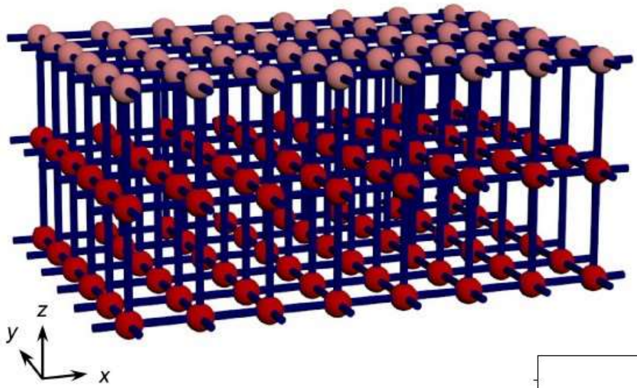
OUR FINDING: At high disorder, conductivity and spin relaxation time increase with disorder in contrast with common belief

A practical strategy for enhancement of surface spin polarization is the increase of nonmagnetic impurity concentration (A. Peng, Y. Yang, R. Singh, SS, D. Yu Nat.Comm. 2016).

Simulations of Transport in TI Surface

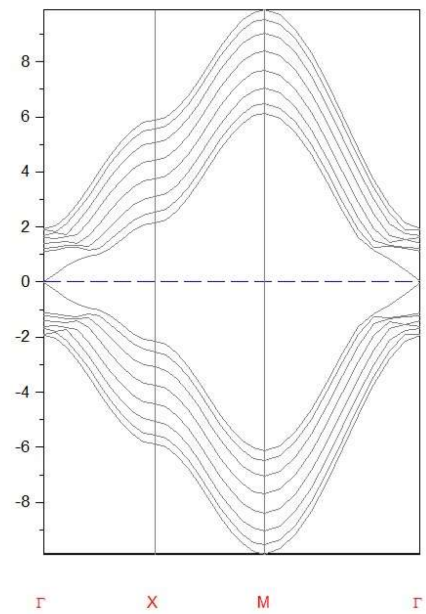
A realistic 4-band tight-binding model with parameters fitted to Bi2Se3

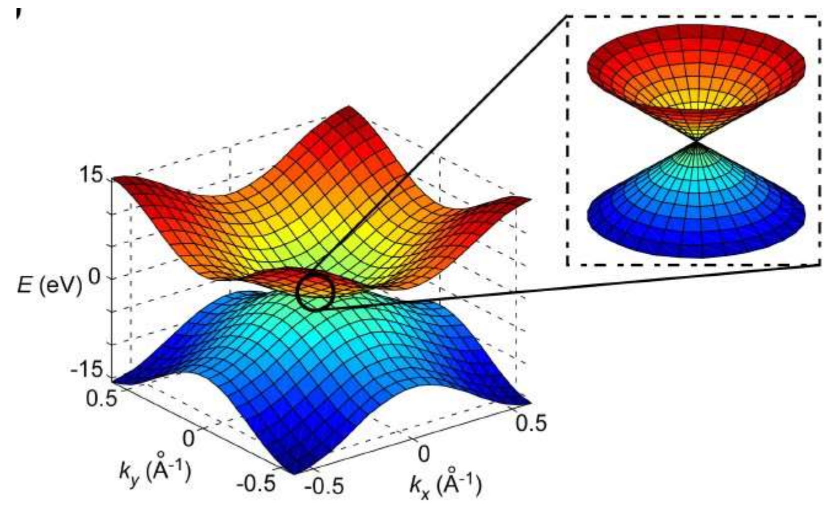
$$H_0(\boldsymbol{k}) = \left(A \sum_{i=x,y} \sin k_i a \alpha_i + A_z \sin k_z a_z \alpha_z \right) + \left[\Delta - 4 \left(B \sum_{i=x,y} \sin^2 \frac{k_i a}{2} + B_z \sin^2 \frac{k_z a_z}{2} \right) \right] \beta$$



The slab is infinite in xy directions and has a total number of N = 10 layers in the z direction (c-axis).

The energy dispersion of the surface states of a clean system. A Dirac cone exists around the Gamma point





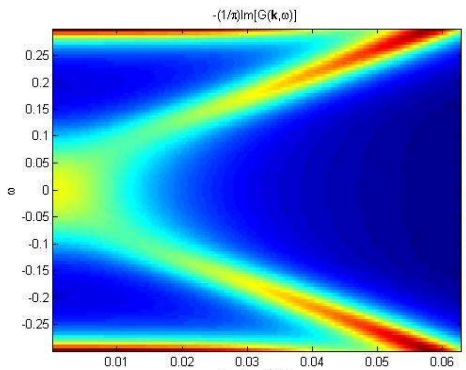
CPA Simulation of Disorder Affected Surface States

Top and bottom layers are subject to vacancies, each surface atom has a probability of c to be occupied by a vacancy and (1 - c) to be intact.

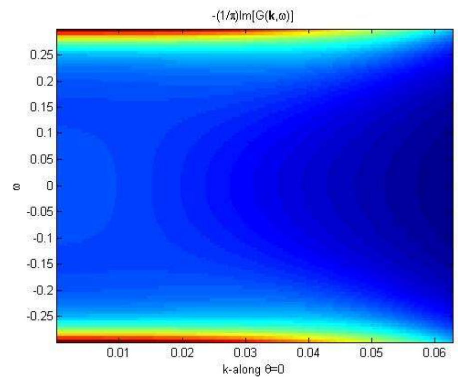
$$\Sigma(\omega) = cU[1 - G(\omega)(U - \Sigma(\omega))]^{-1} \qquad G(\omega) = \sum_{\boldsymbol{k}} [\omega - H_0(\boldsymbol{k}) - \Sigma(\omega)]^{-1}$$

The spectral function $-(1/\pi)\mathrm{Im}G(\boldsymbol{k},\omega)$ obtained via CPA plotted along the $\Gamma - \mathrm{X}$

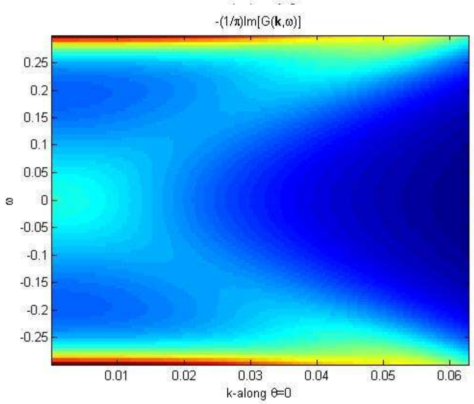
c=0.001



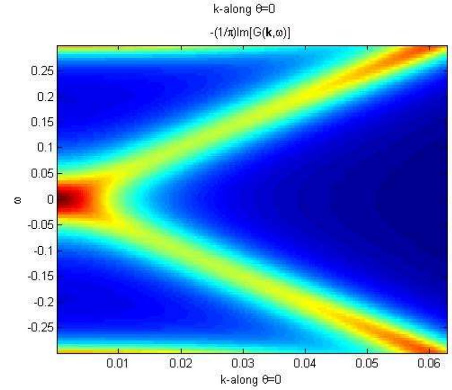
c=0.01



c=0.1



c=0.5



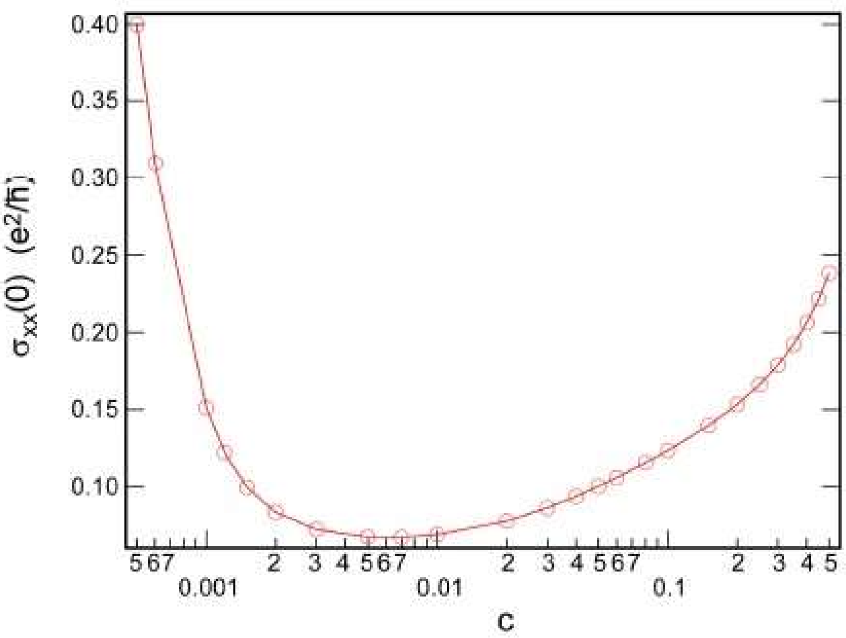
Dirac cone reappears at high disorder!

Surface Charge Conductivity

Calculations of conductivity based on Kubo-Greenwood formalism

$$\sigma_{xx}(0) = \frac{e^2}{4\pi^3} \int \mathrm{Tr}[v_x(\boldsymbol{k})\mathrm{Im}G(\boldsymbol{k},\mu)v_x(\boldsymbol{k})\mathrm{Im}G(\boldsymbol{k},\mu)]\mathrm{d}^2\boldsymbol{k}$$

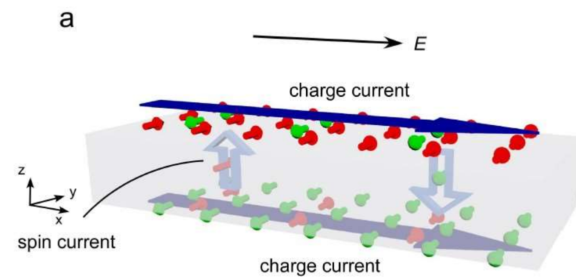
Conductivity σ_{xx} plotted against the impurity concentration (c). The Fermi level position was fixed at 0.13 eV.



Contrasted to conductivity of a single layer of atoms with same band structure (identical shape as TI surface state, but no spin current via bulk): conductivity monotonically decreases towards zero, even in high disorder range (similar to graphene)

Computation of Bulk Spin Hall Conductivity

Spin Hall conductivity has two contributions: Fermi states and Berry phase term contributed by all states occupied! (Sinova et. al, RMP in press 2015)

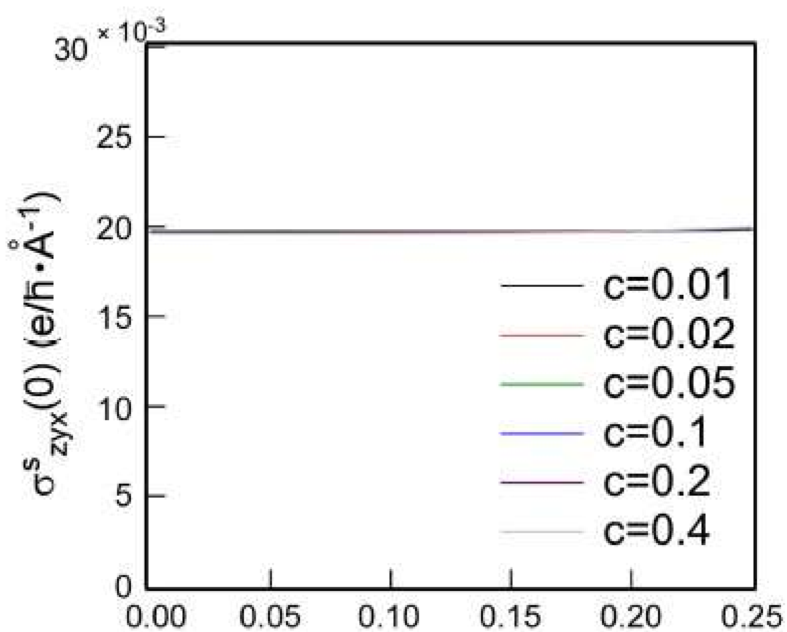


$$j^s_{ij} = \sum_k \sigma^s_{ijk} E_k$$

$$\begin{aligned}\sigma^s_{zyx}(0) &= \frac{e}{4\pi}\mathrm{Tr}[j^s_{zy}G(\mu)v_xG^\dagger(\mu) - j^s_{zy}G^\dagger(\mu)v_xG(\mu)] \\ &+\frac{e}{4\pi}\int_{-\infty}^{\mu}\mathrm{d}\lambda\mathrm{Tr}\left[-j^s_{zy}\frac{\mathrm{d}G(\lambda)}{\mathrm{d}\lambda}v_xG(\lambda) + j^s_{zy}G(\lambda)v_x\frac{\mathrm{d}G(\lambda)}{\mathrm{d}\lambda} + \mathrm{h.c.}\right]\end{aligned}$$

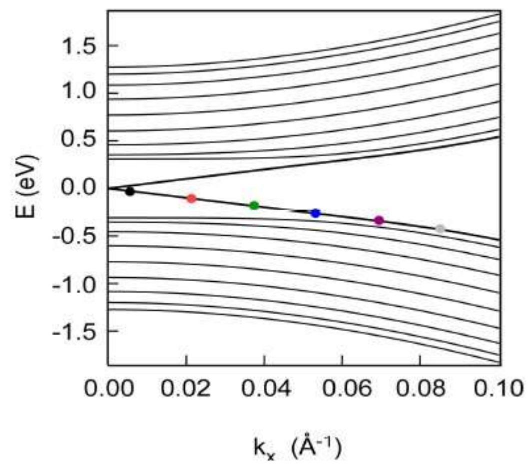
Spin Hall conductivity is insensitive to disorder, all-states term dominates!

