Clustering & Global Challenges
April 07-09, 2021
Online international conference
Health
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ICN2 Institut Català de Nanociència i Nanotecnologia
EXCELENCIA SEVERO OCHOA
BIST Barcelona Institute of Science and Technology

Topological Spin Transport in Quantum Materials and Entanglement

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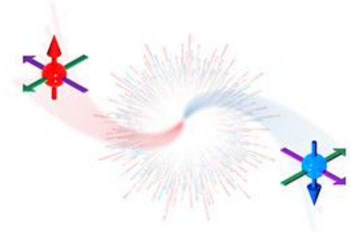
ICREA

Institució CERCA Centres de Recerca de Catalunya
Generalitat de Catalunya
CSIC Consejo Superior de Investigaciones Científicas
UAB Universitat Autònoma de Barcelona

OUTLINE

- *Motivation- Spin Transport Physics in* ***Quantum Materials & Entanglement….***



- ***Theoretical methodologies*** to explore spin transport in (disordered) strong SOC topological materials

  M Vila et al. **Phys. Rev. Lett.** 124 (19), 196602 (2020)

  Z. Fan, J.H. Garcia et al **Physics Reports** 903, 1-69 (2021)

- Multiple components Spin Hall Effect in $MoTe_2$ monolayer

  M. Vila et al. **arXiv:2007.02053**

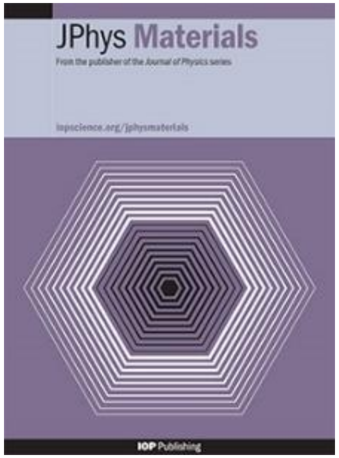
- Canted Quantum Spin Hall Effect in WTe_2 monolayer

  J.H. Garcia et al. **Phys. Rev. Lett. 125, 256603 (2020)**

cea

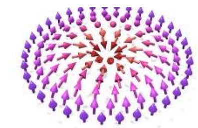
NUS National University of Singapore

Centre for Advanced 2D Materials

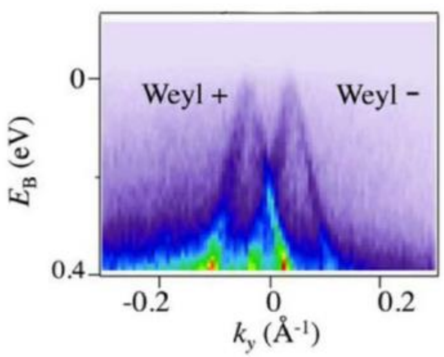


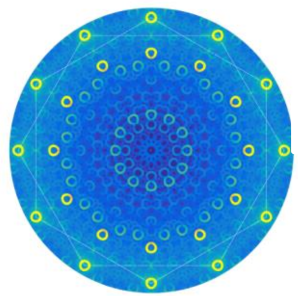
ROADMAP

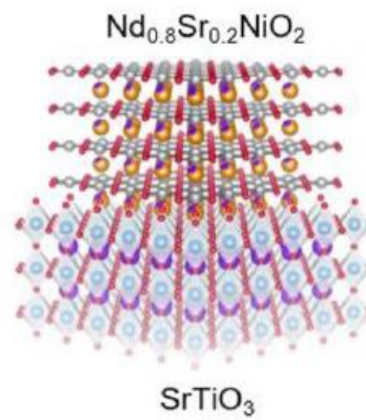
The 2021 quantum materials roadmap

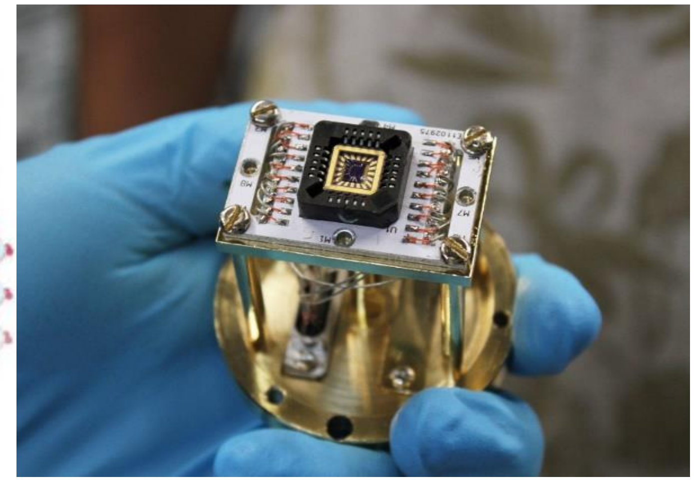


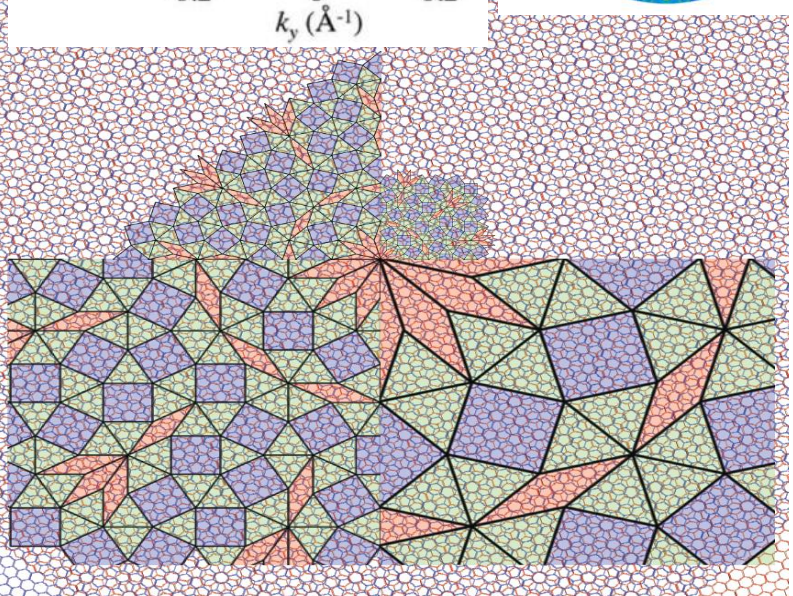
Feliciano Giustino[1,2], Jin Hong Lee[3], Felix Trier[3], Manuel Bibes[3], Stephen M Winter[4], Roser Valentí[4], Young-Woo Son[5], Louis Taillefer[6,7], Christoph Heil[8], Adriana I Figueroa[9], Bernard Plaçais[10], QuanSheng Wu[11], Oleg V Yazyev[11], Erik P A M Bakkers[12], Jesper Nygård[13], Pol Forn-Díaz[14,15], Silvano De Franceschi[16], J W McIver[17], L E F Foa Torres[18], Tony Low[19], Anshuman Kumar[20], Regina Galceran[9], Sergio O Valenzuela[9,21], Marius V Costache[9], Aurélien Manchon[22], Eun-Ah Kim[23], Gabriel R Schleder[24,25], Adalberto Fazzio[24,25] and Stephan Roche[9,21]

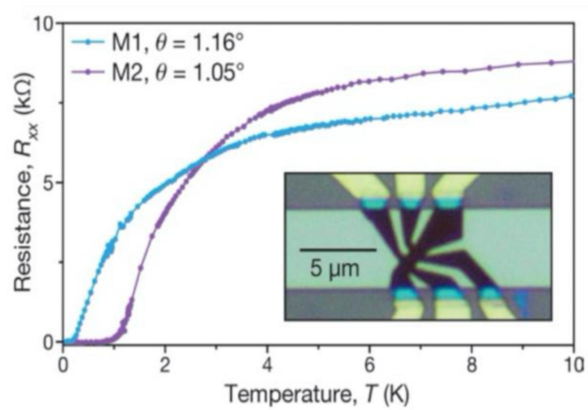


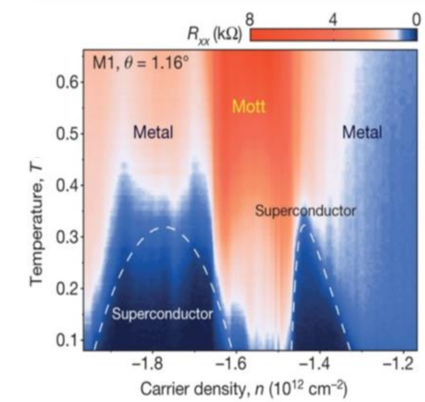












Einstein Podosly Rosen

« *thought experiment*»

Quantum Entanglement

A. Einstein B. Podolsky N. Rosen

MAY 15, 1935 PHYSICAL REVIEW VOLUME 47

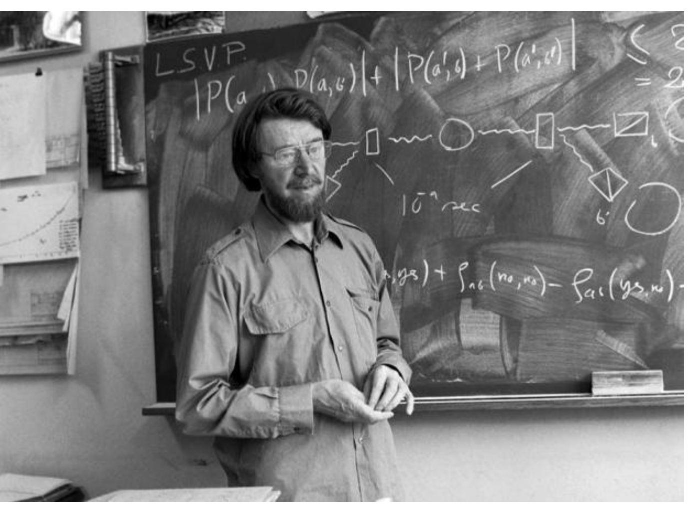
Can Quantum-Mechanical Description of Physical Reality Be Considered Complete?

A. EINSTEIN, B. PODOLSKY AND N. ROSEN, *Institute for Advanced Study, Princeton, New Jersey*

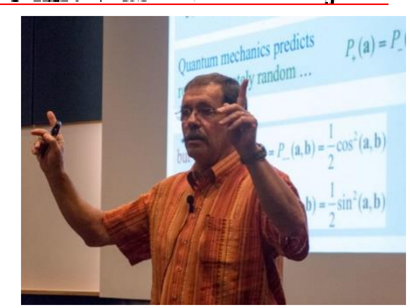
(Received March 25, 1935)

In a complete theory there is an element corresponding to each element of reality. A sufficient condition for the reality of a physical quantity is the possibility of predicting it with certainty, without disturbing the system. In quantum mechanics in the case of two physical quantities described by non-commuting operators, the knowledge of one precludes the knowledge of the other. Then either (1) the description of reality given by the wave function in quantum mechanics is not complete or (2) these two quantities cannot have simultaneous reality. Consideration of the problem of making predictions concerning a system on the basis of measurements made on another system that had previously interacted with it leads to the result that if (1) is false then (2) is also false. One is thus led to conclude that the description of reality as given by a wave function is not complete.

of them with a representative of its own. I would not call that *one* but rather *the* characteristic trait of quantum mechanics, the one that enforces its entire departure from classical lines of thought. By the interaction the two representatives (or ψ-functions) have become entangled. To disentangle them we must gather further information by experiment, although we knew as much as any-



"Problem solved by violation Of the Bell´s inequality…"



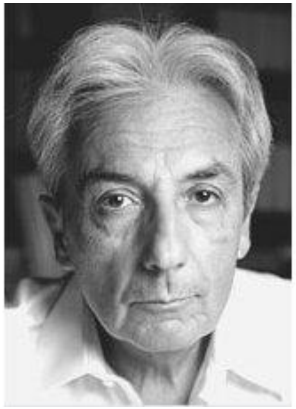
(practical?) **Quantum Computers**

- **IBM** – Q System One : 56-qubit machine
- **INTEL**; **D-Wave** 2000Q quantum annealer
- **Microsoft** –Quantum Lab-Delft
- **Google** –Quantum Artificial Intelligence Lab
- **Bristlecone**: 72-qubit quantum chip

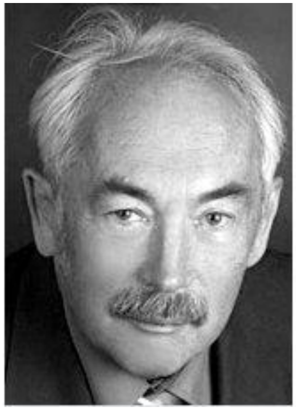
aims to build quantum processors and develop novel quantum algorithms to dramatically accelerate computational tasks for machine learning

Spintronics and its industrial/Societal impact

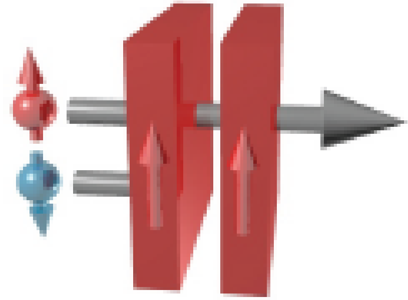
Albert Fert

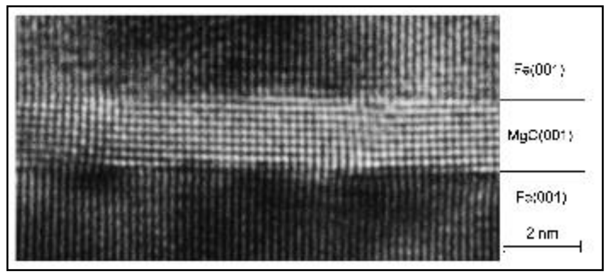


Peter Grünberg

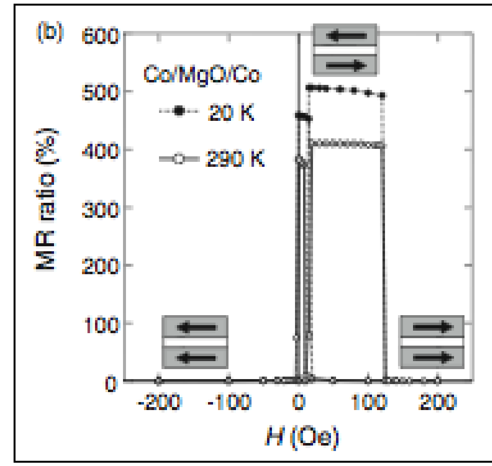


2007 Physics Nobel Laureates





$$MR = \frac{R_{AP} - R_P}{R_P}$$



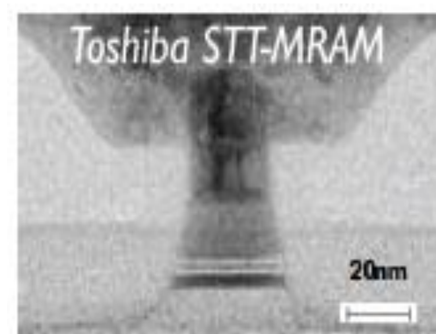
Magnetic field sensors used to read data in hard disk drives,

microelectromechanical systems (MEMS), minimally invasive surgery

Automotive sensors for fuel handling system, Anti-skid system, speed control & navigation

***Magnetoresistive random-access memory** (MRAM)*

Spin transfer Torque MRAM

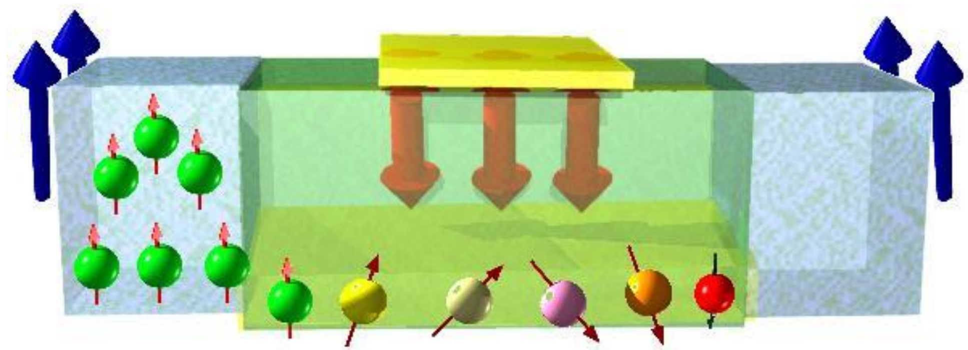


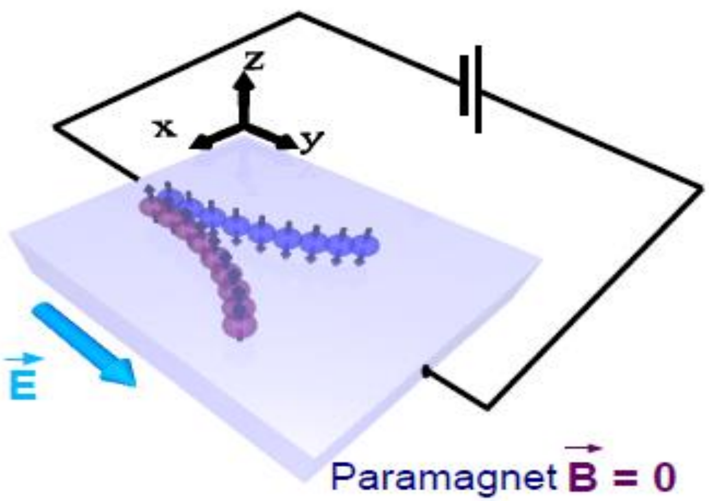
Spin-based information processing ?

Need for spin information transport on long distance (room T)
Spin injection and detection (ferromagnets/non magnetic materials)

Active devices based on **Spin manipulation** ?

Datta-Das spin transistor

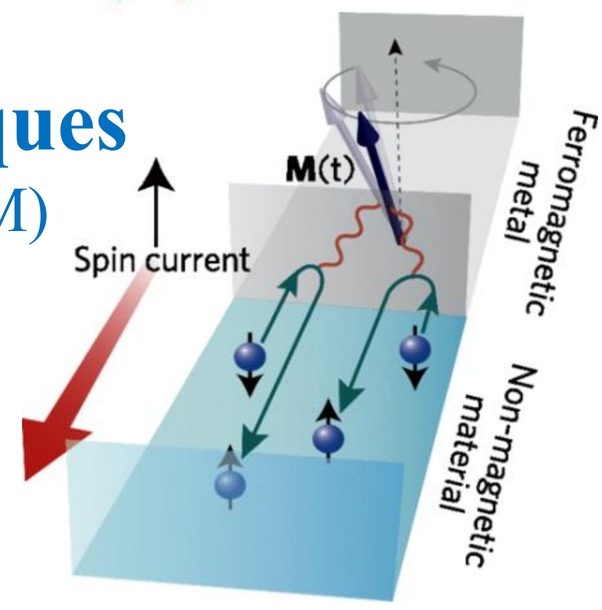




Spin Hall Effect

Spin torques

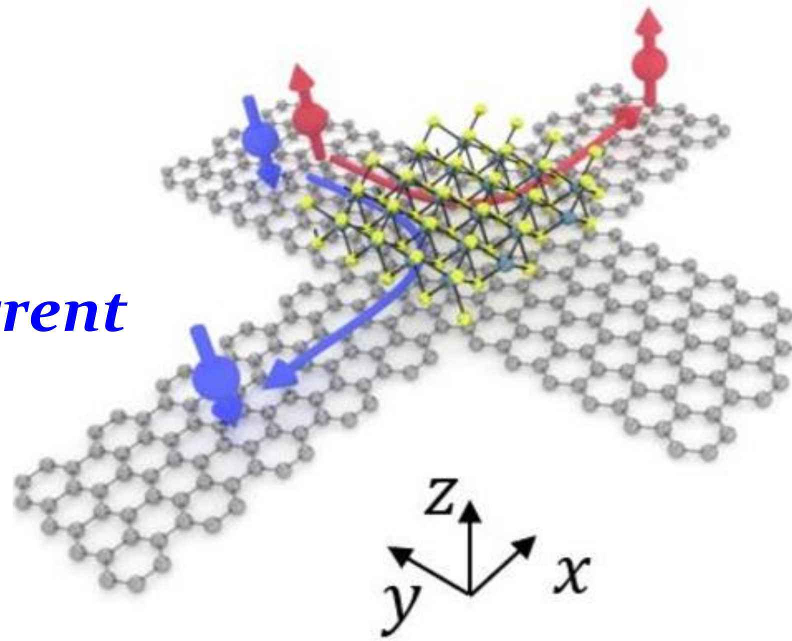
(SOT-MRAM)



Spin Hall effect

(strong spin-orbit coupling materials)

(Pure) **spin current** generation, manipulation & detection



Spin- orbit coupling fields

(effective magnetic field)

Generates (bulk) transversal spin current

(spin polarization orthogonal to both currents)

$$\vec{J}_s = \theta_{sH} \vec{\sigma} \wedge \vec{J}_c$$

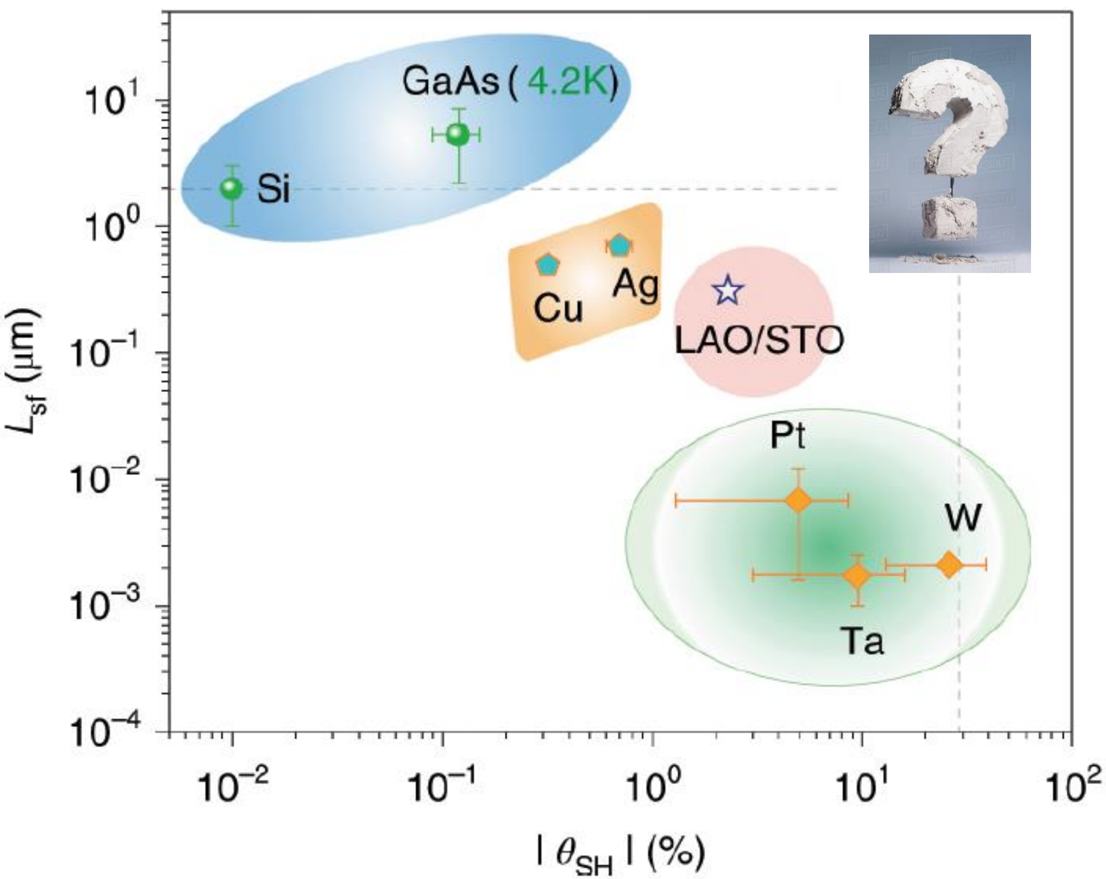
Spin Hall angle :

measures how much spin current is generated from a charge current

$$\theta_{sH} \sim \frac{|J_s|}{|J_c|}$$

Long sought-after spintronic materials

λ_s ***Spin diffusion length*** *: measures upper limit for spin transmission*



Problem !

SOC $\nearrow$

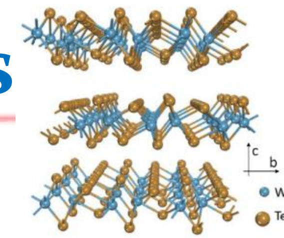
$\theta_{sH} \nearrow$

$\lambda_s \searrow$

$$\lambda_s.\theta_{sH} \sim 0.1 - 0.2 \text{ nm} \quad (\text{Pt}, \beta - W, \beta\text{-Ta or Au})$$

J. Sinova, S. O. Valenzuela et al. **Rev. Mod. Phys. 87, 1213 (2015)**

SHE in Low-symmetry multilayers TMDs

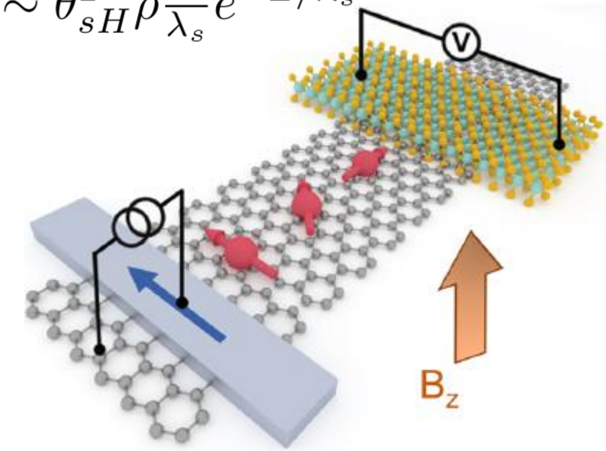


C. K. Safeer, et al. *Nano Letters* **19** (12), 8758-8766 (2019)

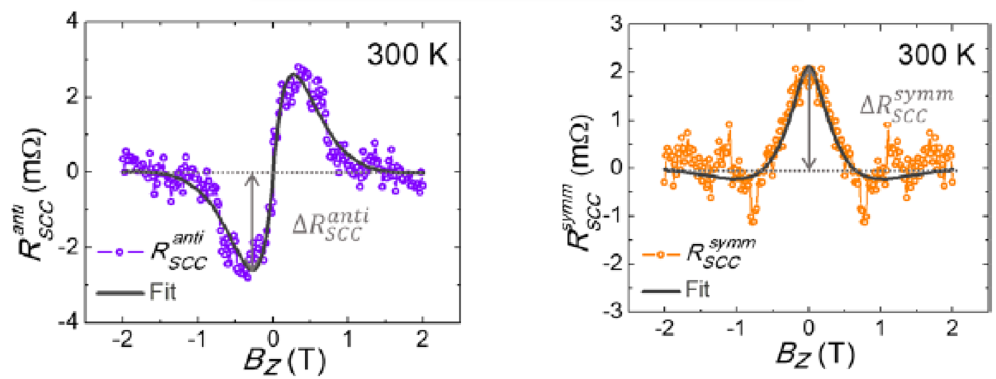
Multidirectional spin-to-charge conversion in multilayers **$MoTe_2$** (11 nm thick sample)

$$\Delta R_{sH} \sim \theta_{sH}^2 \rho \frac{W}{\lambda_s} e^{-L/\lambda_s}$$

Pure spin current injected in graphene channel & adsorbed in MoTe2 – converted into charge current (nonlocal voltage)

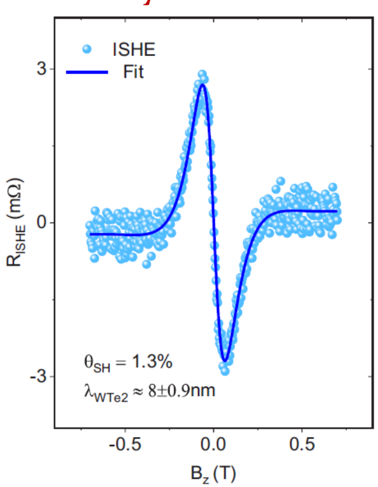


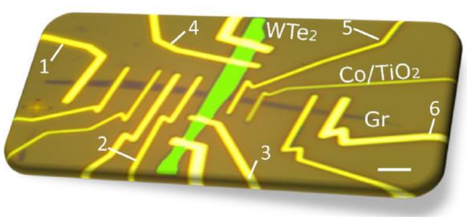
$$\lambda_s . \theta_{sH} \sim 1 \text{ nm}$$



P. Song et al. *Nat. Mater.* **19**, 292–298 (2020)

WTe_2
multilayers





$$\lambda_s . \theta_{sH} \sim 0.1 \text{ nm}$$

B. Zhao et al.
Phys. Rev. Research 2, 013286 (2020)

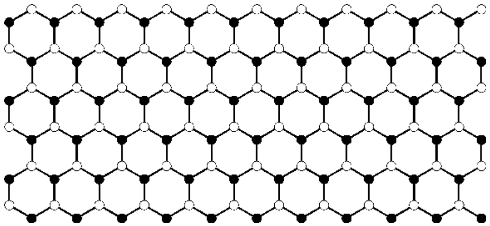
$MoTe_2$
multilayers

$$\theta_{sH} \sim 30\%$$

$$\lambda_s \sim 1 \mu m$$

$$\lambda_s . \theta_{sH} \sim 300\text{nm} \text{ !!}$$

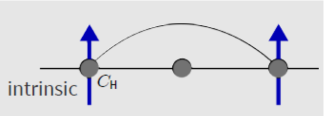
Quantum Spin Hall Effect

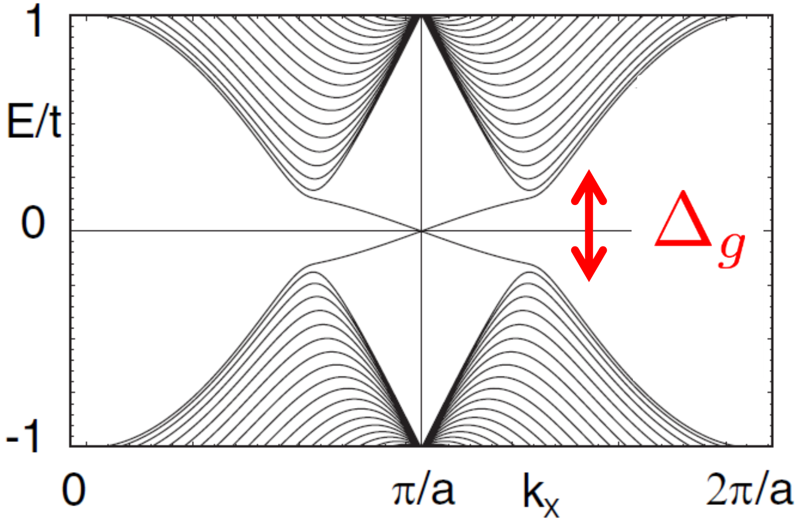


C.L. Kane and E. J. Mele,
Phys. Rev. Lett. 95, 26801 (2005)

Zigzag graphene ribbon with intrinsic SOC

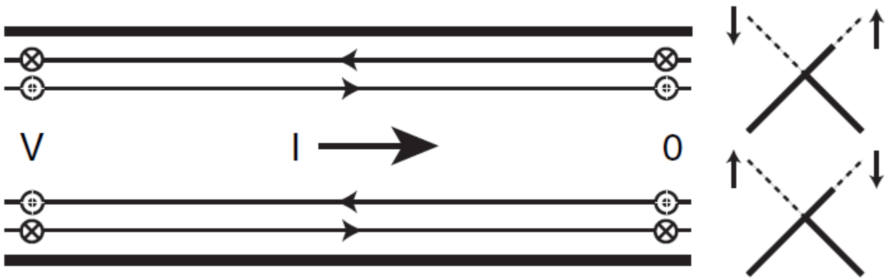
$$\mathcal{H} = t\sum_{\langle ij\rangle} c_i^\dagger c_j + i(8\lambda_{SO}/a^2)\sum_{\langle\langle ij\rangle\rangle} c_i^\dagger \mathbf{s}.(\mathbf{d}_{ij}^1 \times \mathbf{d}_{ij}^2)c_j$$





Gapless helical edge states

States with opposite spins counterpropagate at the edges

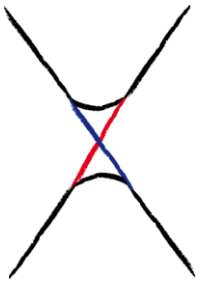


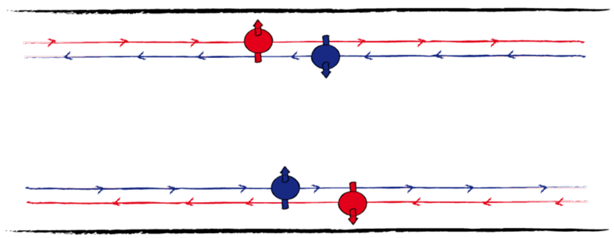
"QHE" in absence of magnetic field

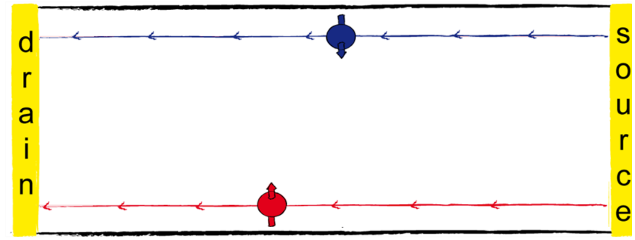
Towards dissipation current **(TRS invariant)….**

$$\Delta_g \sim 0.1\text{meV}$$

First experimental evidence of 2D topological insulators



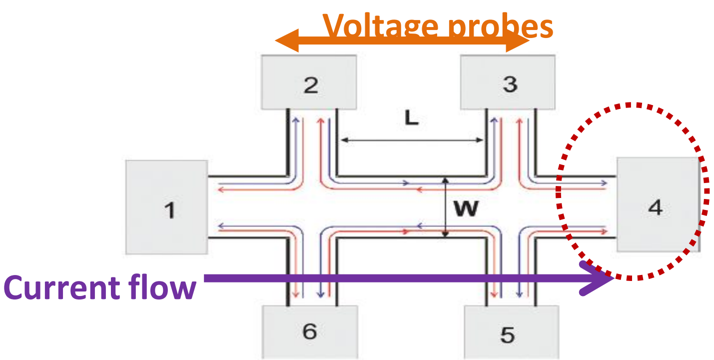




$$G = G_{\Uparrow} + G_{\Downarrow} = \frac{e^2}{h} + \frac{e^2}{h}$$

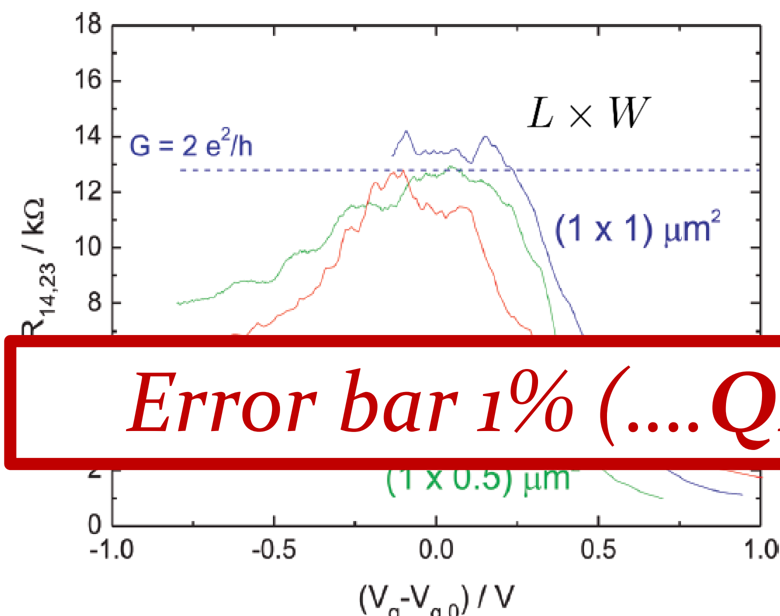
“Quantization” of the conductance

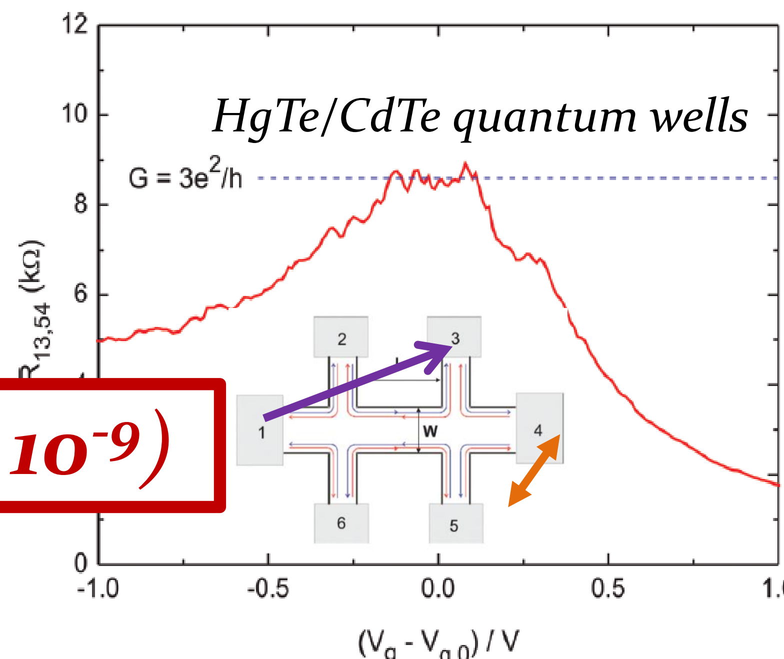
(regardless device aspect ratio)



Nonlocal transport geometry

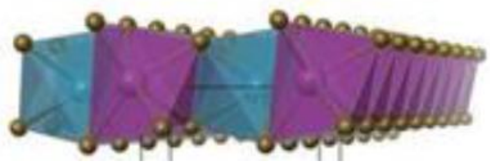
Conductance agrees with predictions





Error bar 1% (….QHE 10^{-9})

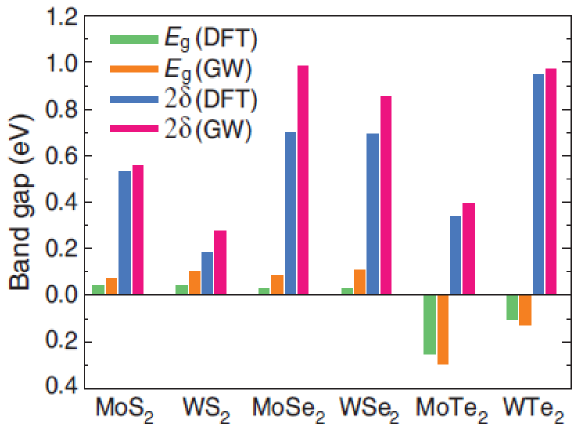
1T′-TMD monolayer as QSH insulators

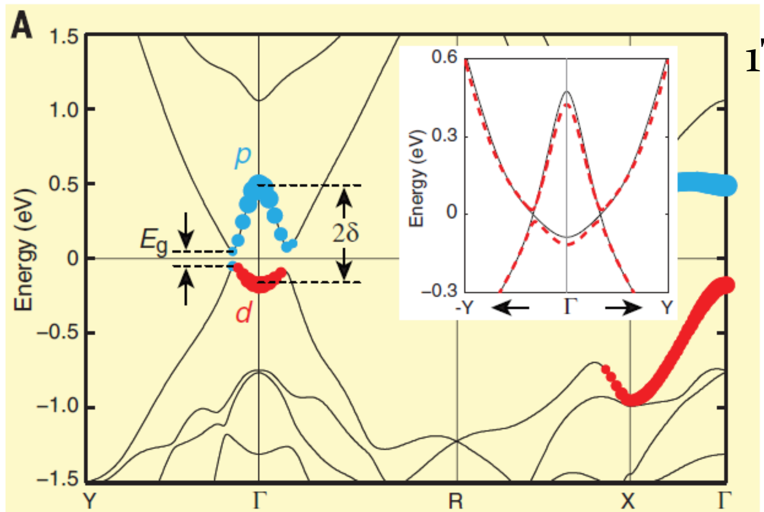


Prediction in 2014

X. Qian, J. Liu, L. Fu, J. Li, **Science 346, 1344 (2014)**

*Structural distortion causes an intrinsic band inversion between chalcogenide-p and metal-d bands (**gap in order of 0.1 eV**)*