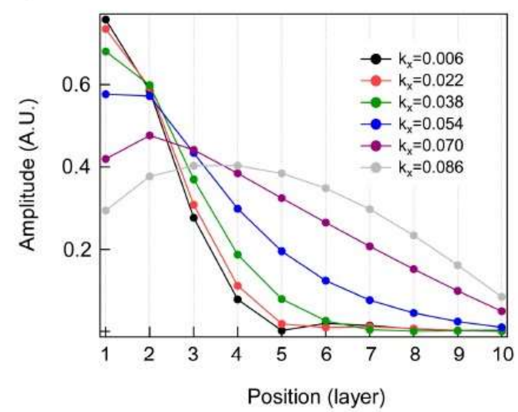
Non-dissipative nature of the spin current, as already demonstrated for a wide class of traditional semiconductors, Murakami, Nagaosa, Zhang Science, 301, 1348-1351 (2003)



Physical Picture of Spin Current via Topological Connection between Bulk and Surface States

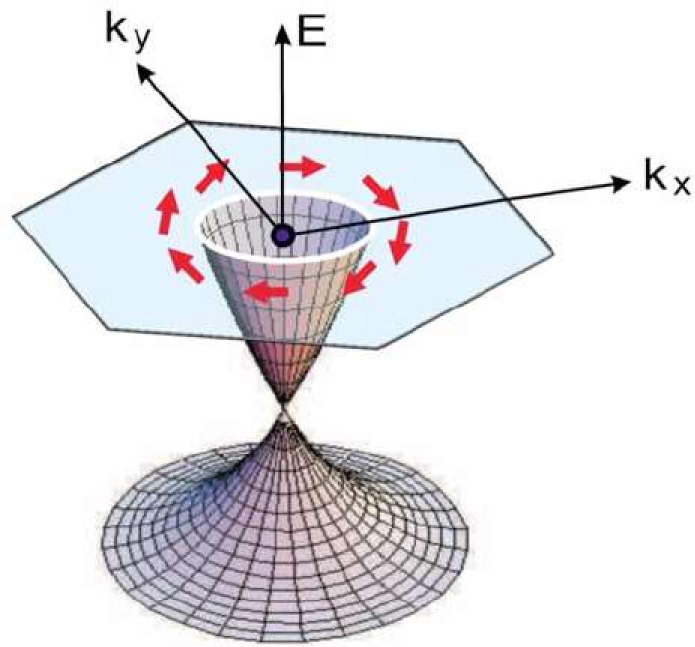
Evolution of wave functions along the colored dots: As wave vector becomes larger, wave function evolves from being localized @ surface to the bulk.

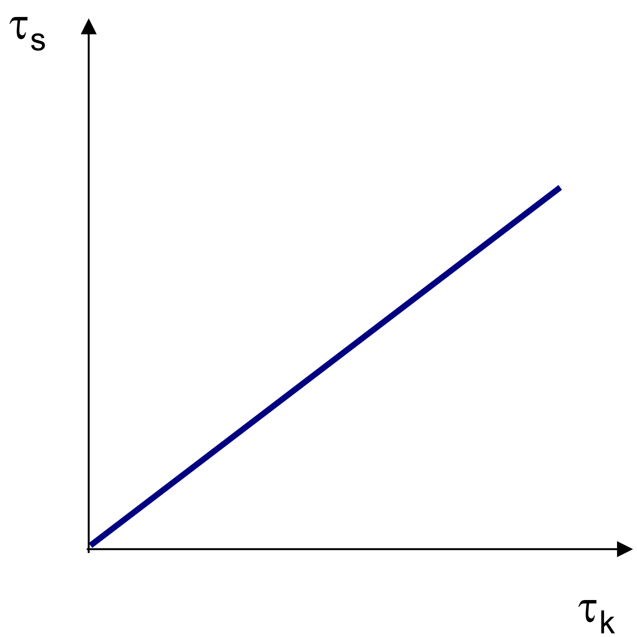




Spin Relaxation Mechanism

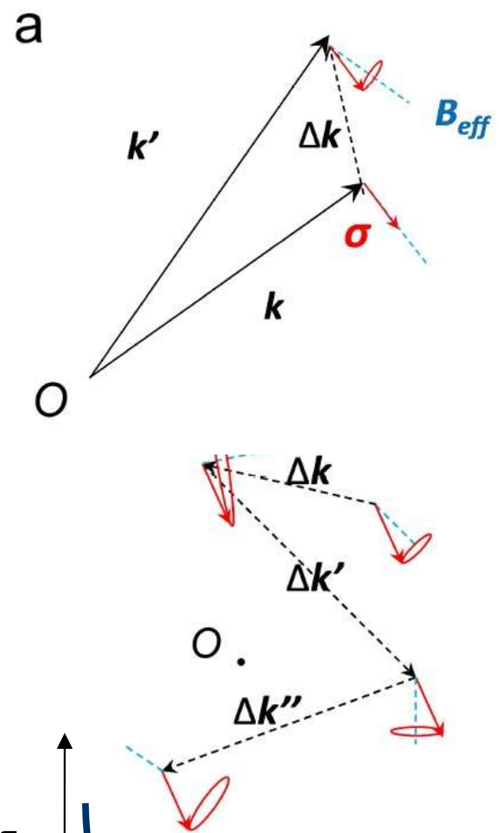
Spins injected onto the surface suffer from immediate relaxation when it scatters from k to k' due to famous spin-momentum locking property of TIs:





Spin relaxation time τ_s determines spin density accumulated on the surface. If disorder is small, spin relaxation τ_s and momentum relaxation times τ_k are proportional to each orther due to spin-momentum lock-up

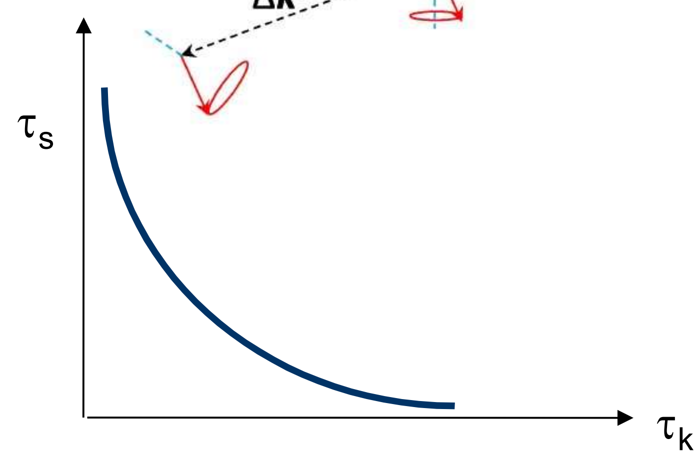
Spin Relaxation Mechanism under High Disorder



• Frequent scatterings: electrons rapid momentum change, spin does not have time to follow the instantaneous energy eigenstate. Instead, spin precesses about instantaneous energy eigenstate, serving as "magnetic field"

• Frequent scatterings change the precession axis. During the interval of two consecutive scatterings the spin can only precess for a small angle. The more frequent the scatterings are and consequently spin can preserve its original direction for a longer time.

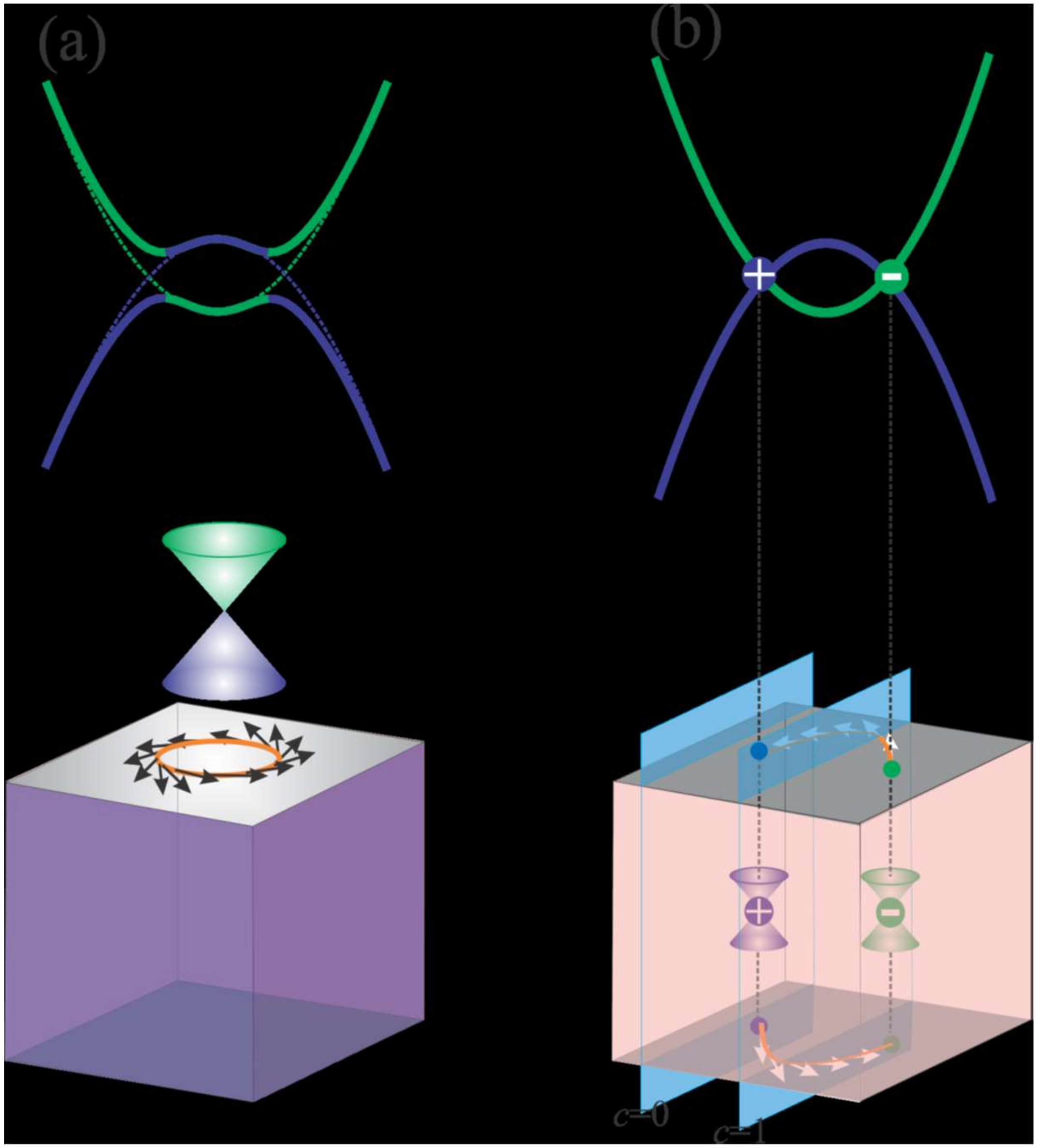
Achieved by higher concentration of disorder!