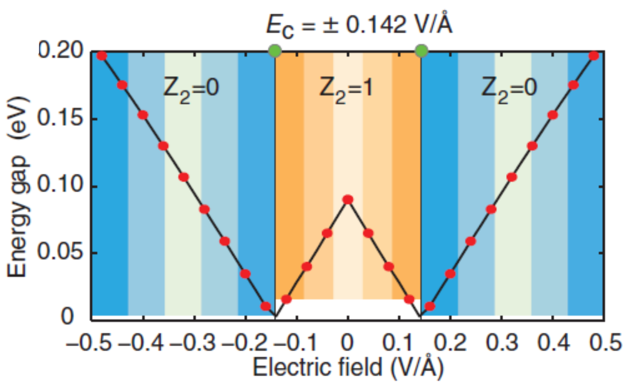


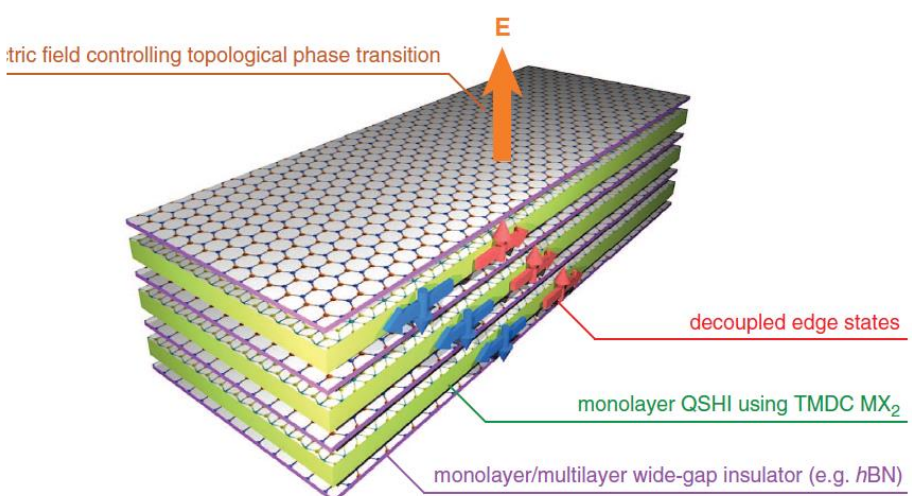


$1T'$-MoS_2

Topological field effect transistor

(low-power quantum electronics)





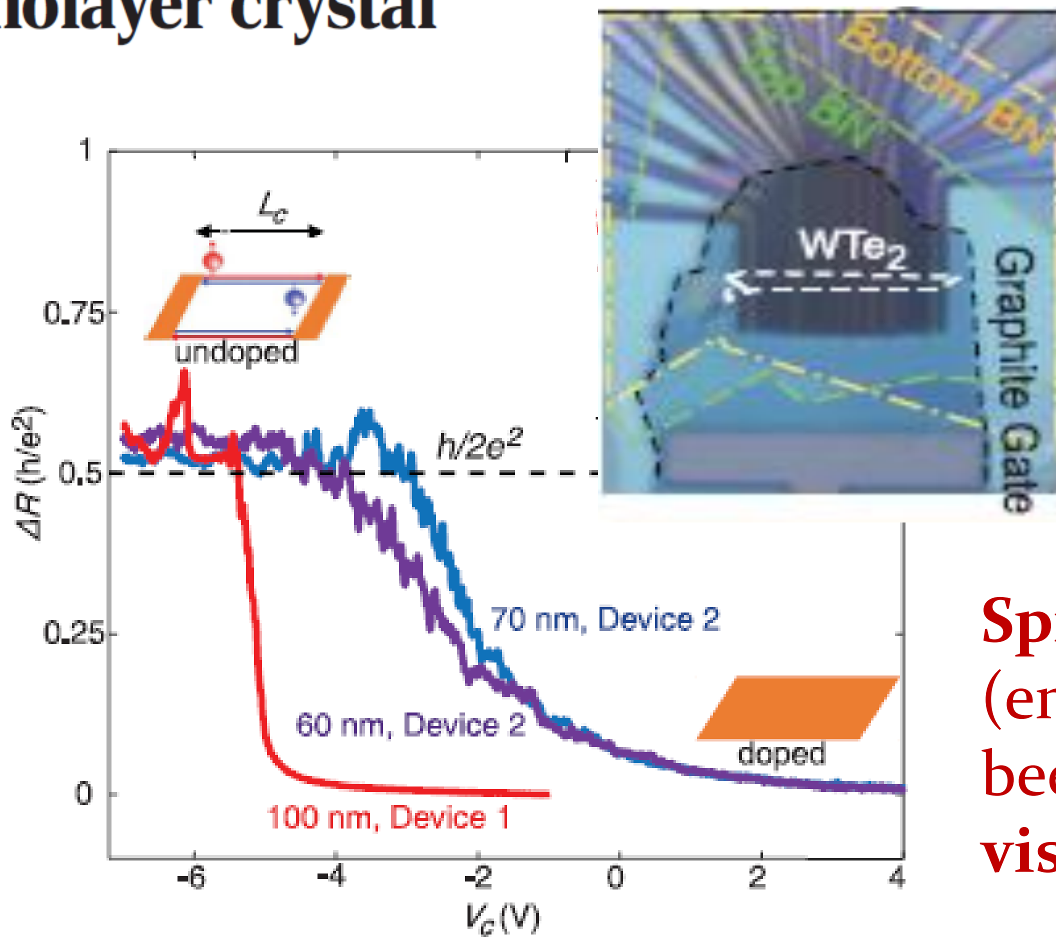
1T-WTe_2 as Quantum Spin Hall insulator

TOPOLOGICAL MATTER

Observation of the quantum spin Hall effect up to 100 kelvin in a monolayer crystal

Wu et al.

Science 359, 76-79 (2018)



Purely electrical measurements

Spin-momentum locking (entanglement) has not yet been directly **visualized/demonstrated**

OUTLINE

- *Motivation- Spin Transport Physics in Quantum Materials*

- *Theoretical methodologies* to explore spin transport in (disordered) strong SOC topological materials

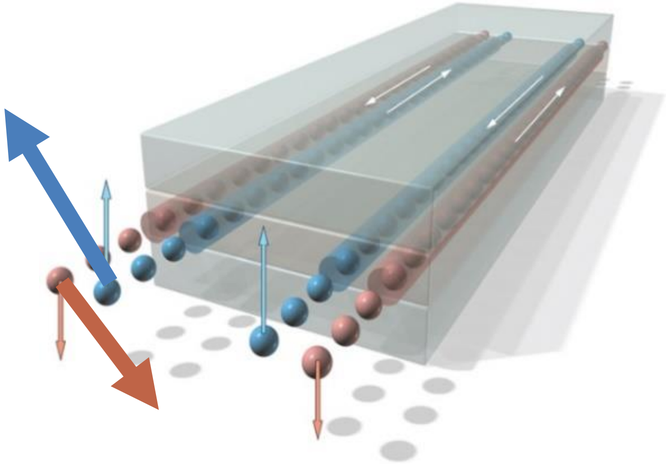
  M Vila et al. **Phys. Rev. Lett.** 124 (19), 196602 (2020)

  Z. Fan, J.H. Garcia et al **Physics Reports** 2021 **(**arXiv:1811.07387)

- Multiple components Spin Hall Effect in $MoTe_2$ monolayer

  M. Vila et al. **arXiv:2007.02053**

- **Canted Quantum Spin Hall Effect**
  in WTe_2 monolayer
  J.H. Garcia et al. **Phys. Rev. Lett. 125, 256603 (2020)**



Order N quantum transport methods

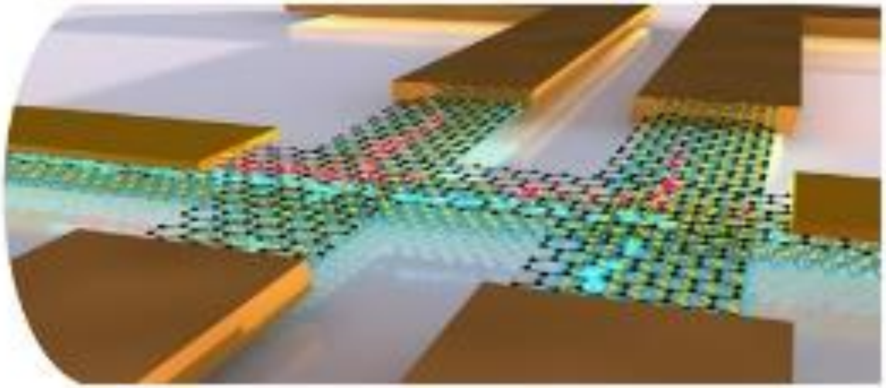
(Kubo, (Spin)-Hall Kubo, Landauer-Büttiker)

Linear Scaling Quantum Transport Methodologies

Zheyong Fan,[1,2] Jose Hugo Garcia,[3] Aron W. Cummings,[3] Jose-Eduardo Barrios,[3] Michel Panhans,[4] Ari Harju,[5] Frank Ortmann,[4] and Stephan Roche[3,6]

Disorder systems, Magnetic fields,
Charge transport
Thermal transport *(phonon dynamics-harmonic approx.)*
Electron-phonon coupling *(molecular dynamics, T-dependence)*
Polaron transport , Spin transport (SOC)

LSQUANT
LINEAR SCALING QUANTUM TRANSPORT



www.lsquant.org

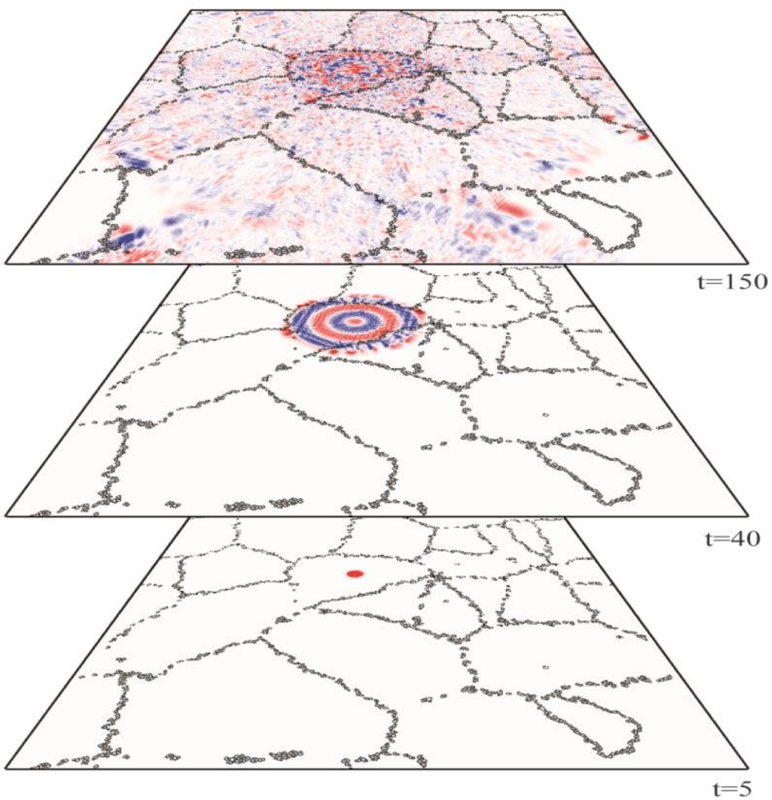
Spin dynamics of propagating wavepacket

$$|\Psi_\perp(0)\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} |\varphi_{RP}\rangle \qquad |\Psi(t)\rangle = e^{-i\hat{\mathcal{H}}t/\hbar}|\Psi(0)\rangle$$

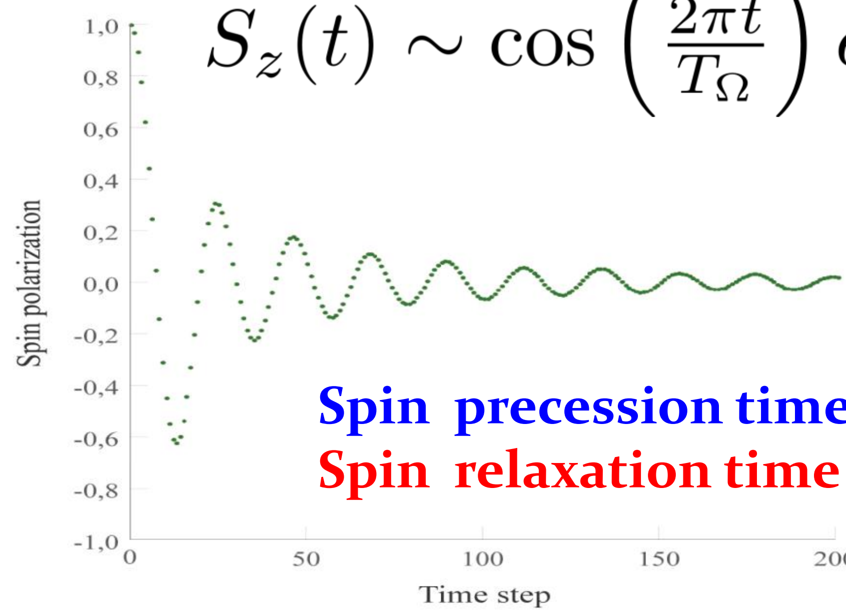
$$s_i(t) = |\Psi_i^\uparrow(t)|^2 - |\Psi_i^\downarrow(t)|^2$$

(time-dependent)
Local spin density in real space

$$\frac{\langle\Psi(t)|\sigma_z\delta(E-\hat{\mathcal{H}})+\delta(E-\hat{\mathcal{H}})\sigma_z|\Psi(t)\rangle}{2\langle\Psi(t)|\delta(E-\hat{\mathcal{H}})|\Psi(t)\rangle}$$



$$S_z(t) \sim \cos\left(\frac{2\pi t}{T_\Omega}\right) e^{-t/\tau_s}$$



Spin precession time T_Ω

Spin relaxation time τ_s

Spin Hall Kubo conductivity

(SHE in dissipative regime)

$$\boxed{\sigma_{\rm sH} = \frac{e\hbar}{\Omega}\sum_{m,n}\frac{f(E_m)-f(E_n)}{E_m-E_n}\frac{\mathcal{I}m[\langle m|J_x^z|n\rangle\langle n|v_y|m\rangle]}{E_m-E_n+i\eta},}$$

$J_x^z = \frac{\hbar}{4}\{\sigma_z, v_x\}$ is the spin current operator

$$\theta_{sH} = \frac{\sigma_{xy}^z}{\sigma_{xx}}$$

$$\sigma_{\rm sH} = \frac{e\hbar}{\Omega}\int dudv\frac{f(u)-f(v)}{(u-v)^2+\eta^2}j(u,v),$$

$$j(u,v) = \sum_{m,n}\mathcal{I}m[\langle m|J_x^z|n\rangle\langle n|v_y|m\rangle]\delta(u-E_m)\delta(v-E_n)$$

$$= \sum_{m,n}^{M}(4\mu_{mn}g_m g_n T_m(\hat{u})T_n(\hat{v}))/((1+\delta_{m,0})(1+\delta_{n,0})\pi^2\sqrt{(1-\hat{u}^2)(1-\hat{v}^2)}),$$

$$\mu_{mn} = \frac{4}{\Delta E^2}\mathcal{I}m[Tr[J_x^z T_n(\hat{H})v_y T_m(\hat{H})]]$$

The trace in μ_{mn} is computed by the average on a small number $R \ll N$ of random phase vectors $|\varphi\rangle$

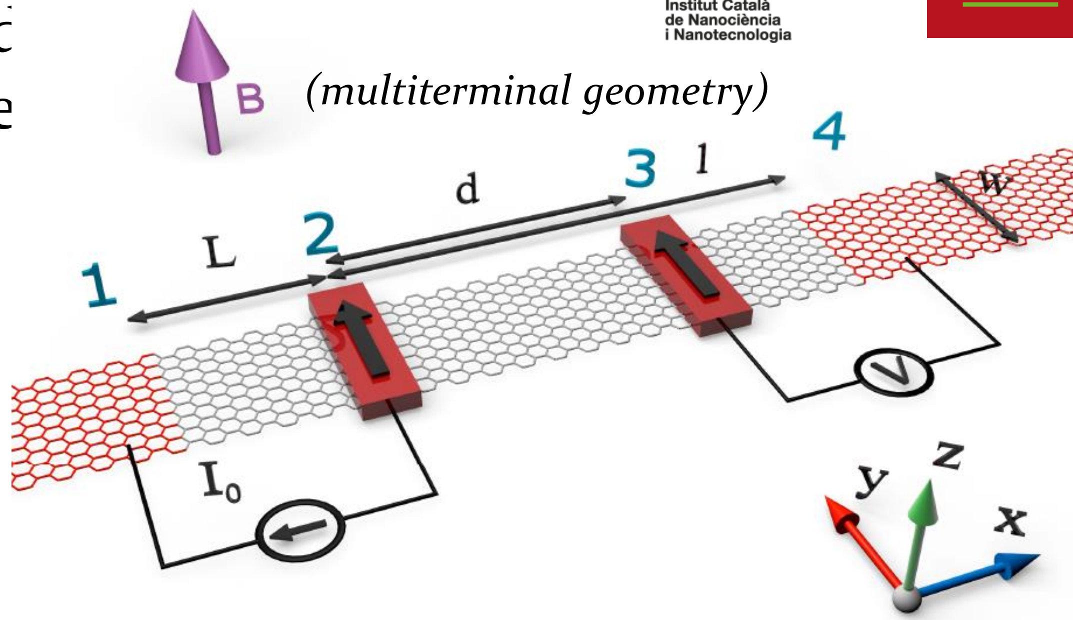
$$\boxed{\sigma_{xx} = \frac{2\hbar e^2}{\pi\Omega}\sum_{m,n=0}^{M}\mathcal{I}m[g_m(\epsilon+i\eta)]\mathcal{I}m[g_n(\epsilon+i\eta)]\mu_{mn}}$$

dc-Kubo conductivity

Nonlocal resistance simulation

I_0 charge current injectec from lead 2 to 1 while a non-local voltage

$$\boxed{R_{\mathrm{NL}} = (V_3 - V_4)/I_0}$$



Charge current

$$I_p = \sum_q G_{pq}(V_p - V_q)$$

kwant

$$G_{pq} = \frac{e^2}{h} \int dE \, \mathrm{Tr}[\mathbf{t}_{pq}\mathbf{t}_{pq}^\dagger](-\partial f/\partial E)$$

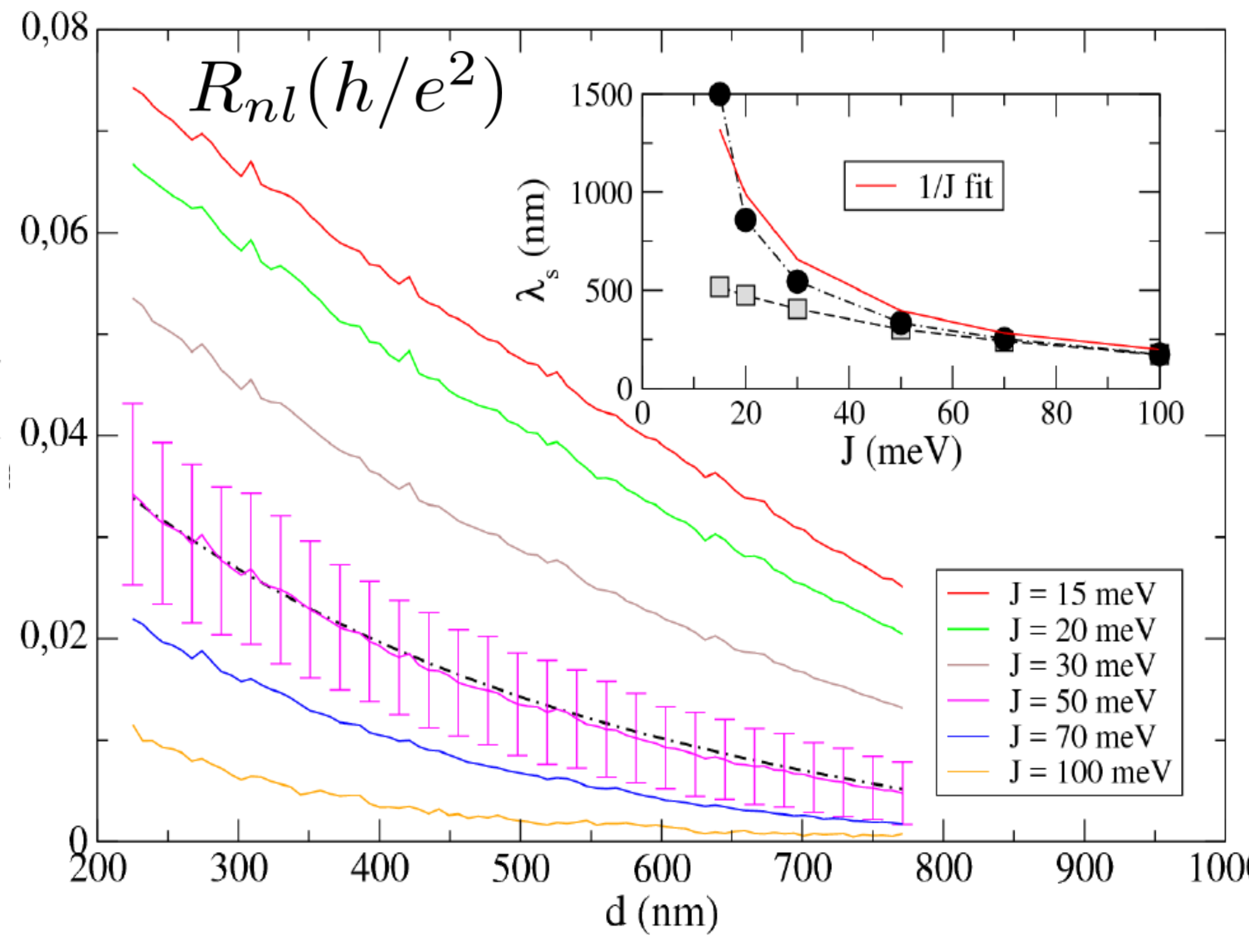
$\mathbf{t}_{pq}$ the transmission matrix between transverse propagating modes within semi-infinite leads p and q

Spin current

$$I_p^{s_\alpha} \quad G_{pq}^{s_\alpha} = \frac{e^2}{h} \int dE \, \mathrm{Tr}[s_\alpha \mathbf{t}_{pq}\mathbf{t}_{pq}^\dagger](-\partial f/\partial E) \qquad \theta_{sH} = \frac{I^{s_z}}{I_0}$$

Study of spin dynamics (crossover)

Brute force simulation of the non-local resistance versus channel length



$$R_{\mathrm{NL}} \propto e^{-d/\lambda_s}$$

understimates spin diffusion length

fails to describe the transition towards ballistic regime **(low J)**

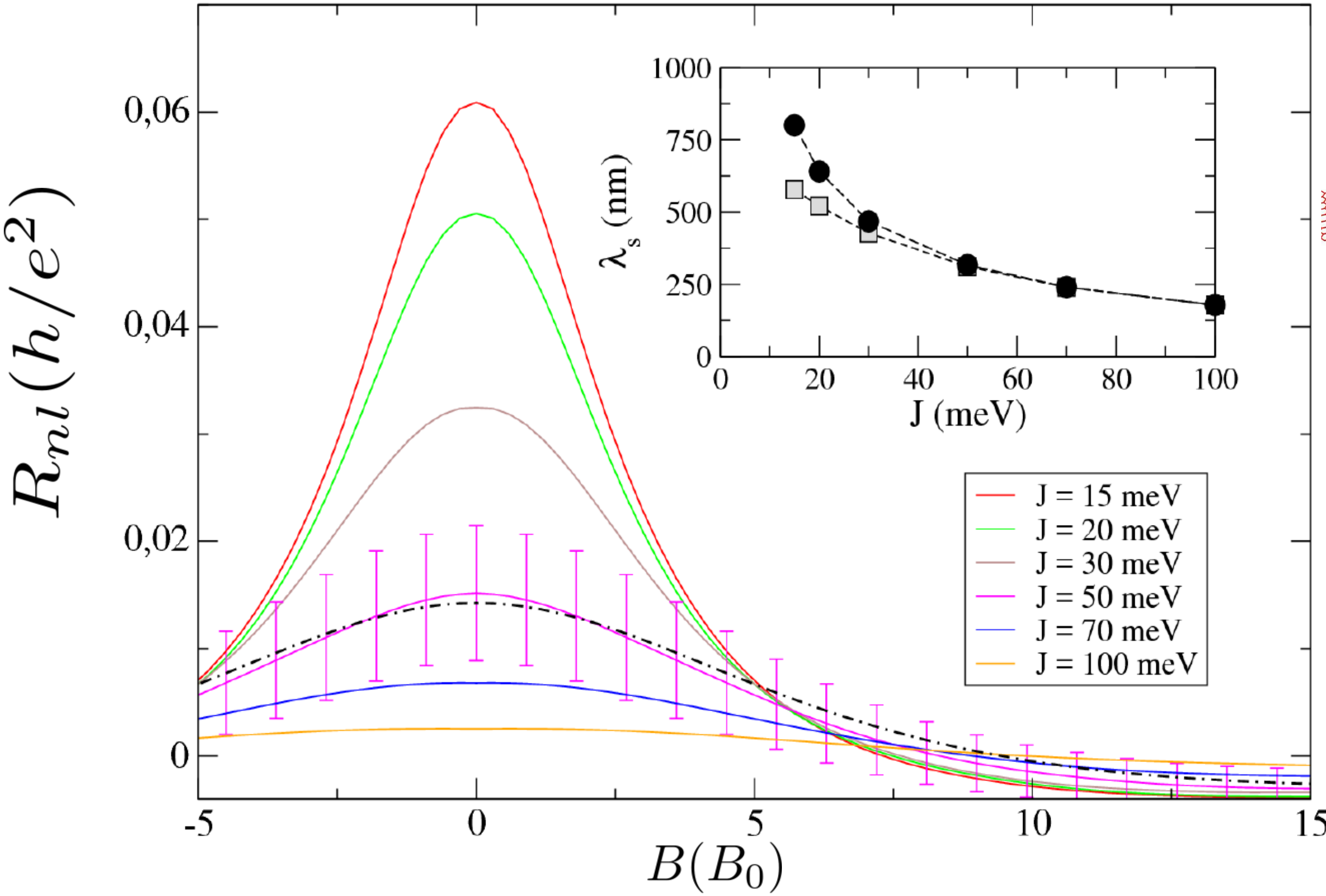
$$J \to 0$$

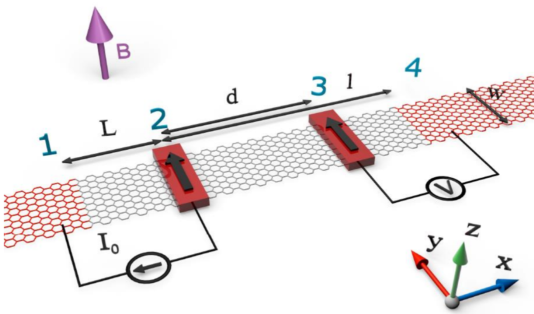
Non-local resistance Still decays....

$$R_{nl} = \frac{(4\frac{L}{w\sigma} + R_c)(-4x + 4l + R_c w\sigma)}{8(2L + 2l + R_c w\sigma)}$$

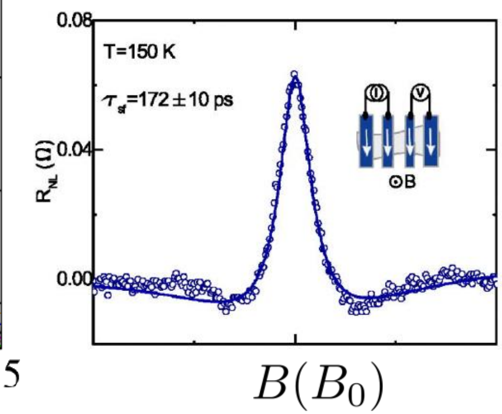
Hanle spin precession simulations

Diffusive regime (graphene with random magnetic impurities) $d \geq L_s$





Consistent extrapolation of spin diffusion length



M. Vila, J.H. Garcia, A.W. Cummings, S. Power, C. Groth, X. Waintal, S. Roche
Physical Review Letters 124 (19), 196602 (2020)

PRL 117, 176602 (2016) PHYSICAL REVIEW LETTERS week ending 21 OCTOBER 2016

Spin Hall Effect and Origins of Nonlocal Resistance in Adatom-Decorated Graphene

D. Van Tuan,[1,2] J. M. Marmolejo-Tejada,[3,4] X. Waintal,[5] B. K. Nikolić,[3,*] S. O. Valenzuela,[1,6] and S. Roche[1,6,†]
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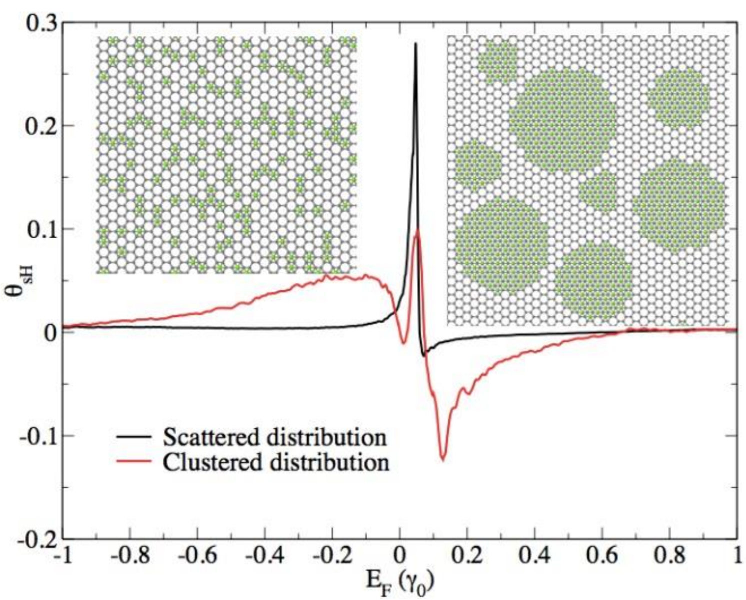
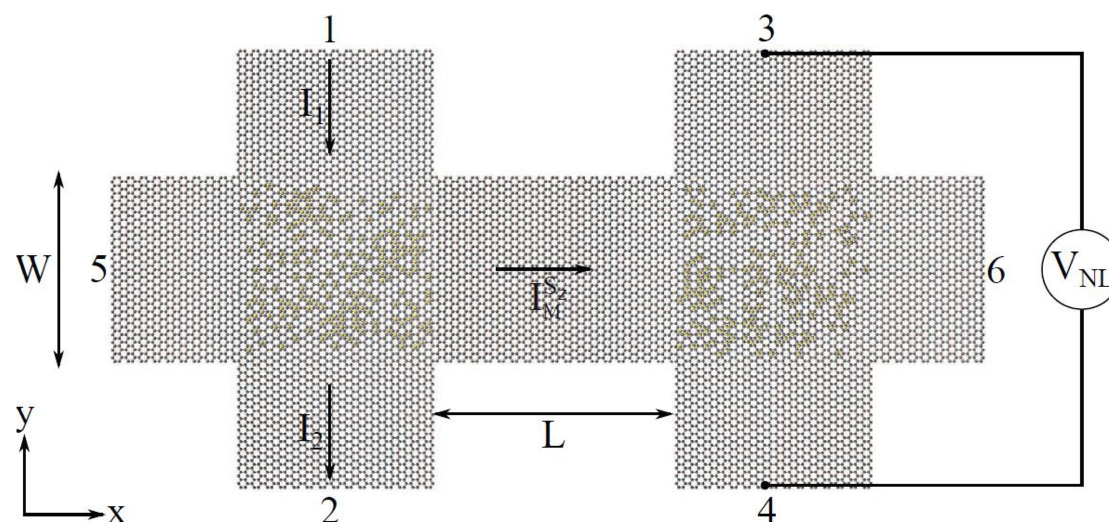
(Received 19 February 2016; published 20 October 2016)

Kubo formalism
(dissipative & Hall conductivities)



$$\theta_{\mathrm{sH}} = \sigma_{\mathrm{sH}} / \sigma_{xx}$$

Multiterminal landauer-Büttiker formalism



$$\theta_{\mathrm{sH}} = I_5^{s_z} / I_1$$

OUTLINE

- *Motivation- spin transport physics*

- *Theoretical methodologies* to explore spin transport in (disordered) strong SOC topological materials

  M Vila et al. **Physical Review Letters** 124 (19), 196602

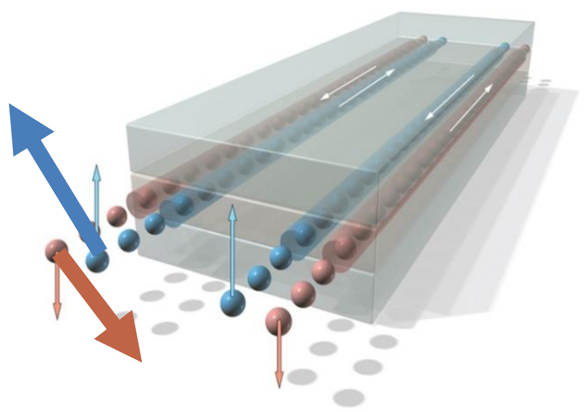
  Z. Fan, J.H. Garcia et al arXiv:1811.07387 (**Physics Reports**)

- **Multiple components Spin Hall Effect** in $MoTe_2$ monolayer

  M. Vila et al. **arXiv:2007.02053**

- **Canted Quantum Spin Hall Effect** in WTe_2 monolayer

  J.H. Garcia et al. **arXiv:2007.05626**



Scalable production of stable 1T′-$MoTe_2$

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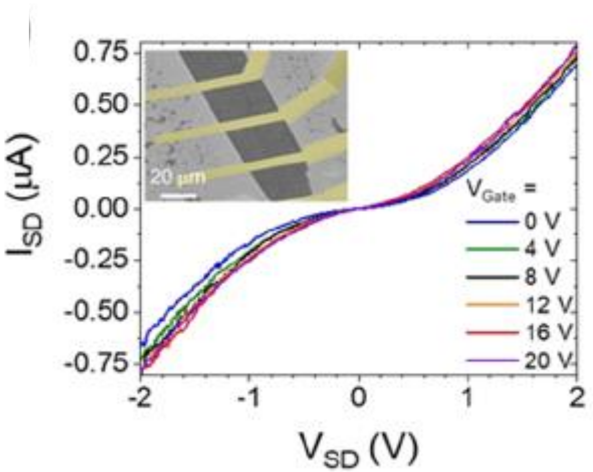
Article

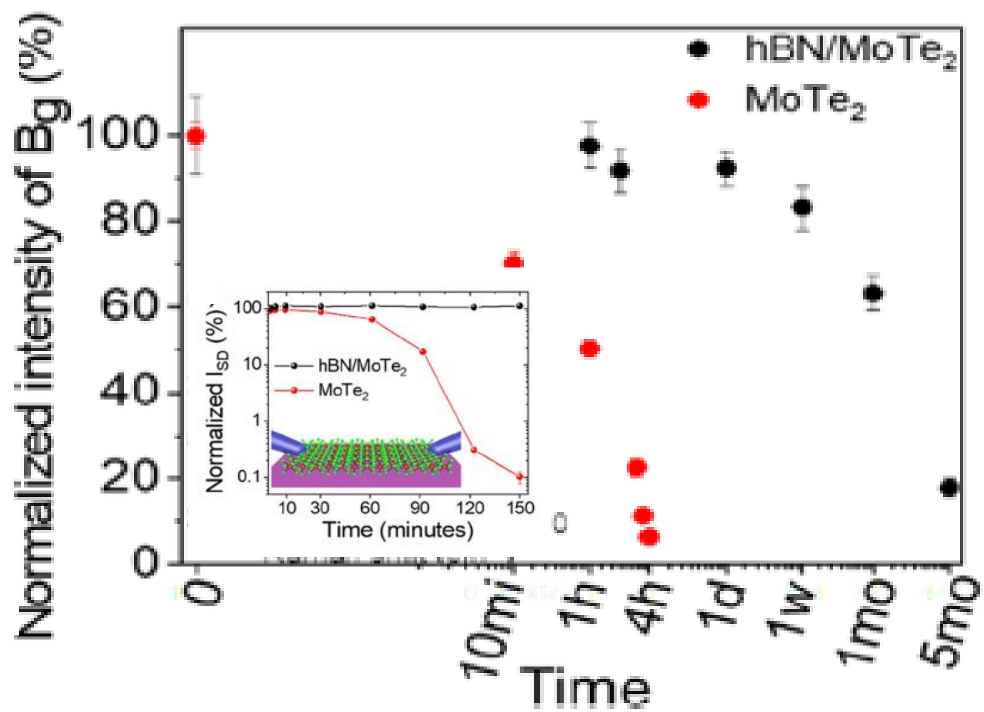
Synthesis of Large-Scale Monolayer 1T′-$MoTe_2$ and Its Stabilization *via* Scalable hBN Encapsulation

Simona Pace,* Leonardo Martini, Domenica Convertino, Dong Hoon Keum, Stiven Forti, Sergio Pezzini, Filippo Fabbri, Vaidotas Mišeikis, and Camilla Coletti*

Optical image of as-grown monolayer 1T′-$MoTe_2$ single crystals on a SiO_2 growth substrate

CVD growth of monolayer 1T′-$MoTe_2$ with a lateral size up to 500 μm & its scalable encapsulation via semidry transfer of few-layer CVD hBN



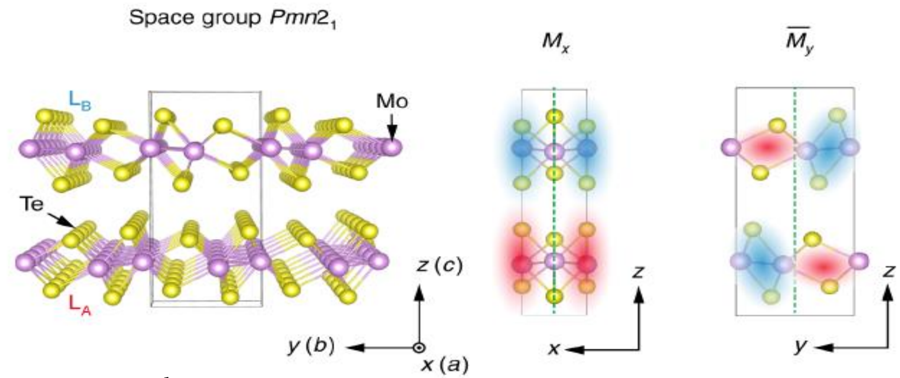


4-band symmetry-based model TMD-1T_d

NUS National University of Singapore
Centre for Advanced 2D Materials

Bulk crystal structure of 1T_d-TMD

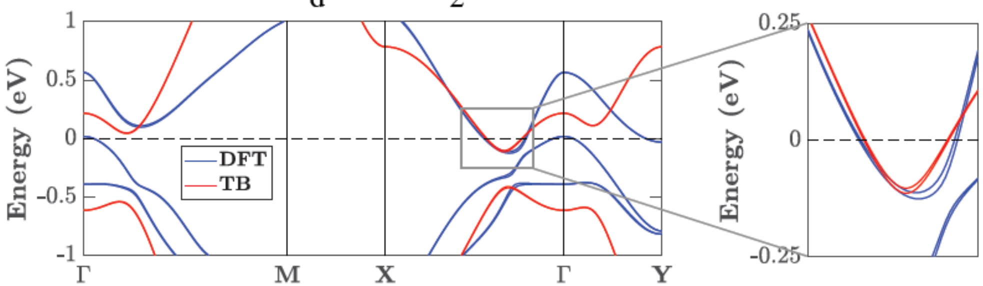
(mirror symmetry in the yz plane (M_x) & a glide mirror symmetry (M_y) along the perpendicular z direction)