Analogous to Dyakonov-Perel (1972) mechanism in semiconductors: spin relaxation time is inverse to momentum relaxation time

Strategy for enhancing surface spin polarization is to increase nonmagnetic impurity concentration

From Topological Insulators to Weyl Semimetals

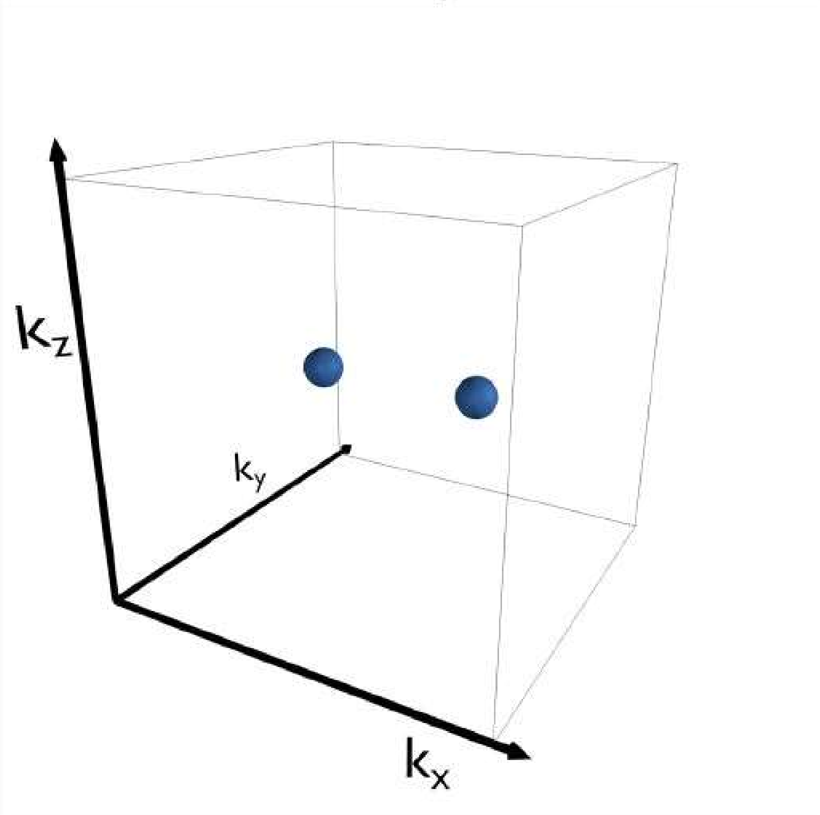


(Wan, Turner, Vishwanath, SS, PRB2011)

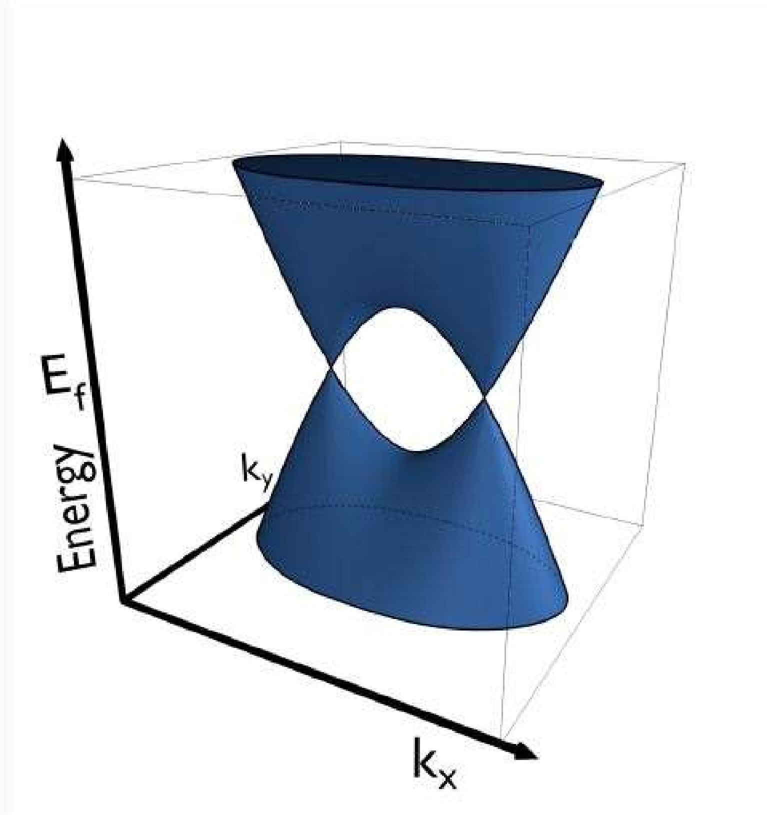
Weyl Semi-Metals

A 3D material with a band structure which is fully gapped except at isolated points where a single conduction and a single valence band touch to form a linear dispersion relation.

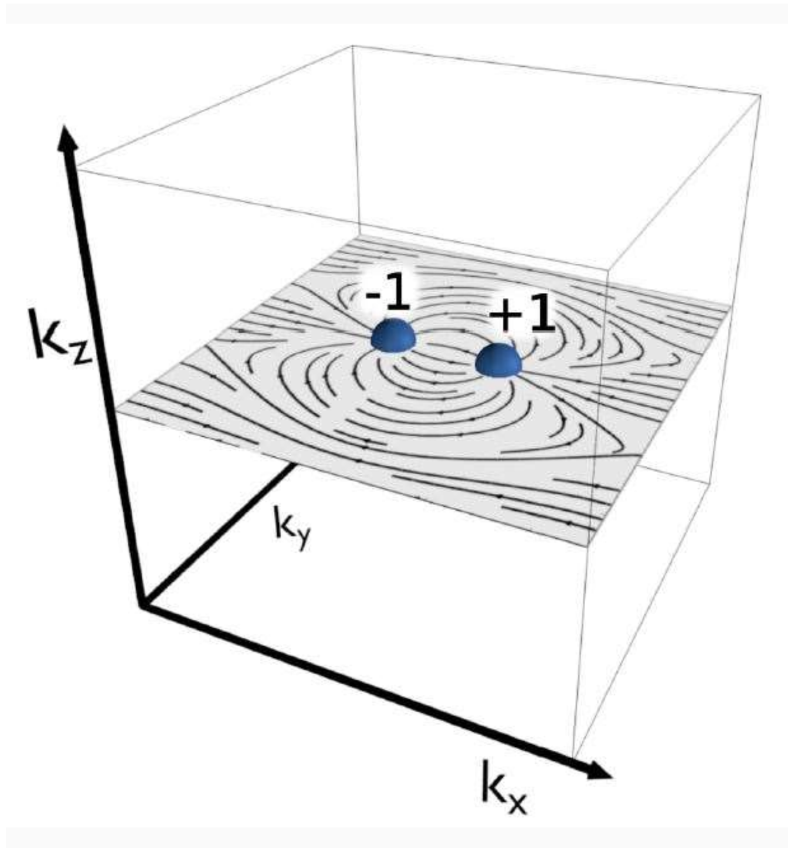
Fixed $E_f \approx 0$



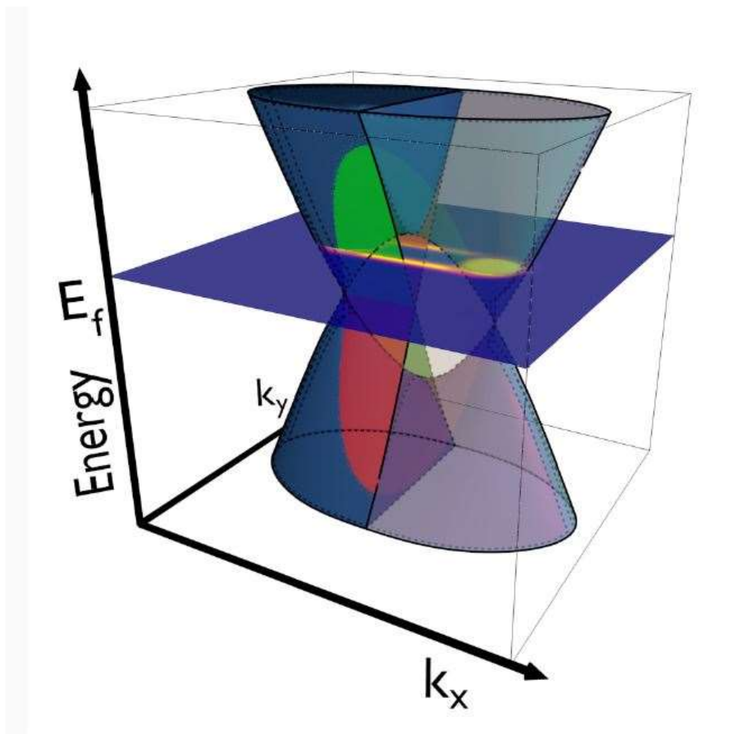
Fixed $k_z = 0$



Weyl Points act as Monopoles of Berry Flux



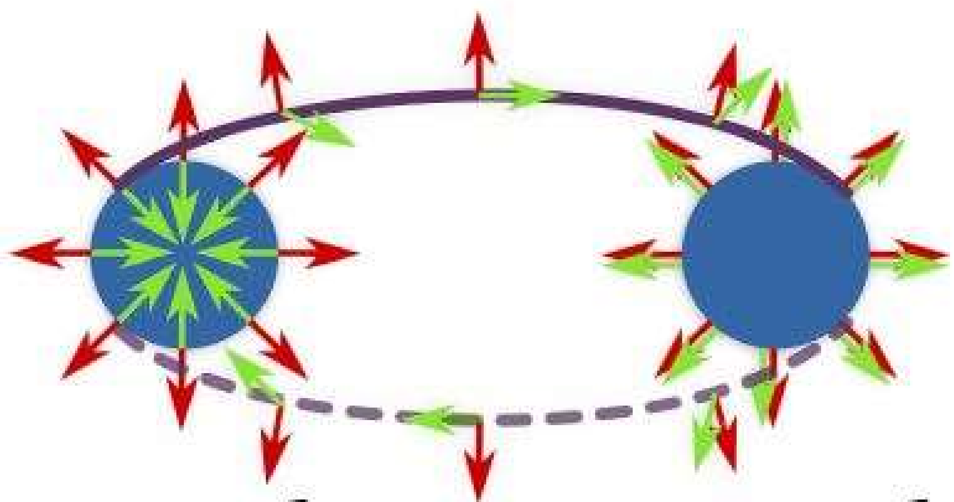
Monopoles Give Rise to Surface States and Fermi Arcs