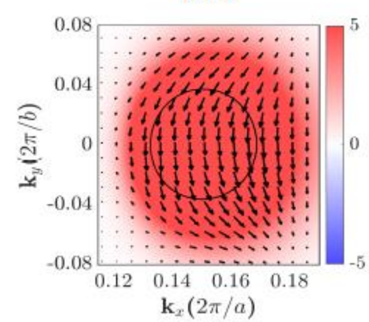
Monolayer 1T_d-TMD: *Lowering symmetry*

2D structure loses translational symmetry along the z direction

1T_d-$MoTe_2$

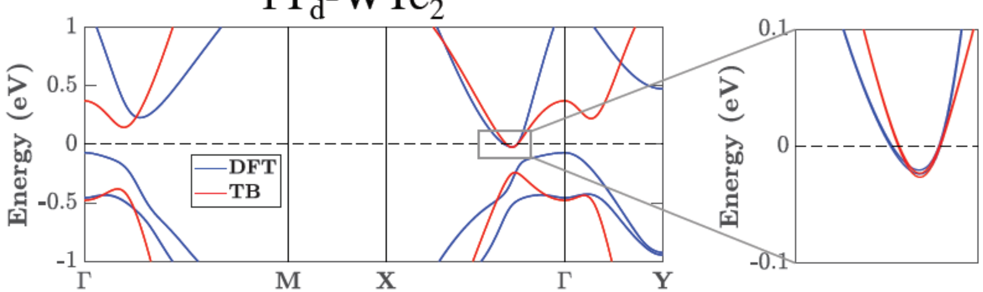


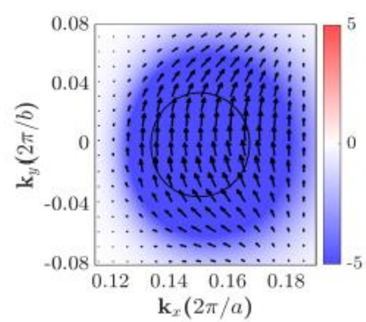
DFT



Persistent-canted spin texture (yz) (k-independent)

1T_d-WTe_2





$$\langle \vec{s} \rangle_{E_F} \approx \langle S_0 \rangle_{E_F} \hat{u}(\theta)$$

4-band symmetry-based model TMD-1T$_d$

NUS National University of Singapore

Centre for Advanced 2D Materials

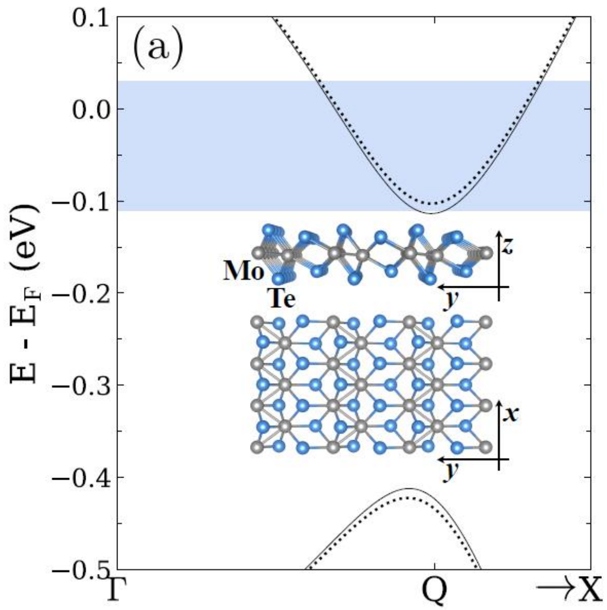
4-band real space tight binding model (*interpolated in Wannier basis (Wanier90)*)
generated by two orbitals (plus spin) / unit cell – p_y of the chalcogens and d_{yz} of the metal ions

$$
\begin{aligned}
H \quad &= \textstyle\sum_i (\Delta_E + 4m_d + \delta) c^\dagger_{i,s} c_{i,s} - \sum_{\langle i,j\rangle} (m_p + m_d) c^\dagger_{i,s} c_{j,s} \\
&\quad + \textstyle\sum_i (\Delta_E - 4m_d - \delta) d^\dagger_{i,s} d_{i,s} - \sum_{\langle i,j\rangle} (m_p - m_d) d^\dagger_{i,s} d_{j,s} \\
&\quad - \textstyle\sum_{\langle i,j\rangle} \frac{\beta}{2} (\hat{\boldsymbol{l}}_{ij} \cdot \hat{\boldsymbol{y}})\, c^\dagger_{i,s} d_{j,s} + \sum_i \eta c^\dagger_{i,s} d_{i,s} \\
&\quad - \textstyle\sum_{\langle i,j\rangle} \frac{i}{2} (\boldsymbol{\Lambda} \times \hat{\boldsymbol{l}}_{ij}) \cdot (\hat{\boldsymbol{y}} + \hat{\boldsymbol{z}}) c^\dagger_{i,s} d_{j,s},
\end{aligned}
$$

Spin-orbit coupling

$$\boldsymbol{\Lambda} \equiv (\Lambda_x \sigma_x, -\Lambda_y \sigma_y, \Lambda_z \sigma_z)$$

Spin texture:
Arrows: *in-plane spin projection*
Color: *spin projection along z*

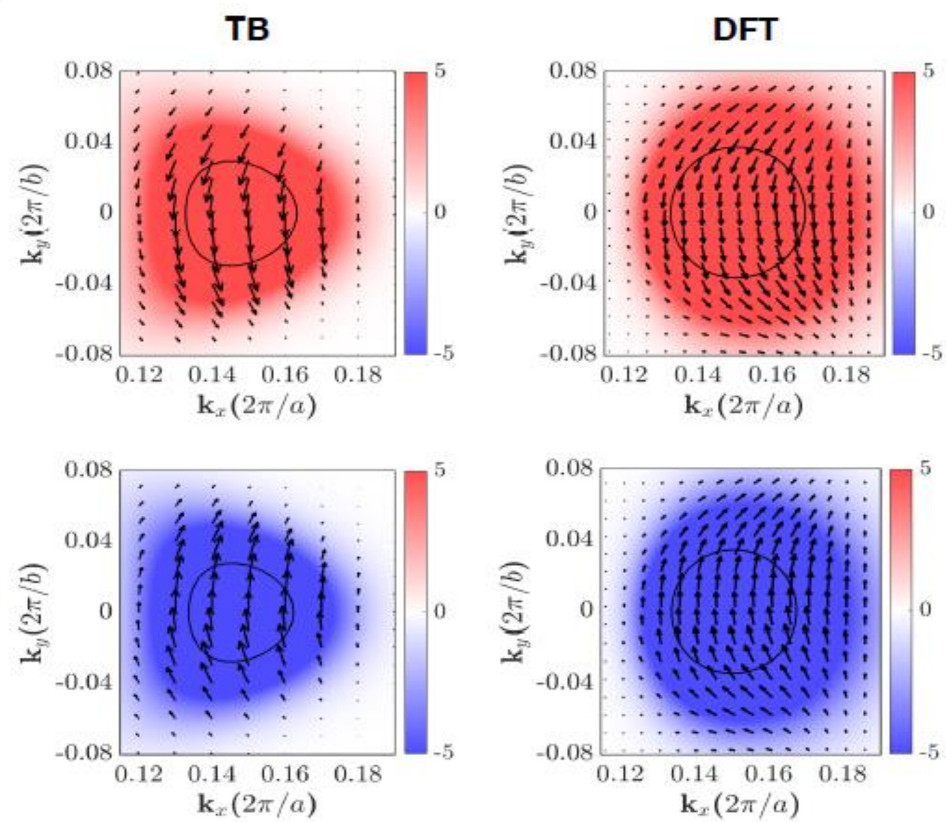


CB1

MoTe$_2$

CB2

WTe$_2$



Anisotropic spin dynamics in $MoTe_2$

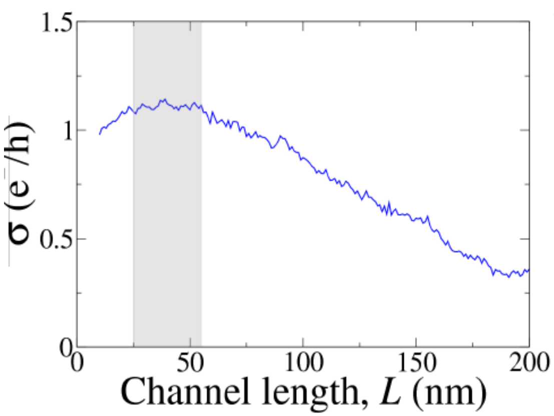
Study of the nonlocal resistance versus channel length to extract spin diffusion length

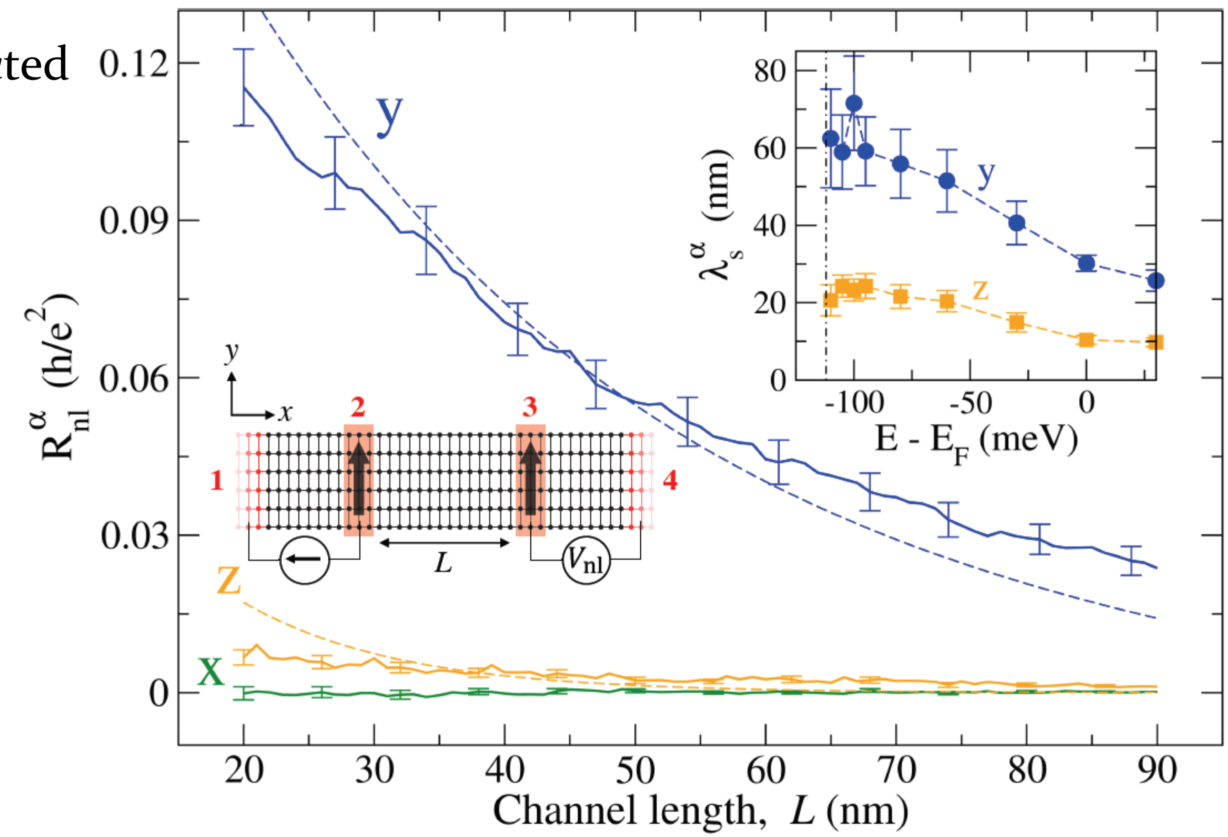
$$I_0^\alpha \quad \alpha \in \{x, y, z\}$$

Spin α-polarized current injected

$$R_{\rm nl}^\alpha \equiv V_{\rm nl}/I_0^\alpha$$

+Anderson disorder
Diffusive regime (MFP<L)





Extract of λ_s by fitting to the solution of a 1D spin diffusion equation

$$\lambda_s^y > \lambda_s^z \gg \lambda_s^x$$

arXiv:2007.02053

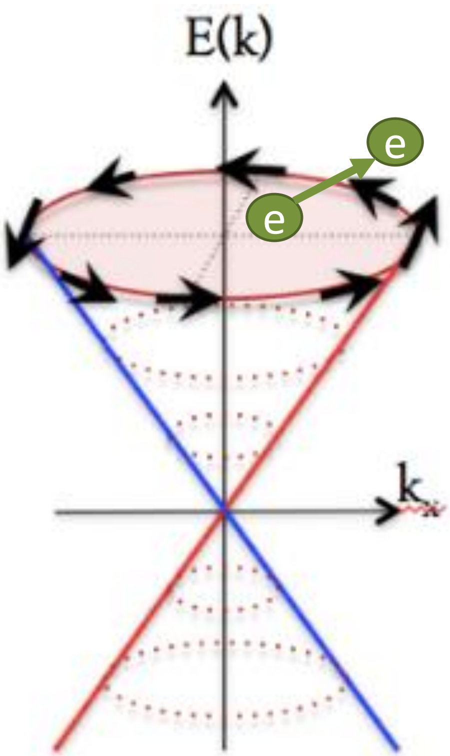
Anisotropic spin dynamics in $MoTe_2$

In 2D Rashba SOC materials

Spin-momentum locking

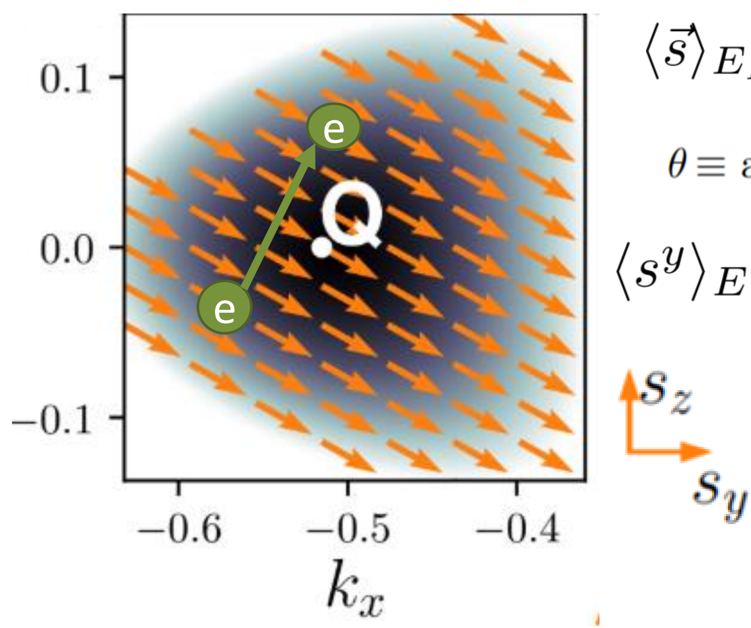
scattering changes effective (in-plane) magnetic field randomly

$$\lambda_s^z \sim \frac{1}{2}\lambda_s^y = \frac{1}{2}\lambda_s^x$$



In 2D Weyl semimetal TMD

Persistent (canted) spin texture



$$\langle \vec{s} \rangle_{E_F} \sim \langle S_0 \rangle_{E_F} \hat{u}(\theta)$$

$$\theta \equiv \arctan(\Lambda_z/\Lambda_y) \approx -56°$$

$$\langle s^y \rangle_E > \langle s^z \rangle_E \gg \langle s^x \rangle_E$$

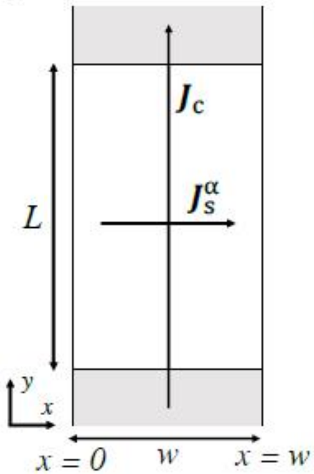
Effective magnetic field is fixed (pointing in the yz plane)

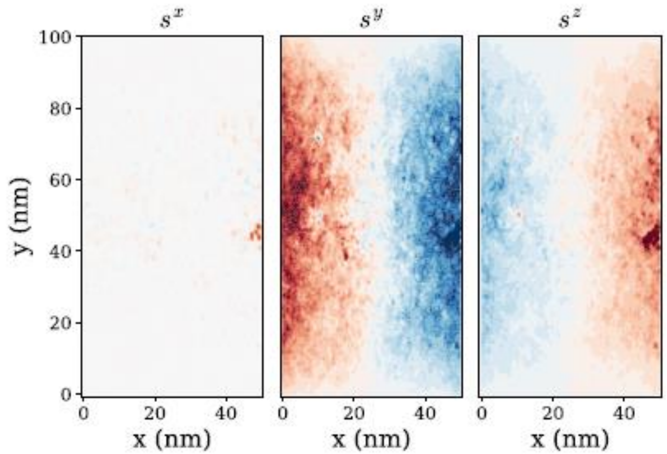
x-polarized spins precess much faster- shorter spin diffusion

z-polarized spins precess faster than y-polarized

$$\lambda_s^y > \lambda_s^z \gg \lambda_s^x$$

Spin accumulation & (Giant) Spin Hall angle



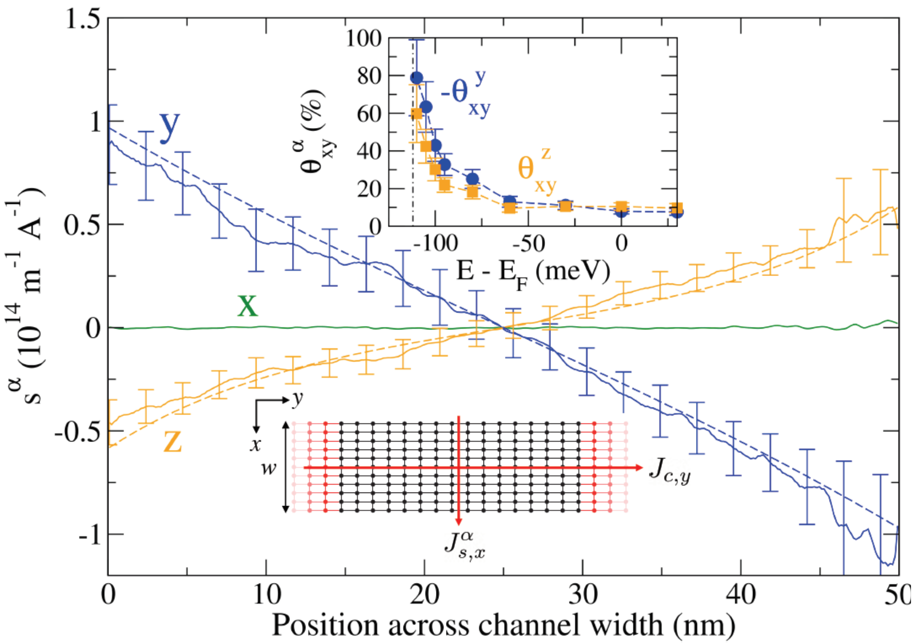


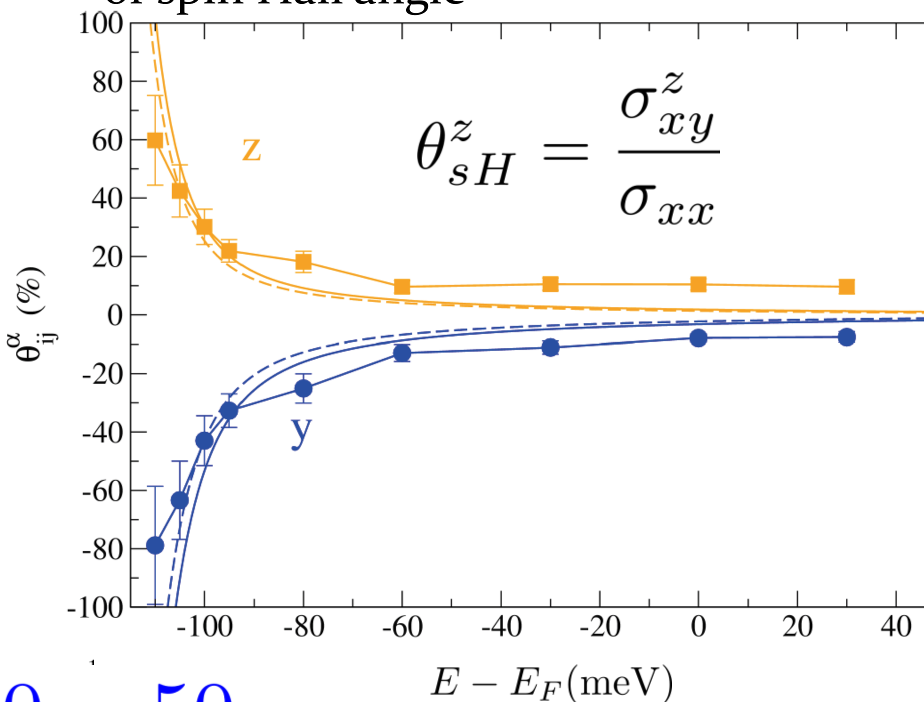
1) Extracting the spin accumulation across the channel