Spin Arrangement along Fermi Arc States

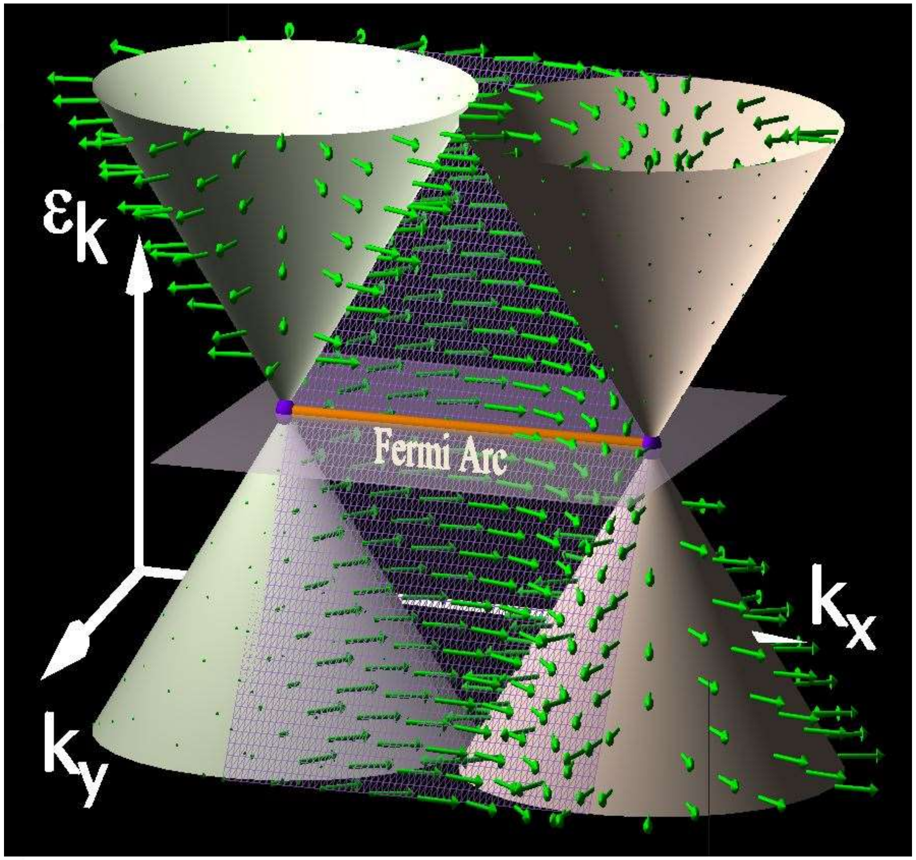
Weyl equation,

$$\hat{H}_{\text{weyl}} = \sum_{i \in \{x,y,z\}} m_i |v_i| k_i \hat{\sigma}_i,$$



m_x = -1 m_x = +1

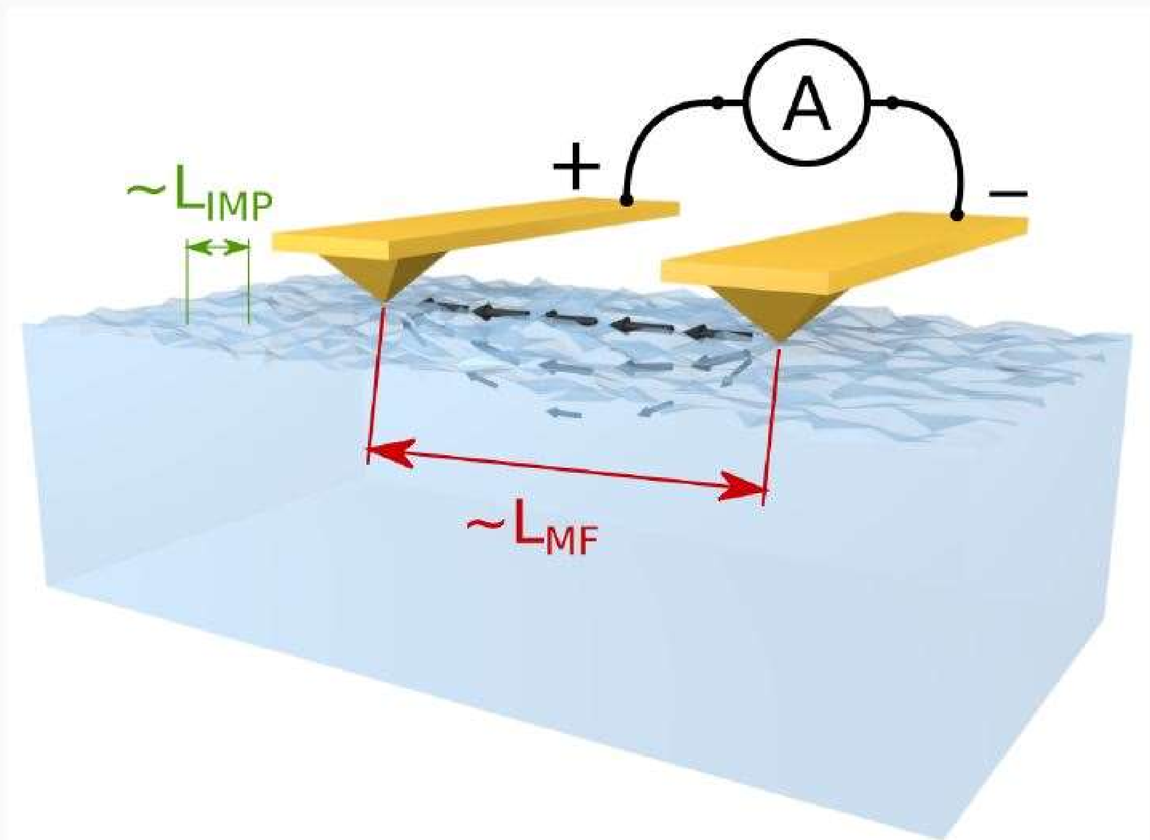
m_y = -1 m_y = +1



Isotropic Weyl nodes

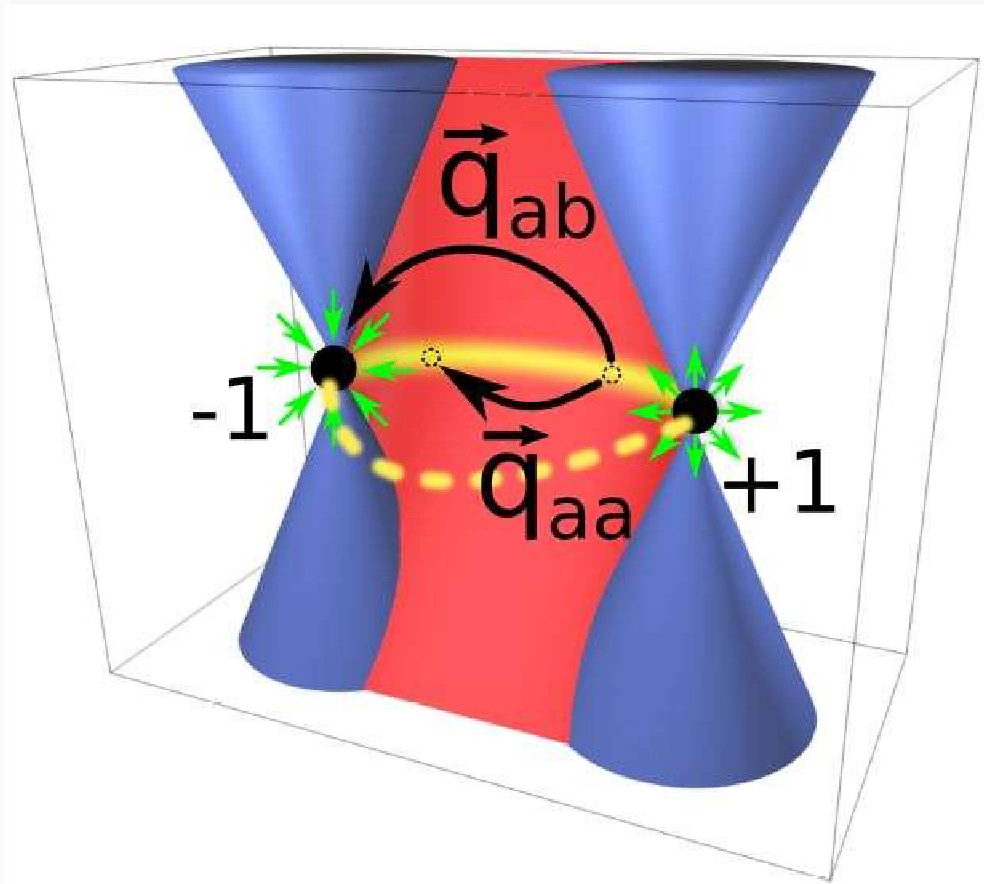
Measuring Surface Transport Effects in Semimetals

$$\vec{j}_{surf}(\vec{r}) = \int \sigma(\vec{r}, \vec{r}') \cdot \vec{E}_{surf}(\vec{r}')d^3r'$$



Intra-Arc and Arc-Bulk Scattering in Weyl Semimetals

There are two scattering processes on a single surface, arc-to-bulk ($\vec{q}_{ab}$) and intra-arc ($\vec{q}_{aa}$) scattering,



With negligible bulk density of states at the Fermi surface, surface transport properties are dominated by intra-arc scattering.

Transport Relaxation Times

Electrical Resistivity $\rho = \sigma^{-1} \sim 1/\tau$

Introducing the transport coefficient,

$$\lambda_{tr}(\vec{q}) = \sum_k (v_{kx} - v_{kx+qx})^2 |V_{k,k+q}|^2 \delta(\epsilon_k - \epsilon_f)\delta(\epsilon_{k+q} - \epsilon_f)$$

$$\lambda_{tr} = \frac{\sum_{\vec{q}} \lambda_{tr}(\vec{q})}{\sum_k v_{kx}^2 \delta(\epsilon_k - \epsilon_f)},$$

the transport relaxation times are given by,

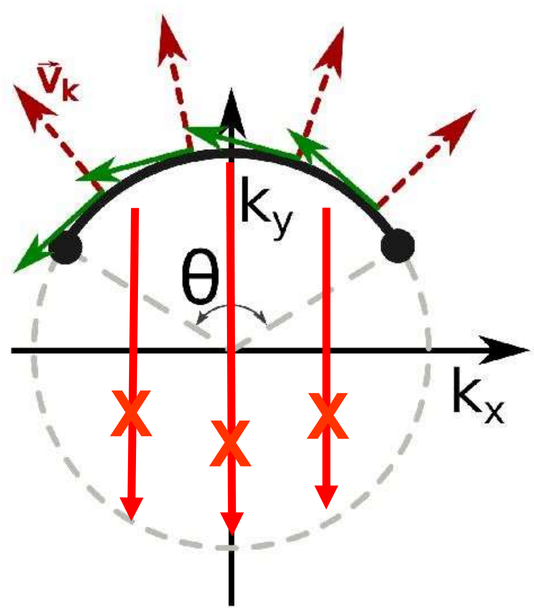
$$\frac{1}{\tau_{imp}} = \frac{2\pi}{\hbar} n_{imp} \lambda_{tr}^{imp},$$

$$\frac{1}{\tau_{ep}} = \frac{2\pi}{\hbar} n_{ph} \lambda_{tr}^{ep},$$

Single Fermi Arc Scattering is Strongly Suppressed

$$\lambda_{tr}(\vec{q}) = \sum_{k}(v_{kx} - v_{kx+qx})^2 |V_{k,k+q}|^2 \delta(\epsilon_k - \epsilon_f)\delta(\epsilon_{k+q} - \epsilon_f)$$

A semicircular arc model: angle q spans from 0 (straight arc) to 2π (circle) by keeping the length $s_F = r_F\theta$ constant