2) fitting the results with solution of the Spin drift-diffusion equation

$$\frac{s^\alpha(x)}{J_c} = -\frac{\theta^\alpha_{xy}\lambda^\alpha_s}{|e|D_s}\frac{\sinh(\frac{w-2x}{2\lambda^\alpha_s})}{\cosh(\frac{w}{2\lambda^\alpha_s})},$$

3) Check with Kubo-Bastin calculations of spin Hall angle





$$\lambda_s\theta^\alpha_{sH} \sim 10 - 50 \text{ nm}$$

Experimental fingerprints (Hanle)

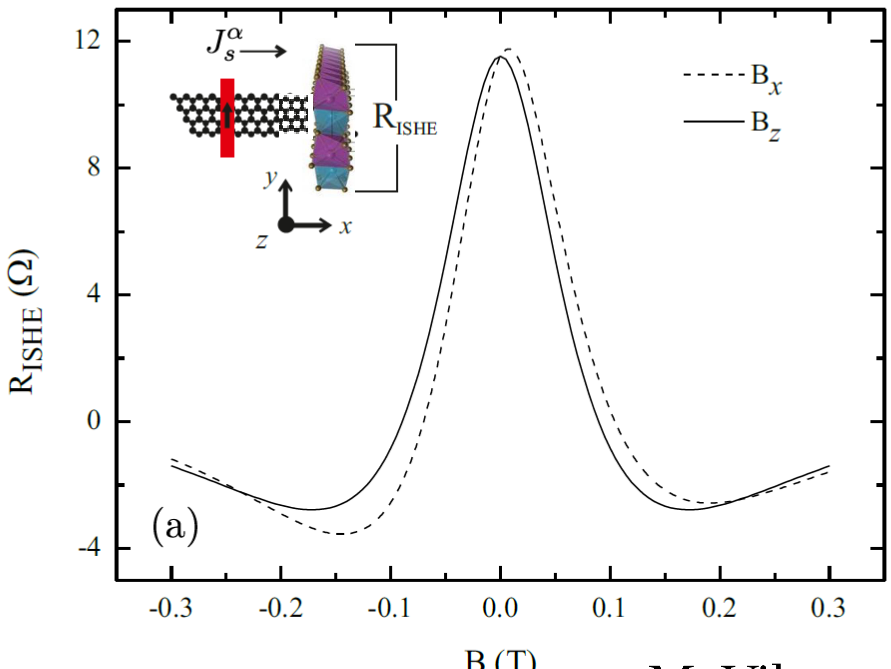
Simulated response of the inverse SHE (R_{ISHE})
to spin precession for two orientations of the TMD crystal (full absorption limit)

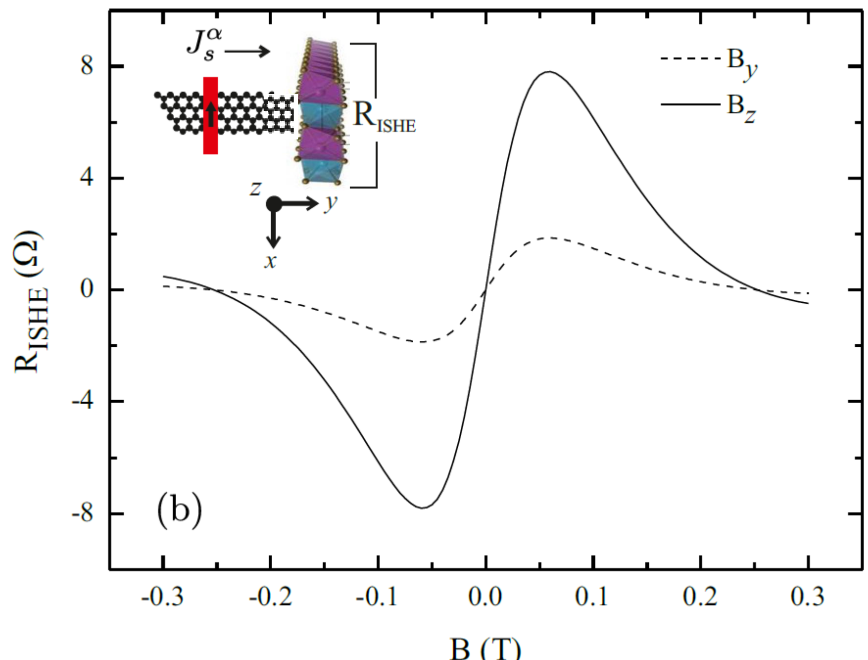
spin current polarization reaching the TMD J_s^{α} controlled externally with a magnetic field orientation

Anisotropic spin diffusion

$$R_{ISHE} = V_{ISHE}/I_0^y$$

- up to 3 orders of magnitude larger than other SHE materials (large SHA)
- symmetric or antisymmetric depending on crystal orientation





M. Vila et al. **arXiv:2007.02053**

OUTLINE

- *Motivation- Spin Transport Physics in Quantum Materials*

- *Theoretical methodologies* to explore spin transport in (disordered) strong SOC topological materials

  M Vila et al. **Phys. Rev. Lett.** 124 (19), 196602 (2020)

  Z. Fan, J.H. Garcia et al **Physics Reports** 2021 **(**arXiv:1811.07387)

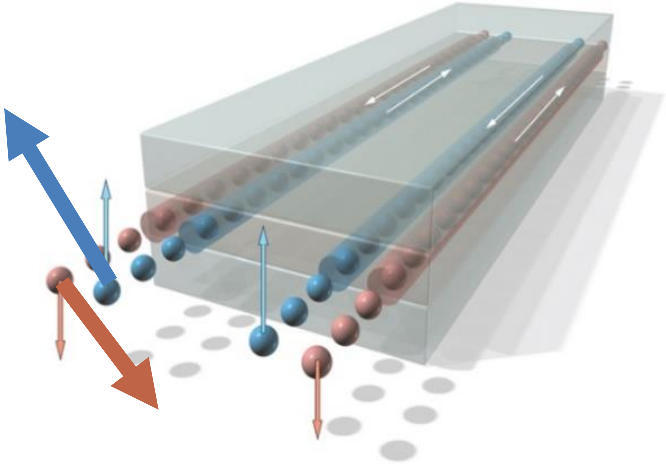
- Multiple components Spin Hall Effect in $MoTe_2$ monolayer

  M. Vila et al. **arXiv:2007.02053**

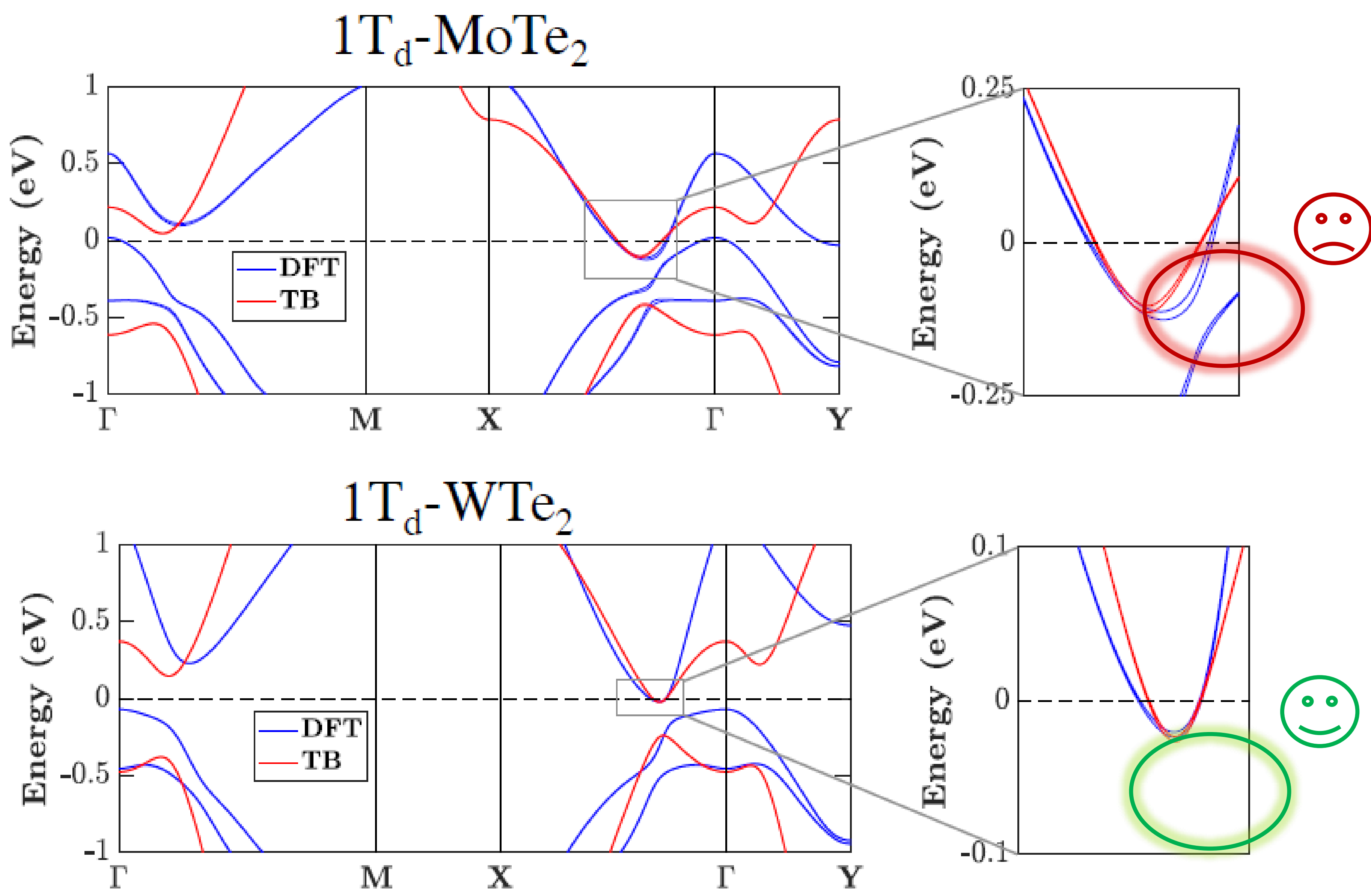
- **Canted Quantum Spin Hall Effect**

  in WTe_2 monolayer

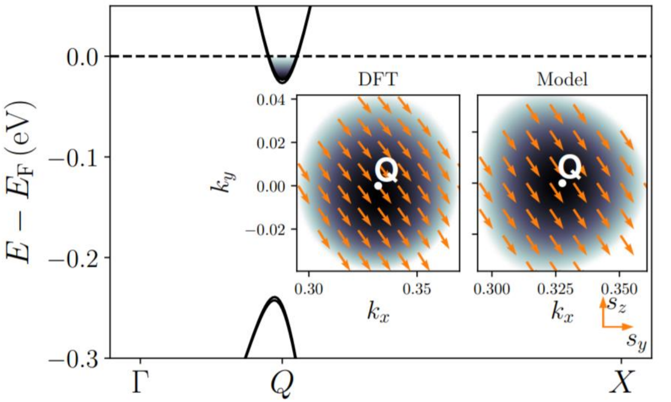
  J.H. Garcia et al. **Phys. Rev. Lett. 125, 256603 (2020)**



QSHE: $MoTe_2$ vs WTe_2



Spin Hall conductivity for WTe_2



$$\mathcal{H}_0 \simeq (k_x^2 + k_y^2)(m_p\tau_0 + m_d\tau_z) + \beta k_y \tau_y + \delta\tau_z + \eta\tau_x$$

$$\mathcal{H}_{\rm soc} \simeq (\Lambda_x k_y \sigma_x + \Lambda_y k_x \sigma_y + \Lambda_z k_x \sigma_z) \otimes \tau_x$$

$$\theta \equiv \arctan(\Lambda_z/\Lambda_y) \approx -56°$$

Simulations on a system with
4 Millions atoms
(*energy broadening = 5meV*)

In the gap

$$|\sigma_{xy}^\alpha| \equiv \sqrt{(\sigma_{xy}^y)^2 + (\sigma_{xy}^z)^2} = \frac{2e^2}{h}$$

two spin-canted topological states
sustaining QSHE in WTe_2

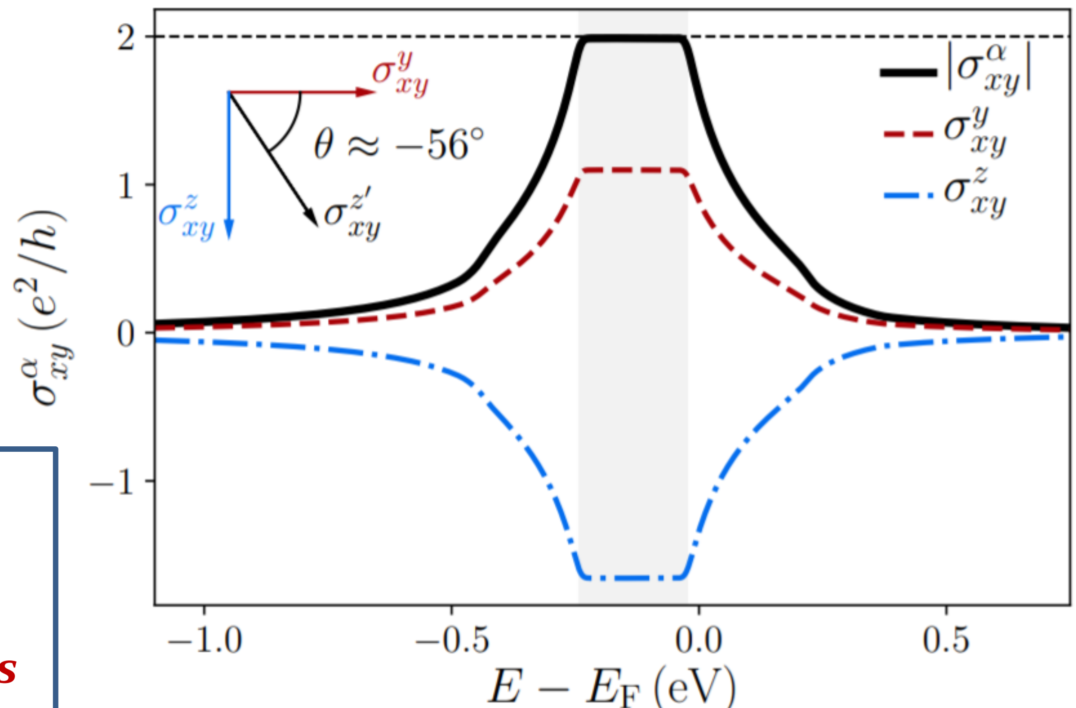
$$\arctan(\sigma_{xy}^z/\sigma_{xy}^y) = -56°$$

(spin quantization axis)

Spin Hall conductivity tensor
(Kubo-Bastin formula)

$\sigma_{ij}^\alpha, \alpha = x, y, z$ *measures of the spin projection onto* α

$$\sigma_{ij}^\alpha = -2\hbar\Omega \int_{-\infty}^{E_F} dE\, \mathrm{Im}\left(\mathrm{Tr}\left[\delta(E-\mathcal{H}) J_{s,i}^\alpha \frac{dG^+}{dE} J_j\right]\right)$$



$$U(\theta) \equiv \cos[(2\theta-\pi)/4]\sigma_0 - i\sin[(2\theta-\pi)/4]\sigma_x$$

$$\mathcal{H}'_{\rm SOC} \equiv U^\dagger(\theta)\mathcal{H}U(\theta) = \Lambda_x k_y \sigma_x + \Lambda_r k_x \sigma_{z'}\tau_x$$

$[\mathcal{H}', \sigma_{z'}] \approx 0$ *(spin preserved along z′)*

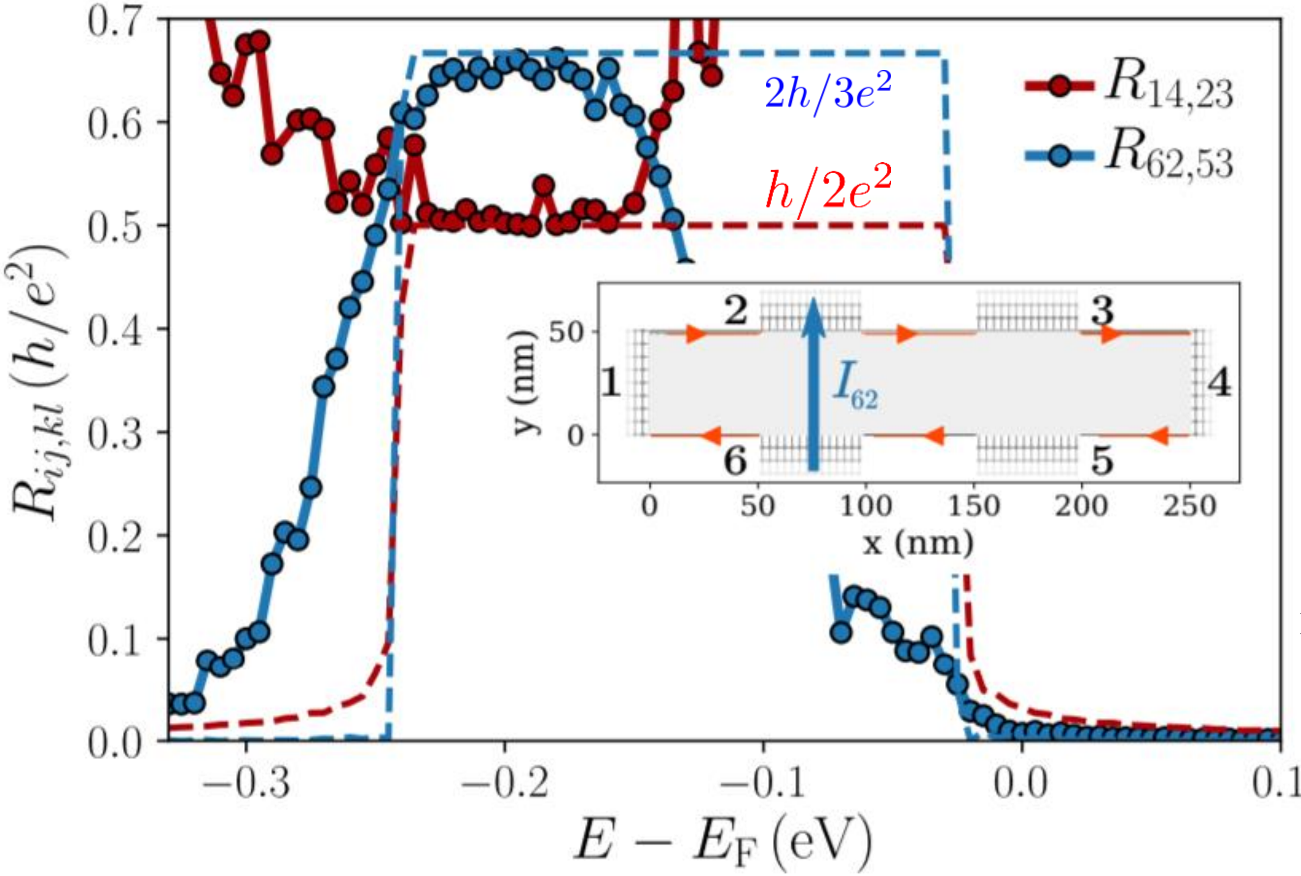
Nonlocal resistance calculations

Topologically protected edge-states

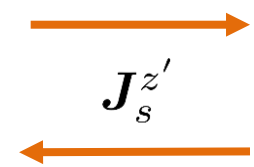
Quantized two-terminal resistance (2 channels) $h/2e^2$