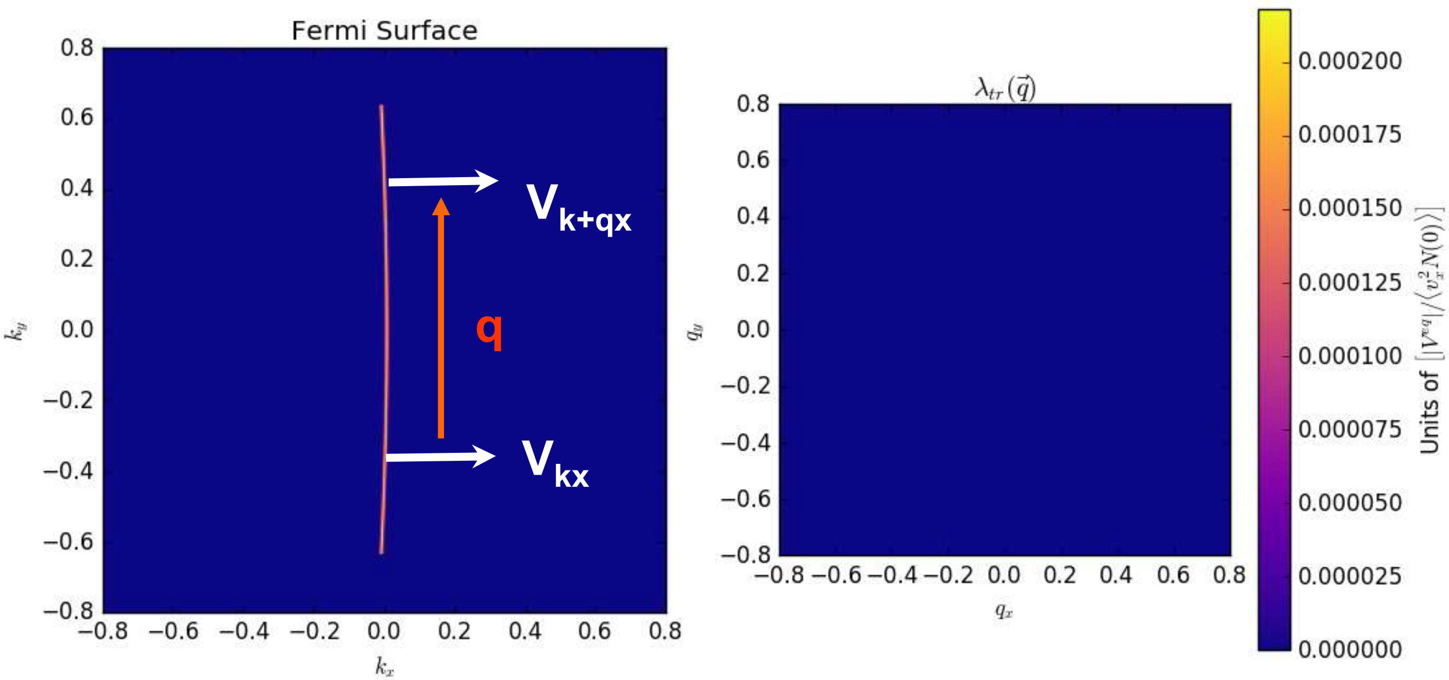


No backscattering for single arc, only side scattering exists

Transport Coefficient as a Function of Arc Curvature

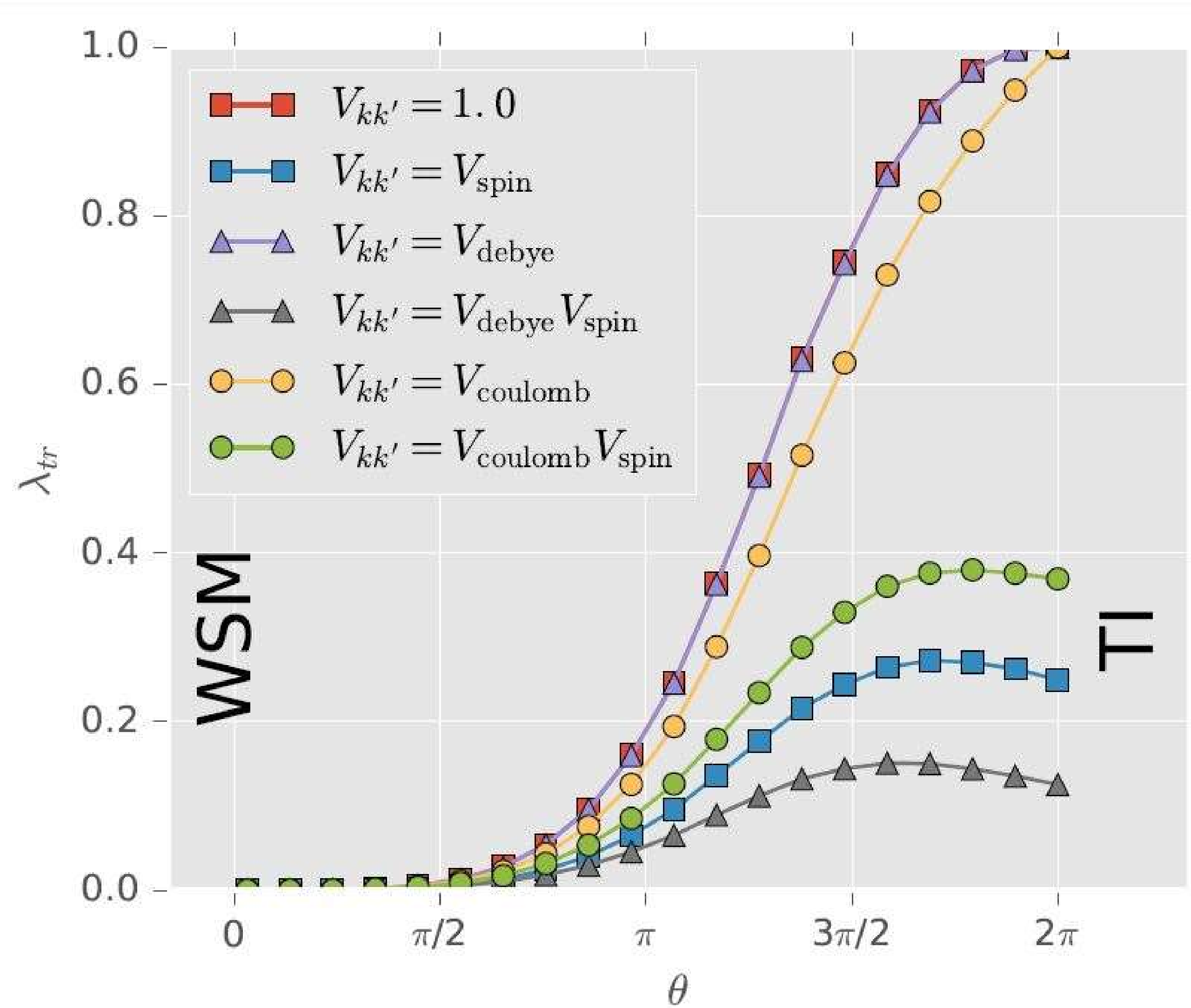
Phase space for transport scattering:

$$\lambda_{tr}(\vec{q}) = \sum_k (v_{kx} - v_{kx+qx})^2 \qquad \delta(\epsilon_k - \epsilon_f)\delta(\epsilon_{k+q} - \epsilon_f)$$



$j_x = \sigma_{xx} E_x$

Transport Coefficient as a Function of Arc Curvature

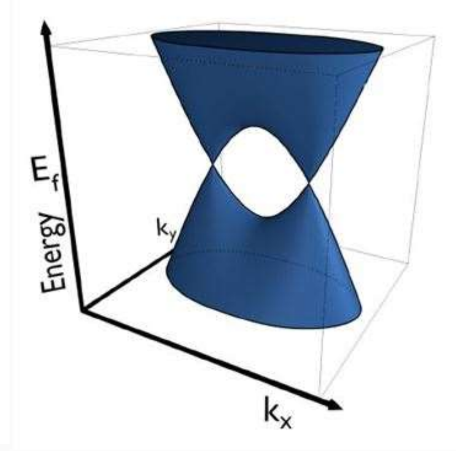


Transport coupling constant calculated for several choices of matrix elements of the electron phonon interaction. It disappears in the limit of straight arc.

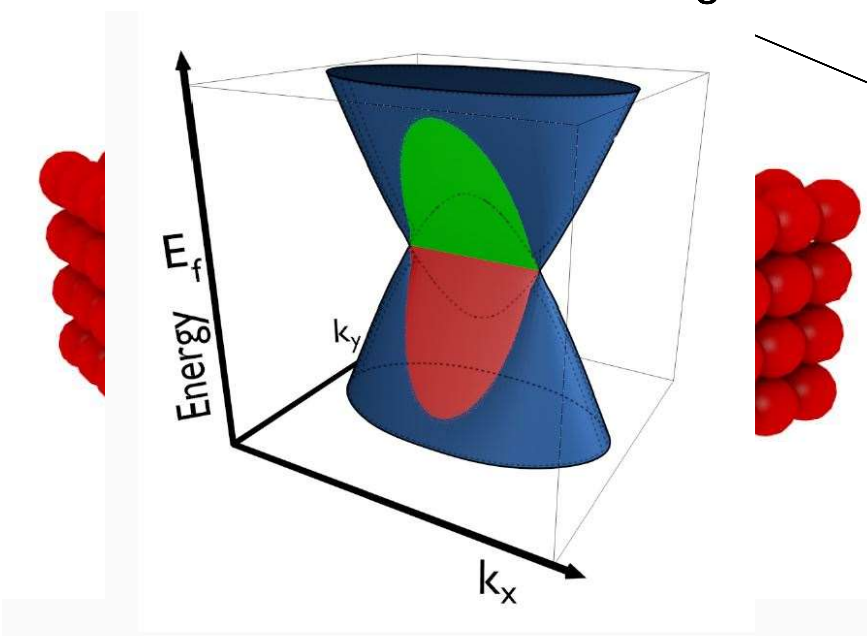
CPA Simulations of Disorder: TB Model for Weyl Semimetal

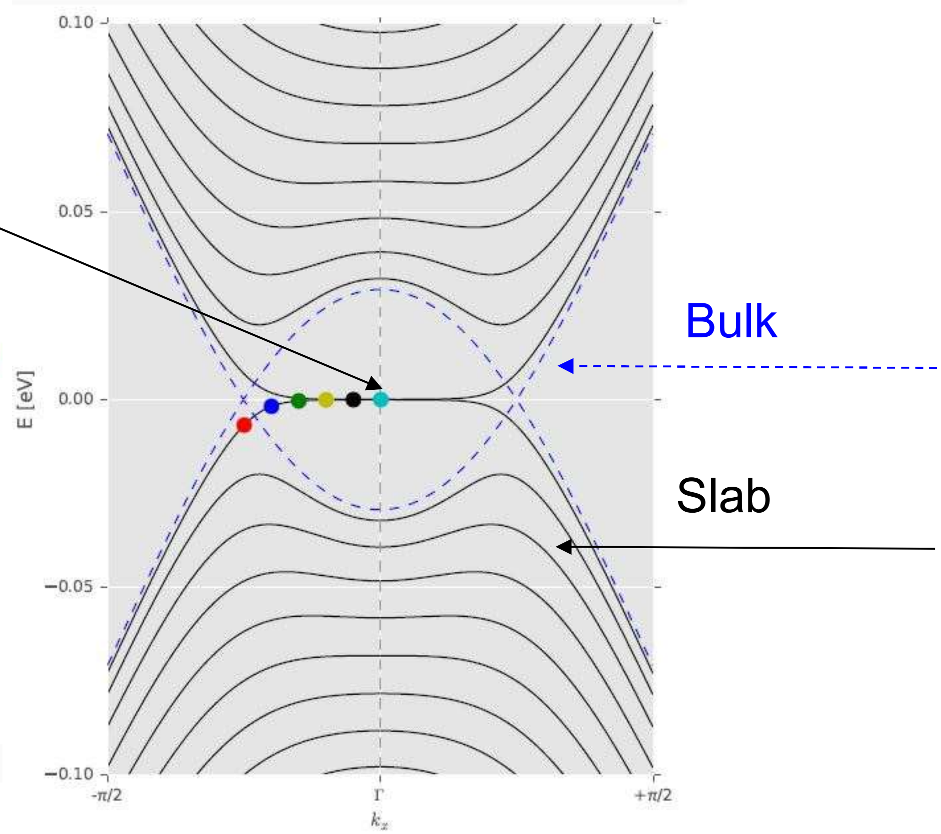
Minimal two-band 3D Weyl semimetal model,

$$\hat{H}(\vec{k}) = [2t_x(\cos(k_x) - \cos(k_0)) + m(2 - \cos(k_y) - \cos(k_z))]\,\hat{\sigma}_x + 2t_y \sin(k_y)\hat{\sigma}_y + 2t_z \sin(k_z)\hat{\sigma}_z$$



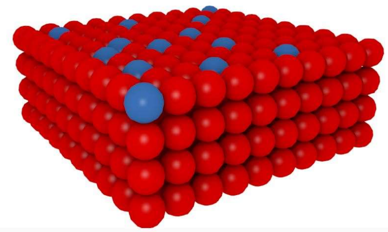
Slab calculation shows the straight arc:



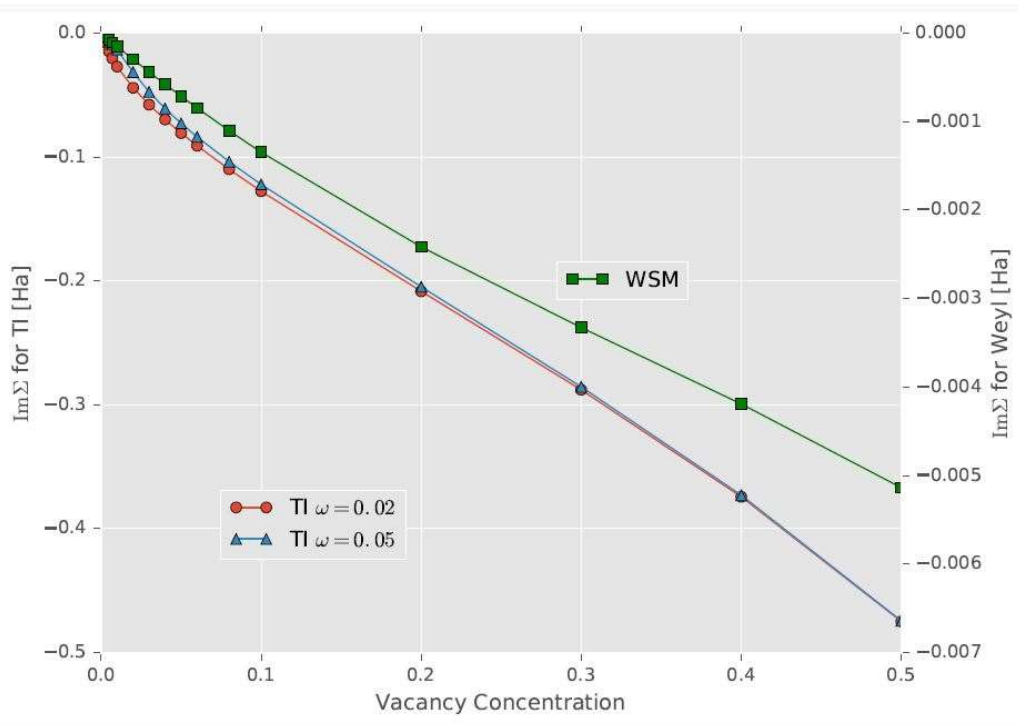


Effect of Surface Vacancies on Electron Self-Energies

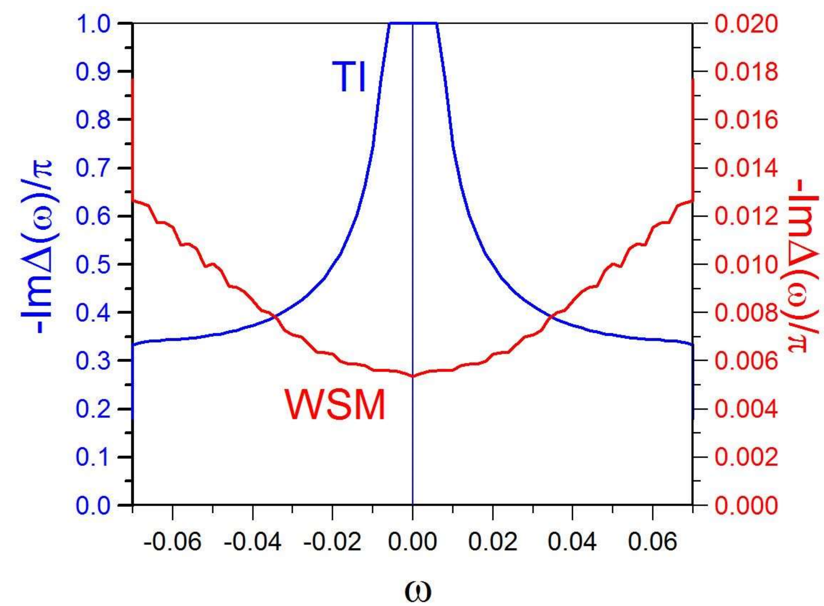
Slab simulations with Coherent Potential Approximation (CPA)



Imaginary part of self-energy for WSM model vs TI model with comparable setups



$$\Delta(\omega) = \omega - G_{loc}^{-1}(\omega)$$

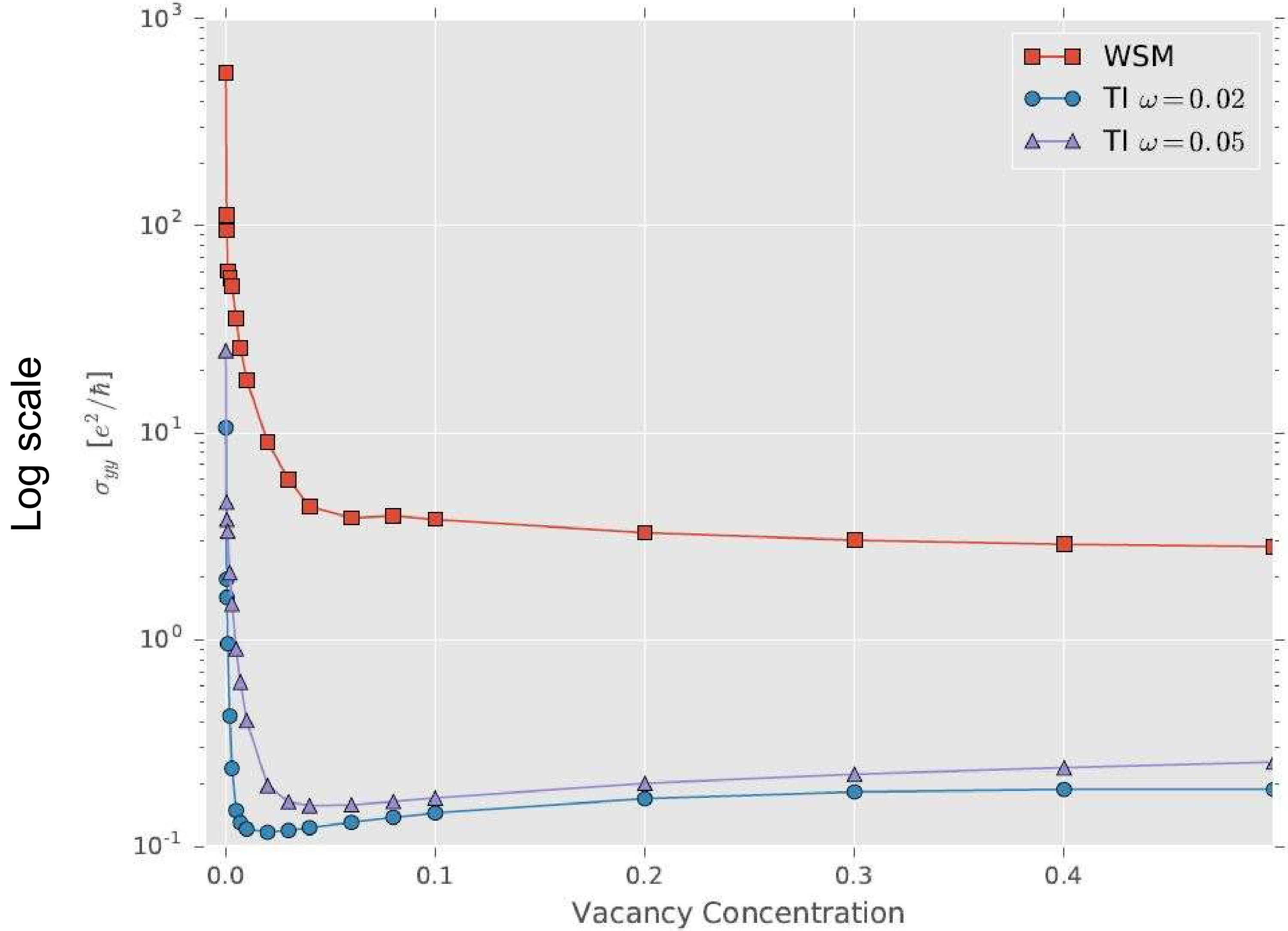


$Im\Sigma_{WSM} << Im\Sigma_{TI}$

Fermi arcs appear to be much more disorder tolerant than Dirac cones states of TIs!

Conductivity vs Surface Vacancy Concentration

Kubo Greenwood conductivity for WSM Model vs TI model with comparable setups



The conductivity of WSM is 10-100 times larger than that of TI

Recent Experimental Discoveries: TaAs

PHYSICAL REVIEW X **5**, 011029 (2015)

Weyl Semimetal Phase in Noncentrosymmetric Transition-Metal Monophosphides

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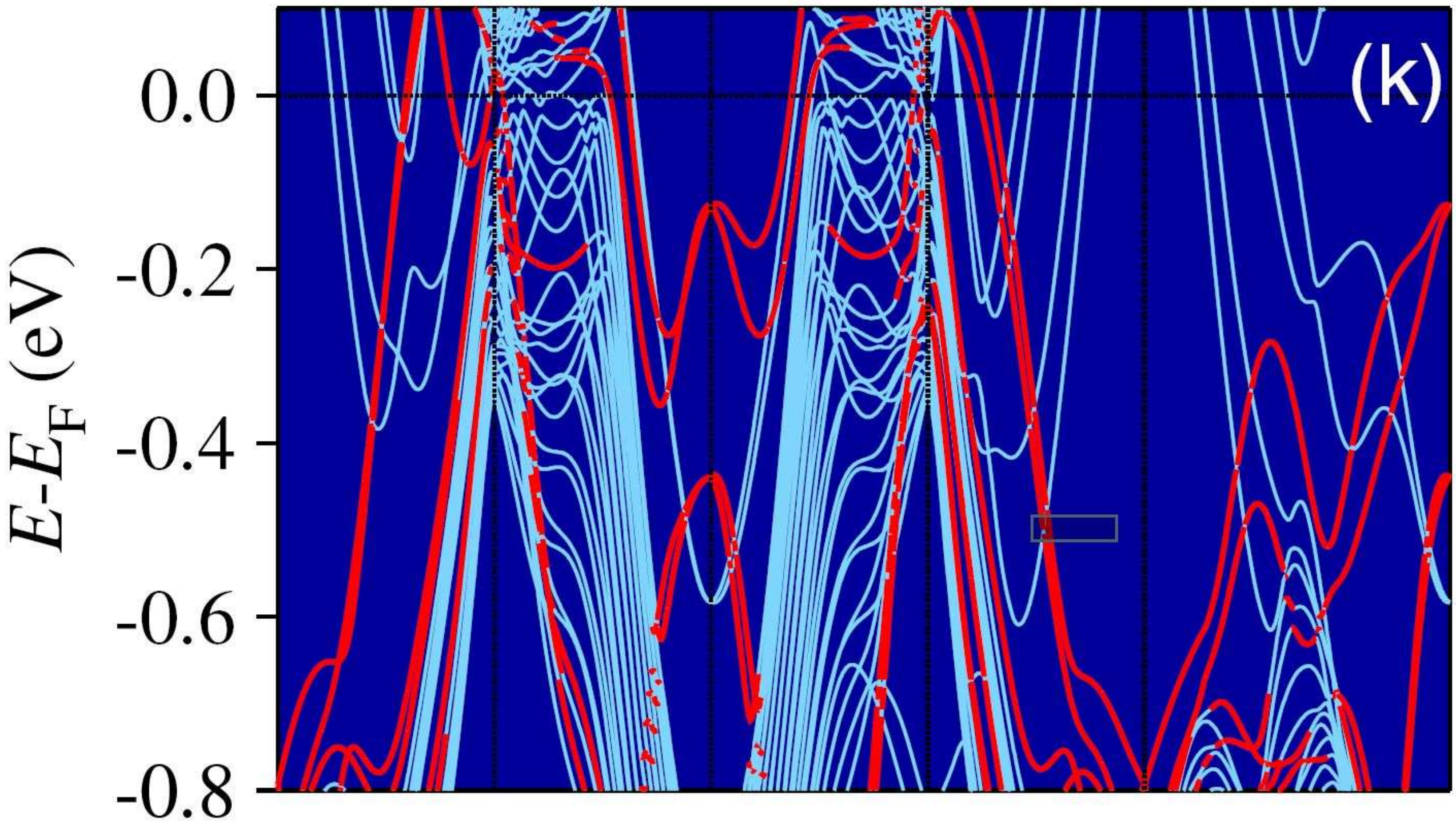
nature physics