Quantized nonlocal resistance $2h/3e^2$

Robustness to disorder *(Anderson model 1 eV)*



Bond-projected spin currents for spins polarized along the (rotated) **z‘ direction**



Bond-projected spin currents for spins polarized along the (rotated) y' direction

$J_s^{y'}$

“vanishing contribution”

M. Vila et al. **arXiv:2007.02053**

Determination of the helical edge and bulk spin axis in quantum spin Hall insulator WTe_2

Wenjin Zhao[1]†, Elliott Runburg[1]†, Zaiyao Fei[1], Joshua Mutch[1], Paul Malinowski[1], Bosong Sun[1], Xiong Huang[2,3], Dmytro Pesin[4], Yong-Tao Cui[2,3], Xiaodong Xu[1,5], Jiun-Haw Chu[1], David H. Cobden[1]*

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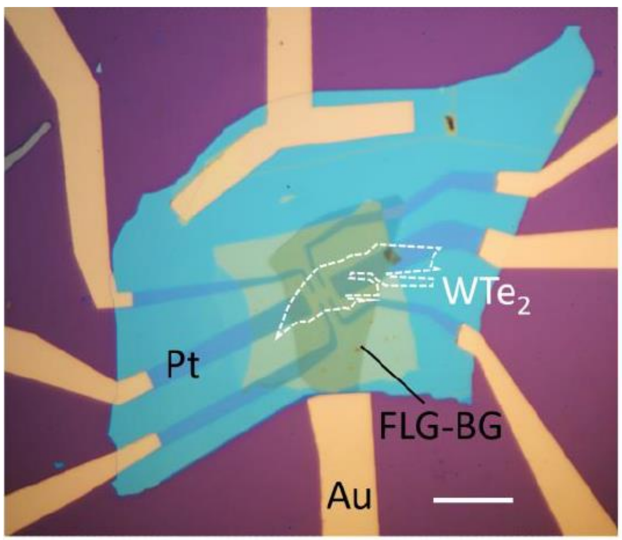
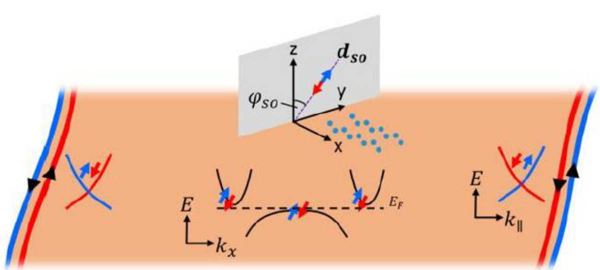
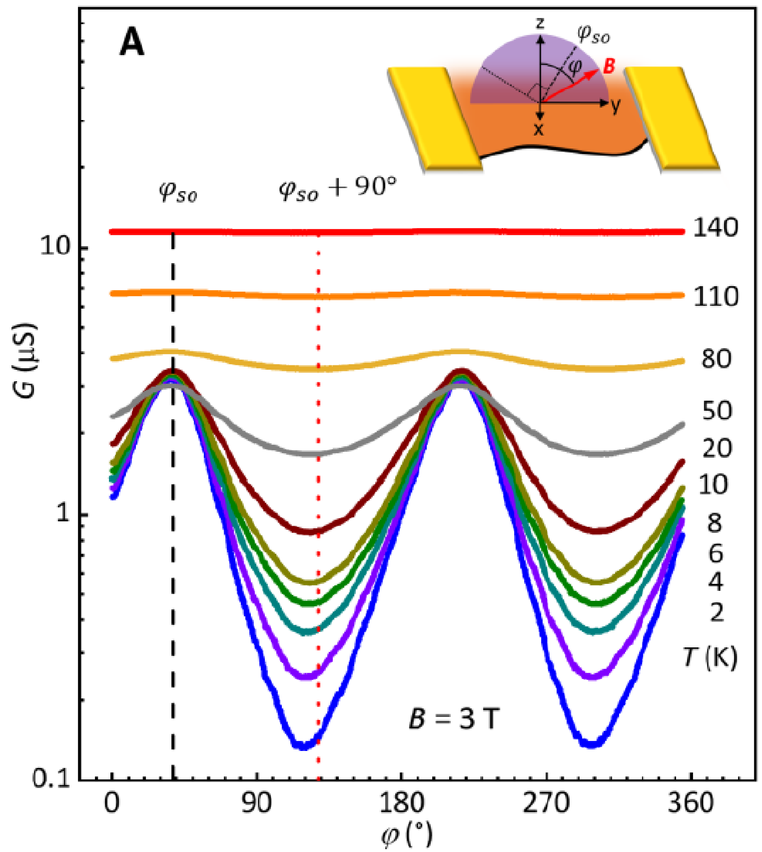
[2]Department of Physics and Astronomy, University of California, Riverside, Riverside CA 92521, USA
[3]Department of Materials Science and Engineering, University of California, Riverside, Riverside CA 92521, USA
[4]Department of Physics, University of Virginia, Charlottesville, Virginia 22904, USA
[5]Department of Materials Science and Engineering, University of Washington, Seattle WA 98195, USA
†These authors contributed equally
*Corresponding author: cobden@uw.edu

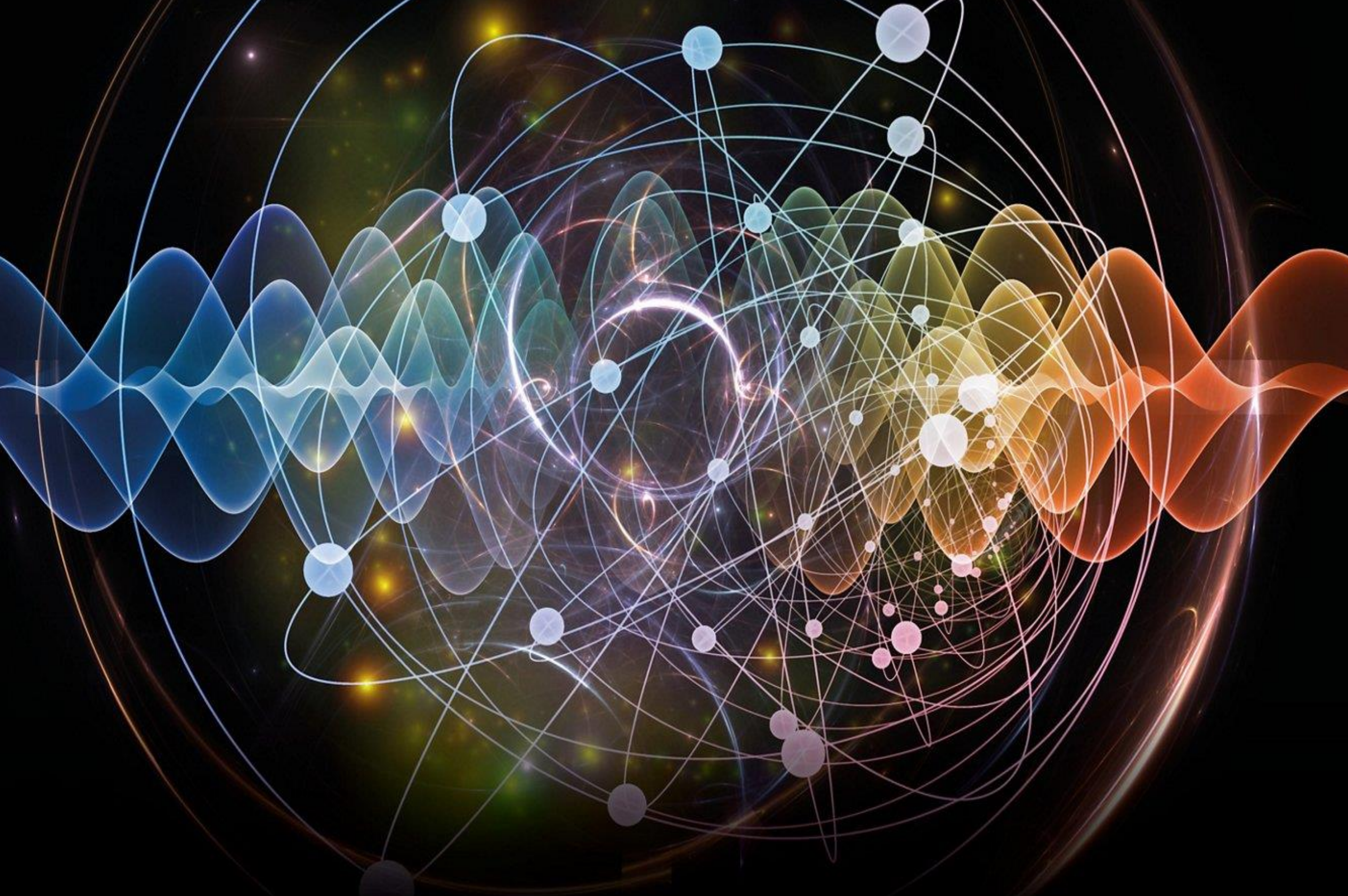
arXiv:2010.09986

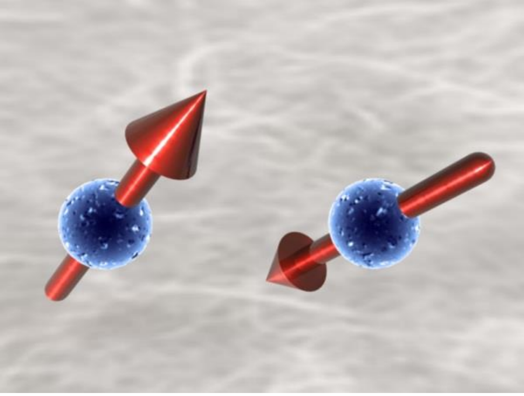






Entanglement in Quantum Materials …..





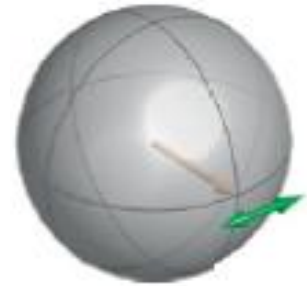
Particles in Graphene

Three intraparticle (quantum) degrees

Spin

Valley "isospín"

Sublattice "pseudospin"



8-components wavefunction

$$\begin{pmatrix} 0 & p_x - ip_y & 0 & 0 & 0 & 0 & 0 & 0 \\ p_x - ip_y & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -p_x + ip_y & 0 & 0 & 0 & \\ 0 & 0 & -p_x + ip_y & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & p_x - ip_y & 0 & 0 \\ 0 & 0 & 0 & 0 & p_x - ip_y & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -p_x + ip_y \\ 0 & 0 & 0 & 0 & 0 & 0 & -p_x + ip_y & 0 \end{pmatrix} \begin{pmatrix} \Psi^{\Uparrow}_{A,+} \\ \Psi^{\Uparrow}_{B,+} \\ \Psi^{\Uparrow}_{A,-} \\ \Psi^{\Uparrow}_{B,-} \\ \Psi^{\Downarrow}_{A,+} \\ \Psi^{\Downarrow}_{B,+} \\ \Psi^{\Downarrow}_{A,-} \\ \Psi^{\Downarrow}_{B,-} \end{pmatrix}$$

No intervalley/spin mixing- Valleys degenerate..

No disorder, No spin-orbit interaction

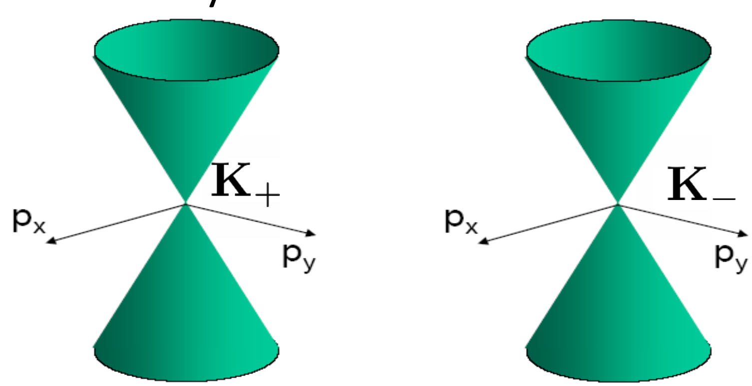
$$\mathcal{H}_{K_+} = v_F \vec{\sigma}.\vec{p}$$

DIRAC Fermions

*GAPLESS **Linear energy dispersion***

and velocity 10⁶m/s

Valley + Valley -

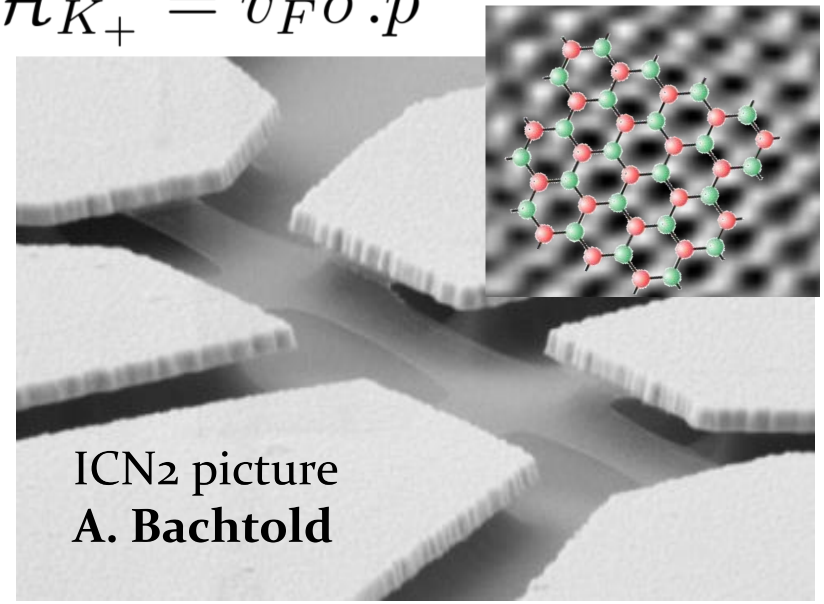


“Unique properties of Clean graphene”

$$\mathcal{H}_{K_+}|\Psi_{\vec{p}}\rangle = E_{\vec{p}}|\Psi_{\vec{p}}\rangle$$

$$\Psi_{\vec{p}} = \frac{1}{\sqrt{2}}\left(\Psi_{\vec{p}}(A)\begin{pmatrix}1\\0\end{pmatrix} + \Psi_{\vec{p}}(B)\begin{pmatrix}0\\1\end{pmatrix}\right)$$

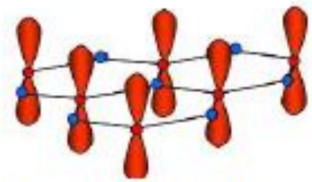
$$\mathcal{H}_{K_+} = v_F\vec{\sigma}.\vec{p}$$



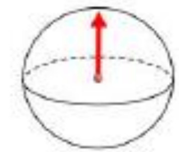
pseudospin

A sublattice : p_z

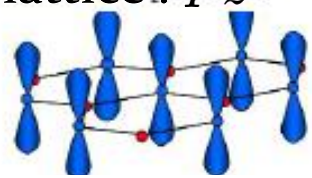
Spinor Representation



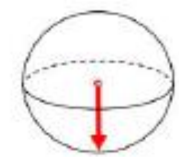
$|\Psi_A\rangle$



B sublattice : p_z



$|\Psi_B\rangle$

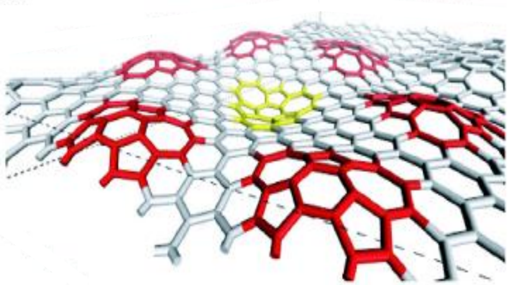


And related Berry´s phase

Long range potential

Intravalley scattering

(short momentum transfer)



Anomalous quantum transport

- Ballistic conductivity $\sigma \sim 4e^2/\pi h$
- Klein tunneling
- Diverging zero-energy Mean free path/mobility
- Weak antilocalization (quantum interferences)
- Anomalous vs conventional QHE
- **Spin transport ?**

nature physics

ARTICLES

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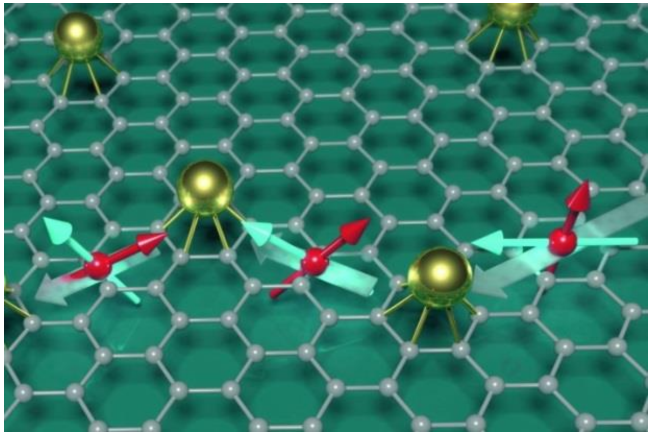
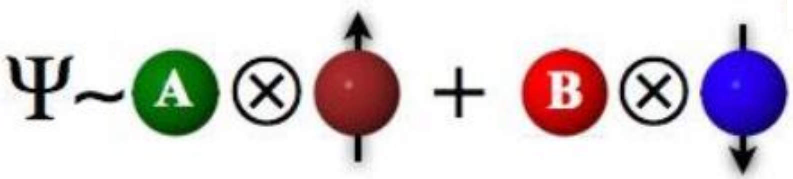
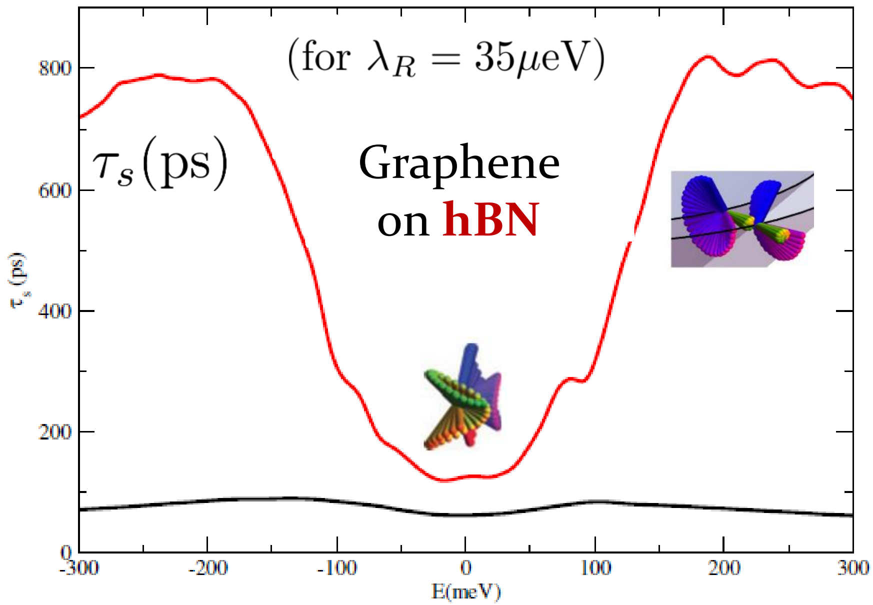
Pseudospin-driven spin relaxation mechanism in graphene