Observation of Weyl nodes in TaAs

B. Q. Lv[1,2†], N. Xu[2,3†], H. M. Weng[1,4†], J. Z. Ma[1,2], P. Richard[1,4], X. C. Huang[1], L. X. Zhao[1], G. F. Chen[1,4], C. E. Matt[2], F. Bisti[2], V. N. Strocov[2], J. Mesot[2,3,5], Z. Fang[1,4], X. Dai[1,4], T. Qian[1★], M. Shi[2★] and H. Ding[1,4★]

Spaghetti for TaAs Slab



PHYSICAL REVIEW X **5,** 031013 (2015)

Experimental Discovery of Weyl Semimetal TaAs

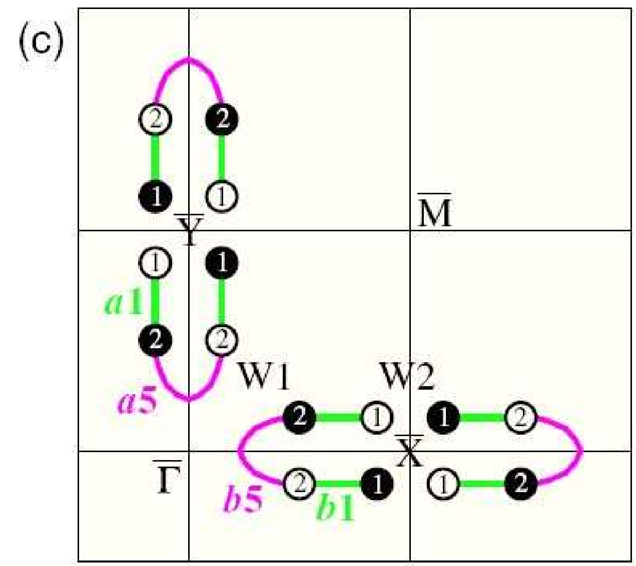
B. Q. Lv,[1] H. M. Weng,[1,2] B. B. Fu,[1] X. P. Wang,[2,3,1] H. Miao,[1] J. Ma,[1] P. Richard,[1,2] X. C. Huang,[1] L. X. Zhao,[1] G. F. Chen,[1,2] Z. Fang,[1,2] X. Dai,[1,2] T. Qian,[1,*] and H. Ding[1,2,†]

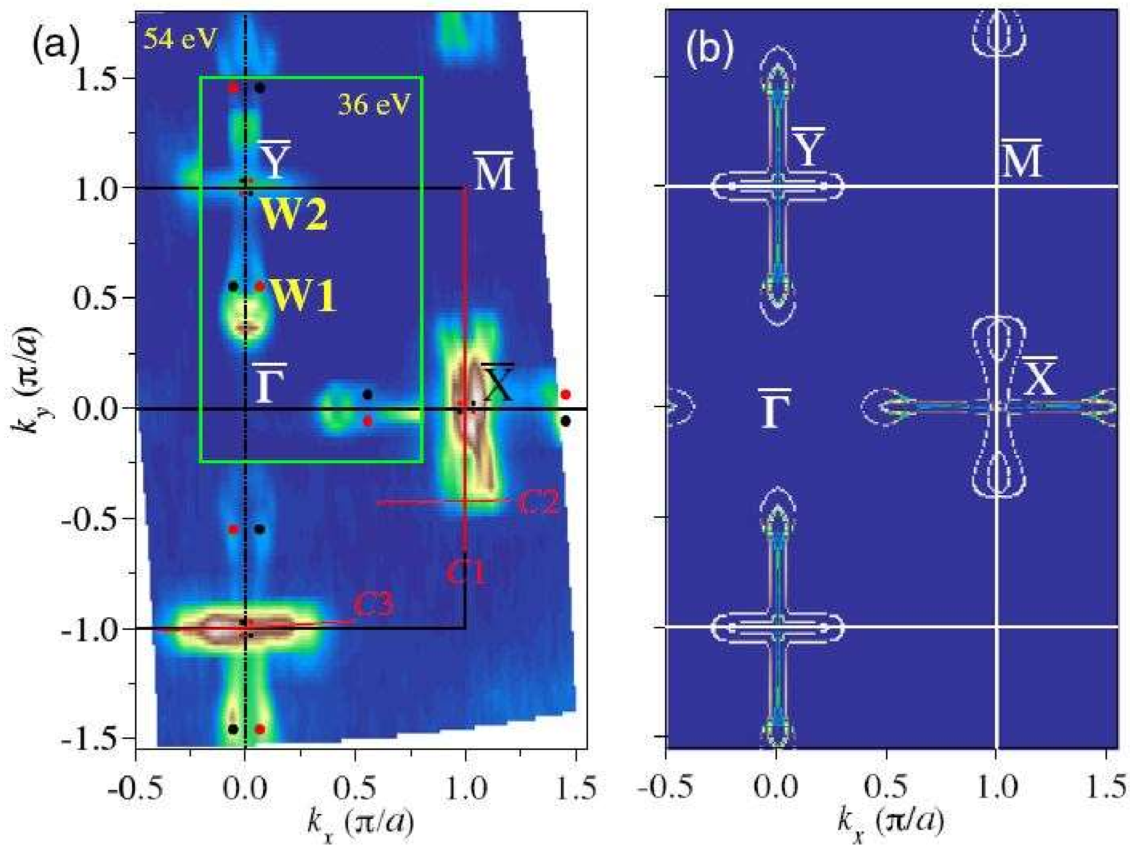
Fermi Arcs in TaAs: LDA and ARPES

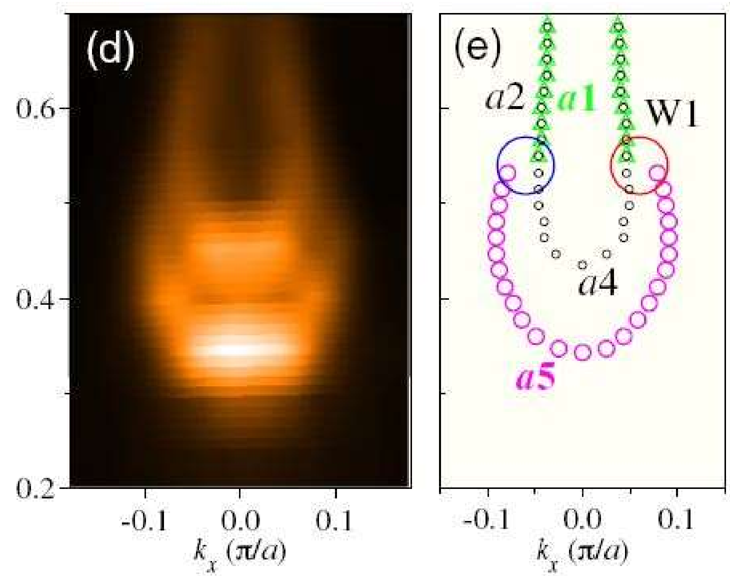
PHYSICAL REVIEW X **5**, 031013 (2015)

Experimental Discovery of Weyl Semimetal TaAs

B. Q. Lv,[1] H. M. Weng,[1,2] B. B. Fu,[1] X. P. Wang,[2,3,1] H. Miao,[1] J. Ma,[1] P. Richard,[1,2] X. C. Huang,[1] L. X. Zhao,[1] G. F. Chen,[1,2] Z. Fang,[1,2] X. Dai,[1,2] T. Qian,[1,*] and H. Ding[1,2,†]

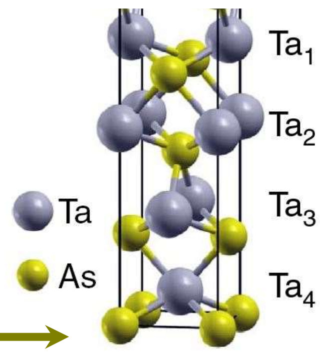






Simulations of Surface Disorder in TaAs

Construct a long slab along z axis (min 6 unit cells per slab, 24 atomic layers)

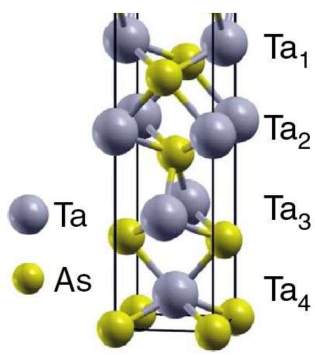


Slab of TaAs unit cells

Vacancies replacing As atoms at bottom surface layer

Vacancies replacing Ta atoms at top surface layer

12A vacuum layer

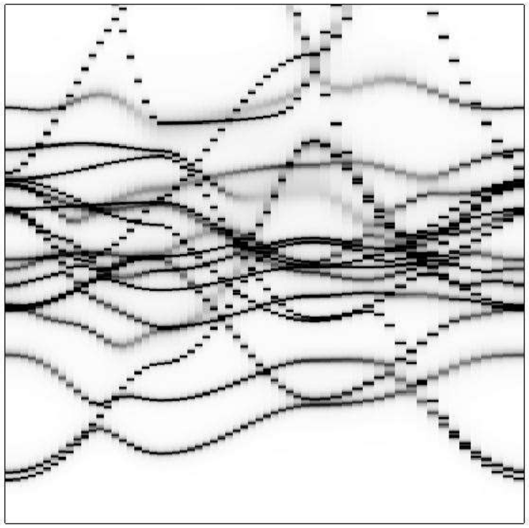


Slab of TaAs unit cells

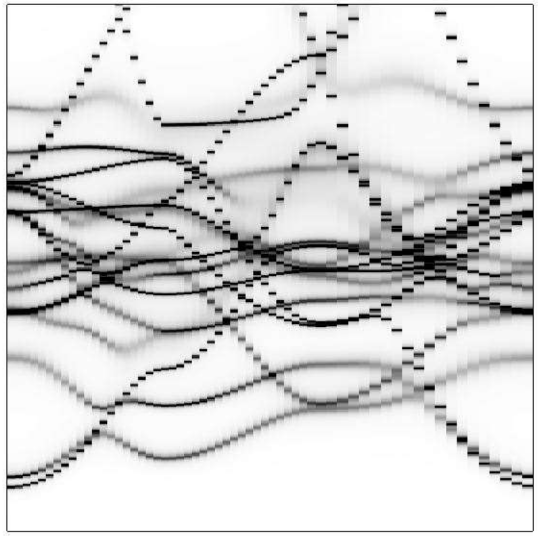
Perform LDA+CPA simulation, burn lot of CPU time

LDA+CPA Band Structures for TaAs (One Unit-Cell Slab)

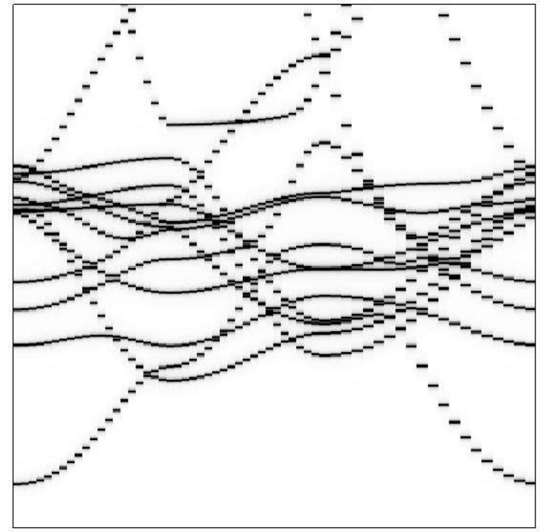
0.05 Ta1 Removed



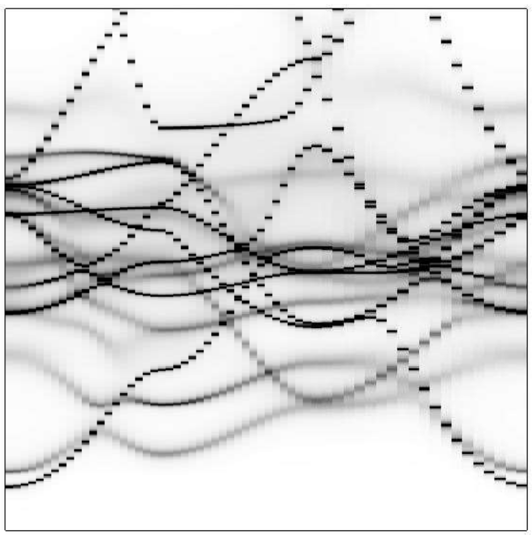
0.10 Ta1 Removed



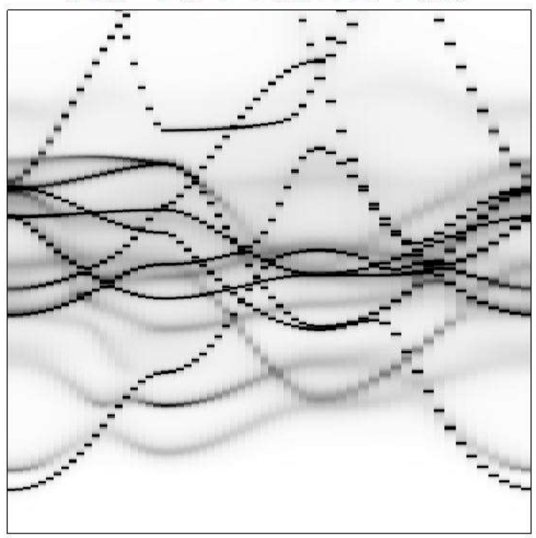
100% Ta1 Removed
using CPA



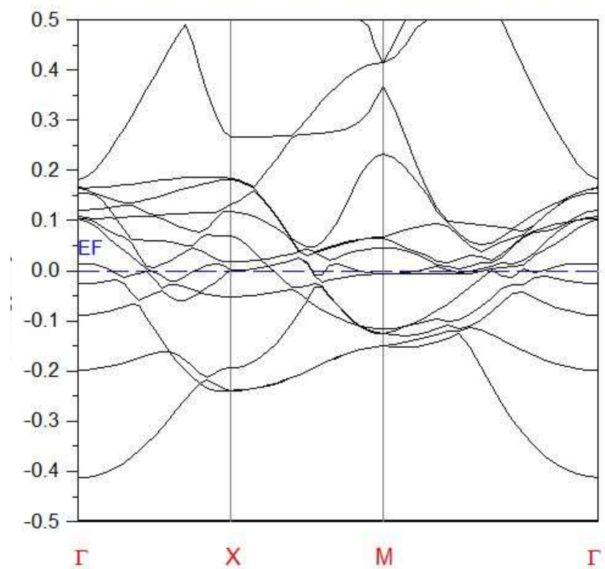
0.20 Ta1 Removed



0.3 Ta1 Removed



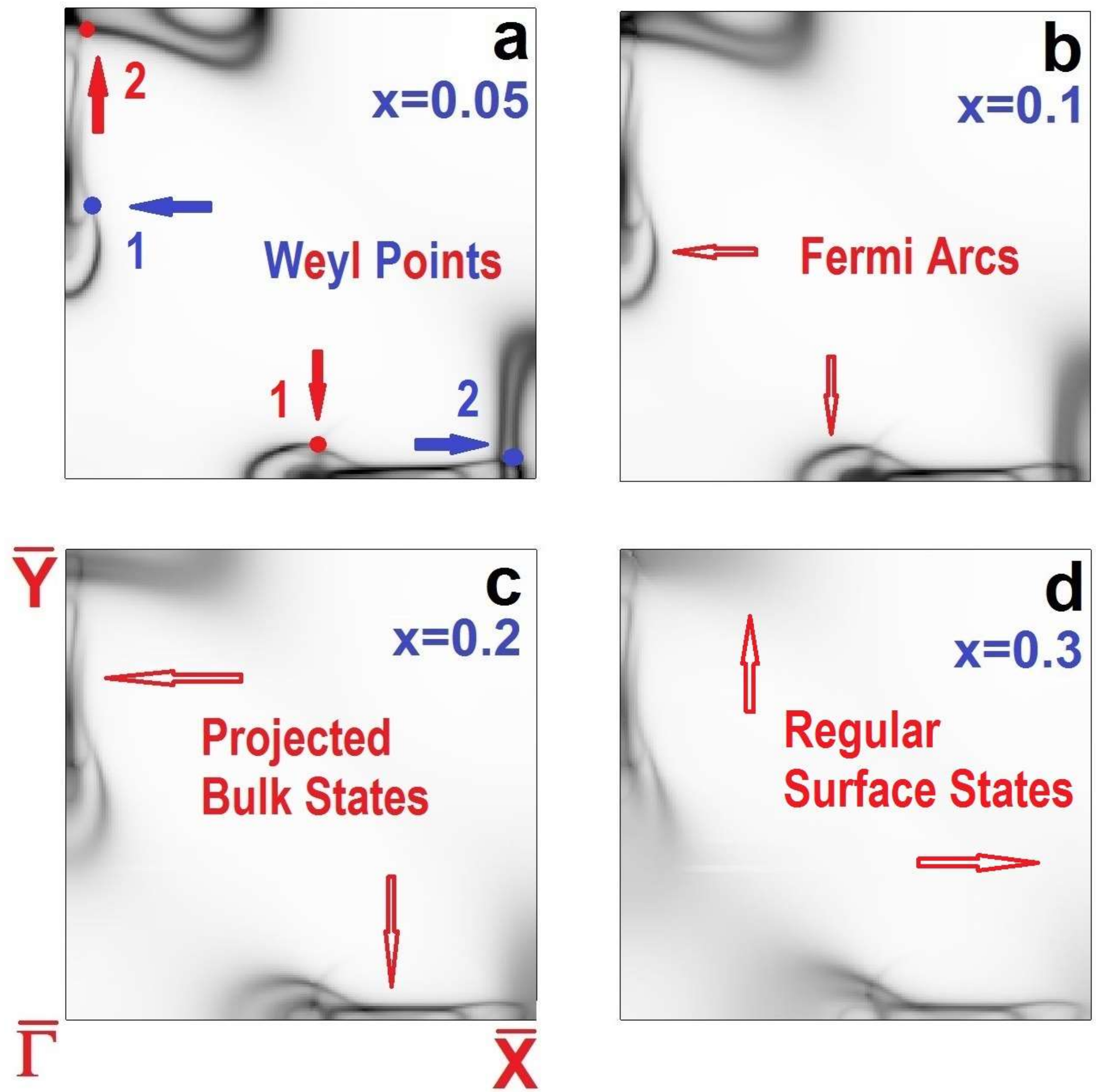
As2-Ta3-As4 with Ta1 removed, SCF LDA



Effect of Disorder on Fermi Arc States in TaAs

Results for 24 layers (6 unit cell slab)

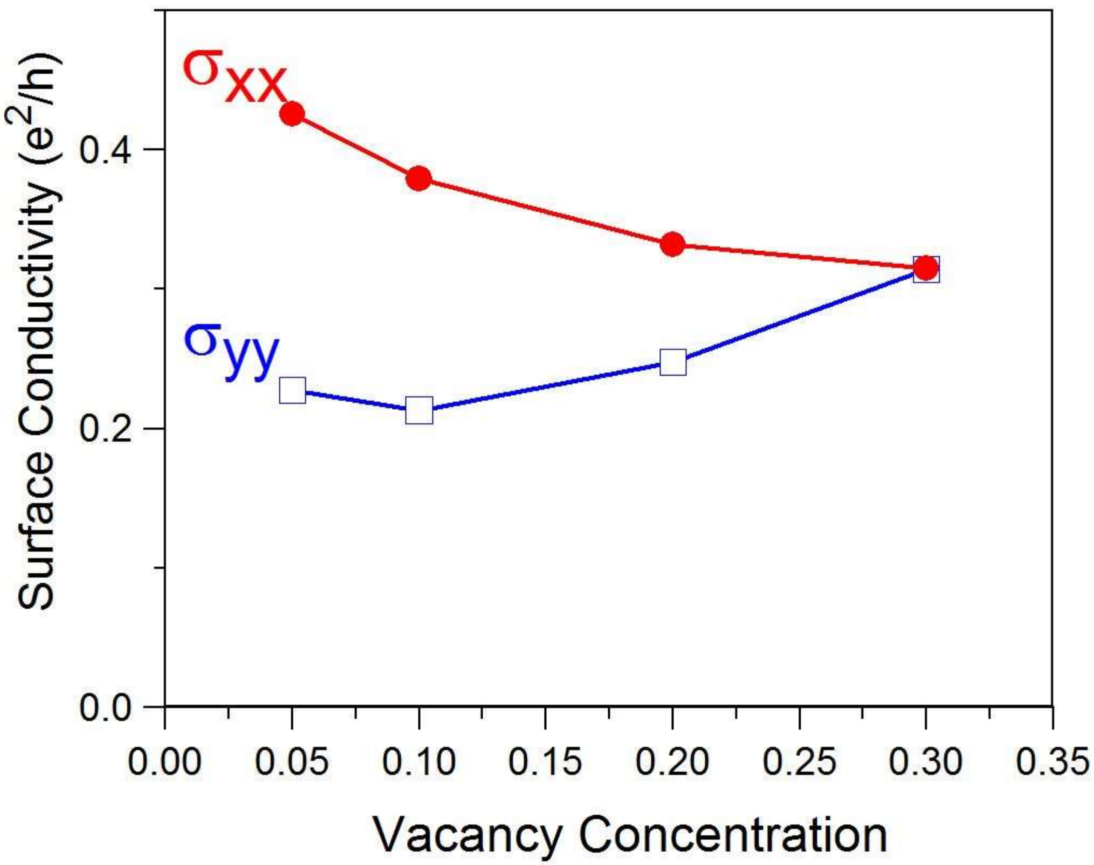
LDA+CPA simulation of surface vacancies effect on electronic states of TaAs for various strengths of disorder



Fermi arcs dissolved much slower than regular surface states (in accord with simulations on models)

Computation of Surface Conductivity in TaAs

Calculated conductivity for top 4 layers of TaAs 24 layers slab using Kubo Greenwood formalism and CPA simulating the effect of surface vacancies at the topmost layer



Conclusion

In Topological Insulators

❑ Topological nature of band structures demands a pure spin current between two opposite surfaces and consequent spin transfer.

❑ High level of nonmagnetic disorder can suppress spin relaxation, allowing substantial increase of spin accumulation at the surfaces.

In Weyl semimetals

❑ Single Fermi arc scattering is strongly suppressed (disappears for straight arc), the result of collapsing phase space in Boltzmann transport.

❑ Fermi arcs show much greater disorder tolerance than Dirac cones, their life times and conductivities are two orders of magnitude larger

❑ Fermi arcs in TaAs are affected by surface disorder, but dissolve much slower than regular surface states. Surface conductivity is weakly disorder dependent

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