Dinh Van Tuan[1,2], Frank Ortmann[1,3,4], David Soriano[1], Sergio O. Valenzuela[1,5] and Stephan Roche[1,5]*

$$\vec{P}(E,t) = \frac{\langle\psi_\uparrow(t)|\,[1_\sigma \otimes \vec{s}]\,\delta(E-\mathcal{H}^{\text{eff}}) + \delta(E-\mathcal{H}^{\text{eff}})\,[1_\sigma \otimes \vec{s}]\;|\psi_\uparrow(t)\rangle}{2\langle\psi_\uparrow(t)|\delta(E-\mathcal{H}^{\text{eff}})\;|\psi_\uparrow(t)\rangle}$$







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Rapid Communications

Emergence of intraparticle entanglement and time-varying violation of Bell's inequality in Dirac matter

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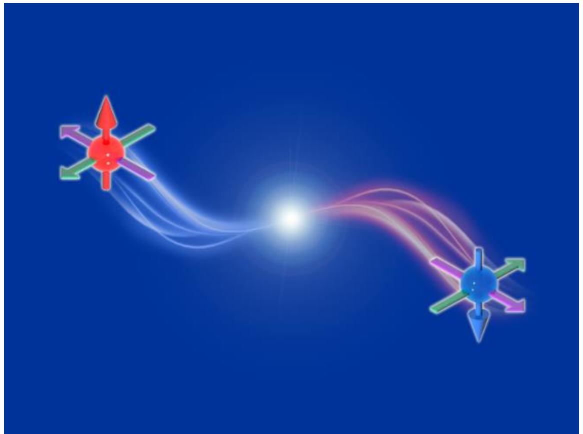
We demonstrate the emergence and dynamics of intraparticle entanglement in massless Dirac fermions. This entanglement, generated by spin-orbit coupling, arises between the spin and sublattice pseudospin of electrons in graphene. The entanglement is a complex dynamic quantity but is generally large, independent of the initial state. Its time dependence implies a dynamical violation of a Bell inequality, while its magnitude indicates that large intraparticle entanglement is a general feature of graphene on a substrate. These features are also expected to impact entanglement between pairs of particles, and may be detectable in experiments that combine Cooper pair splitting with nonlocal measurements of spin-spin correlation in mesoscopic devices based on Dirac materials.



Emerging *entanglement properties between intraparticle degrees of freedom*

Robustness *against decoherence*

Possibility of ***nonlocal manipulation****…*

Concurrence
(entanglement degree)

$$R = \sqrt{\rho_{1,2}(\sigma_{1y} \otimes \sigma_{2y})\rho^*_{1,2}(\sigma_{1y} \otimes \sigma_{2y})}$$

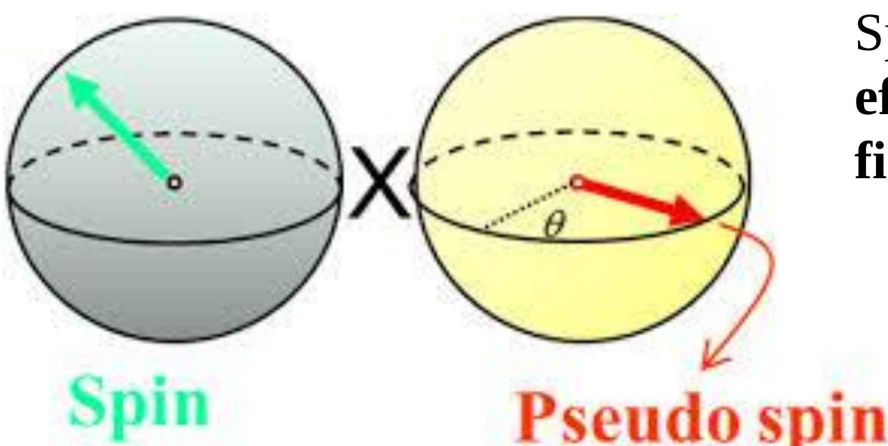
diagonalising an operator R which is built from the general ***two-qubit*** *density matrix*

$$C(\phi) = max\{0, \tilde{\lambda_1} - \tilde{\lambda_2} - \tilde{\lambda_3} - \tilde{\lambda_4}\}$$

Concurrence has a one-to-one correlation with the entanglement of formation, and ranges between **0 (separable state)** and **1 (maximally entangled state)**

Concurrence (spin-pseudospin) for electronic states propagating in Graphene/substrate (SiO_2 or hBN)

$$\hat{\mathcal{H}} = \hbar v_{\mathrm{F}} \left(\tau \hat{\sigma}_x k_x + \hat{\sigma}_y k_y\right) \otimes \hat{s}_0 + \lambda_{\mathrm{R}} \left(\tau \hat{\sigma}_x \otimes \hat{s}_y - \hat{\sigma}_y \otimes \hat{s}_x\right)$$



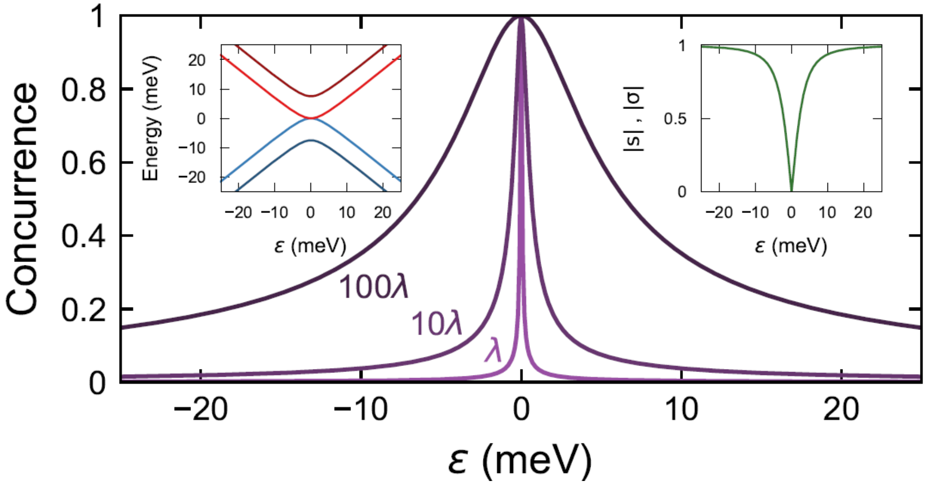
Spin and pseudospin will precess around **effective magnetic and pseudomagnetic fields** (oscillation freq. $\omega_{\mathrm{R}} = 2\lambda_{\mathrm{R}}/\hbar$)

$$\boldsymbol{B}^{\mathrm{eff}}_{\boldsymbol{s}}(t) = \lambda_{\mathrm{R}} \left(-\langle\hat{\sigma}_y\rangle(t)\,,\, \langle\hat{\sigma}_x\rangle(t)\,,\, 0\right),$$

$$\boldsymbol{B}^{\mathrm{eff}}_{\boldsymbol{\sigma}}(t) = \lambda_{\mathrm{R}} \left(\langle\hat{s}_y\rangle(t)\,,\, -\langle\hat{s}_x\rangle(t)\,,\, 0\right) + \varepsilon\,(1\,,\,0\,,\,0)\,,$$

Hamiltonian (Rashba SOC) & **Concurrence** (spin-pseudospin)

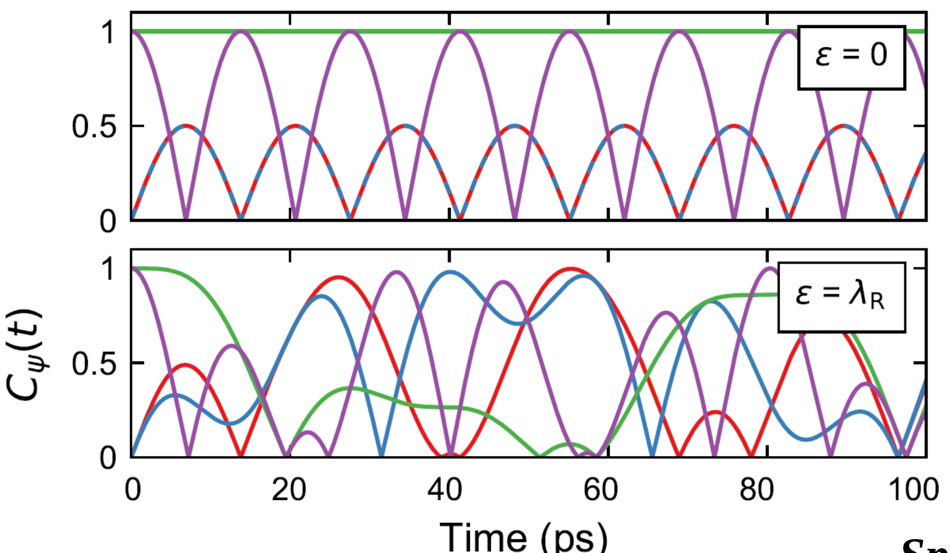
$$\hat{\mathcal{H}} = \hbar v_{\mathrm{F}} \left(\tau \hat{\sigma}_x k_x + \hat{\sigma}_y k_y\right) \otimes \hat{s}_0 + \lambda_{\mathrm{R}} \left(\tau \hat{\sigma}_x \otimes \hat{s}_y - \hat{\sigma}_y \otimes \hat{s}_x\right)$$



$$\left[|A\uparrow\rangle \quad |B\uparrow\rangle \quad |A\downarrow\rangle \quad |B\downarrow\rangle\right]^{\mathrm{T}}$$

In the eigenstates basis of H

$$C_{\phi_{\pm}^{\mathrm{e,h}}} = \lambda_{\mathrm{R}} / \sqrt{\varepsilon^2 + \lambda_{\mathrm{R}}^2}$$



$|\psi_x^{\uparrow}\rangle$ $|\psi_y^{\uparrow}\rangle$ $|\psi_{\mathrm{Bell}}^{1}\rangle$ $|\psi_{\mathrm{Bell}}^{2}\rangle$

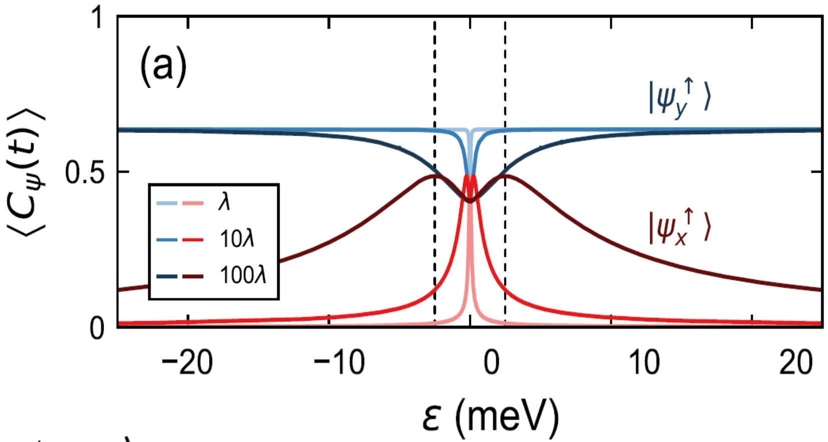
Time-evolution of concurrence
for different initial states

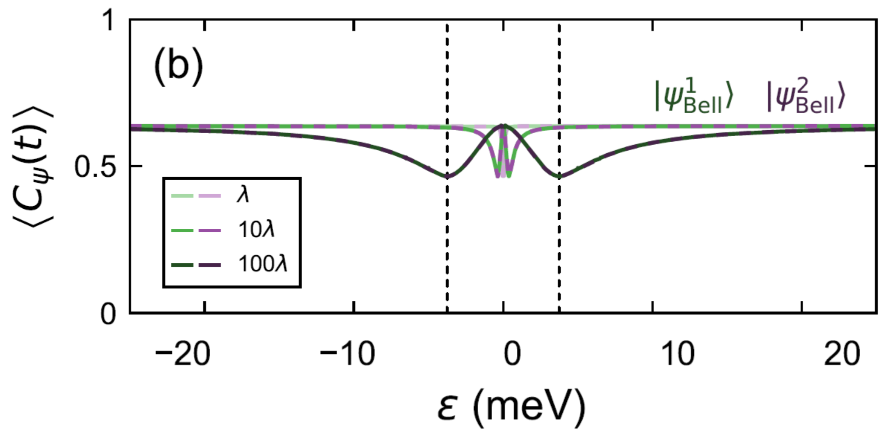
$$\frac{1}{\sqrt{2}}\left[1 \quad 1 \quad 0 \quad 0\right]^{\mathrm{T}} = \frac{1}{\sqrt{2}}\left(|A\rangle + |B\rangle\right) \otimes |\uparrow\rangle = |\psi_x^{\uparrow}\rangle$$

pseudospin along x, spin along z

States initially unentangled acquired
Spin-pseudospin entanglement during propagation

Emergence and Resilience of Spin-Pseudospin entanglement



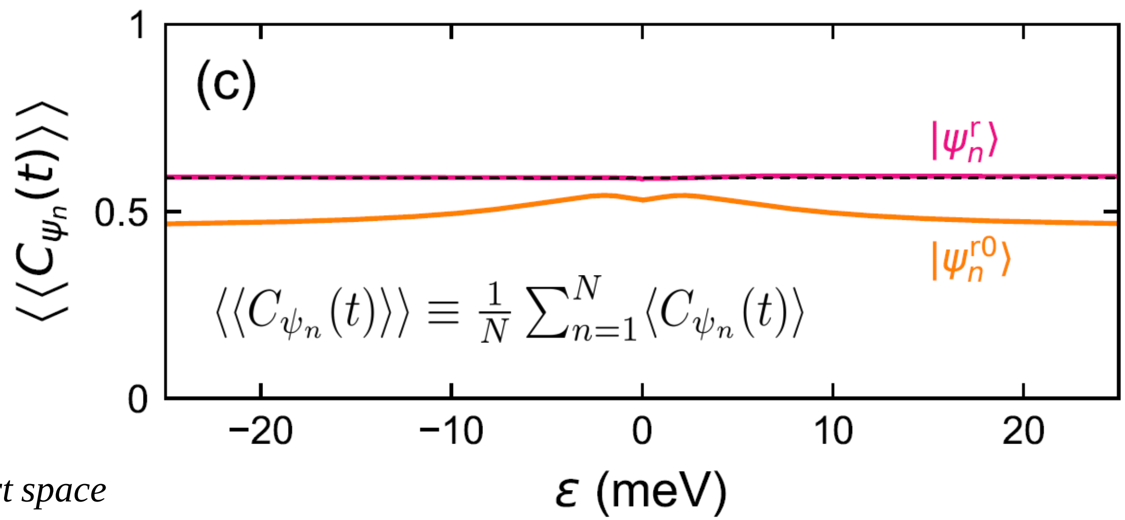


$$|\psi_n^{r_0}\rangle$$

is ***a separable state with*** *random spherical angles defining the orientations of the pseudospin and spin on the Bloch sphere*

$$|\psi_n^r\rangle = \begin{bmatrix} a & b & c & d \end{bmatrix}^{\mathrm{T}}$$

States that are equivalent to the action of a random unitary matrix on some reference state, which are uniform over the four-dimensional Hilbert space



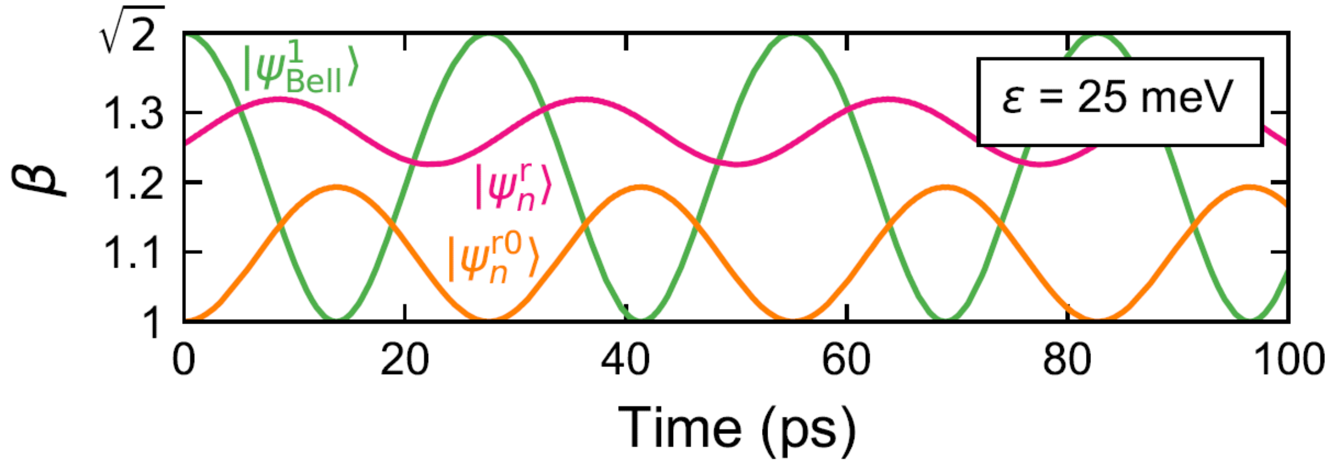
Even arbitrarily initial state develops a final entanglement

(entanglement resilient to scattering)

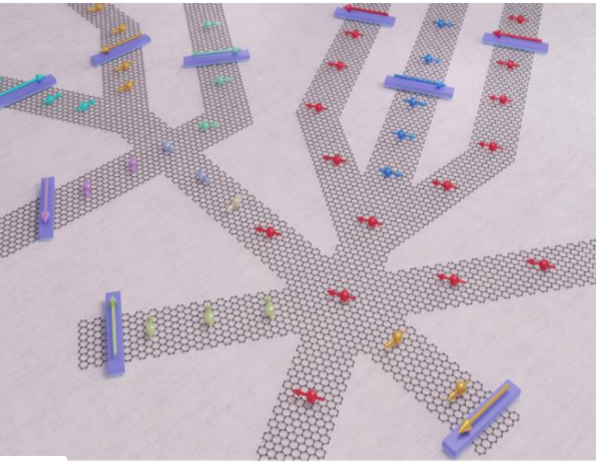
Time-dependent violation of the Bell inequality

(CHSH variant) *for intraparticle degrees of freedom*

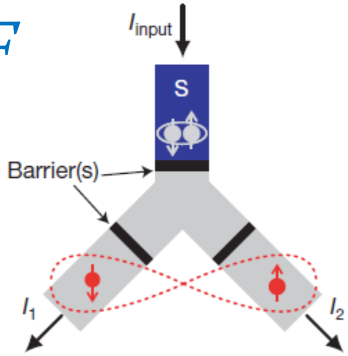
$$\beta = \sqrt{1 + C_\psi^2}$$



Generalization to nonlocal correlations between interparticle DoF



Manipulation ***by gauge fields***
(electromagnetic, deformation fields, proximity effects...)



$$e^{-i\hat{\mathcal{H}}t/\hbar}\,|\Psi_{1,k_0};\Psi_{2,-k_0}\rangle \otimes \left(|\Uparrow_1^z\Downarrow_2^z\rangle - |\Downarrow_1^z\Uparrow_2^z\rangle\right)$$