Conference and Advanced School on Low-Dimensional Quantum Systems

13 - 24 March 2023
An ICTP Meeting
Santiago, Chile

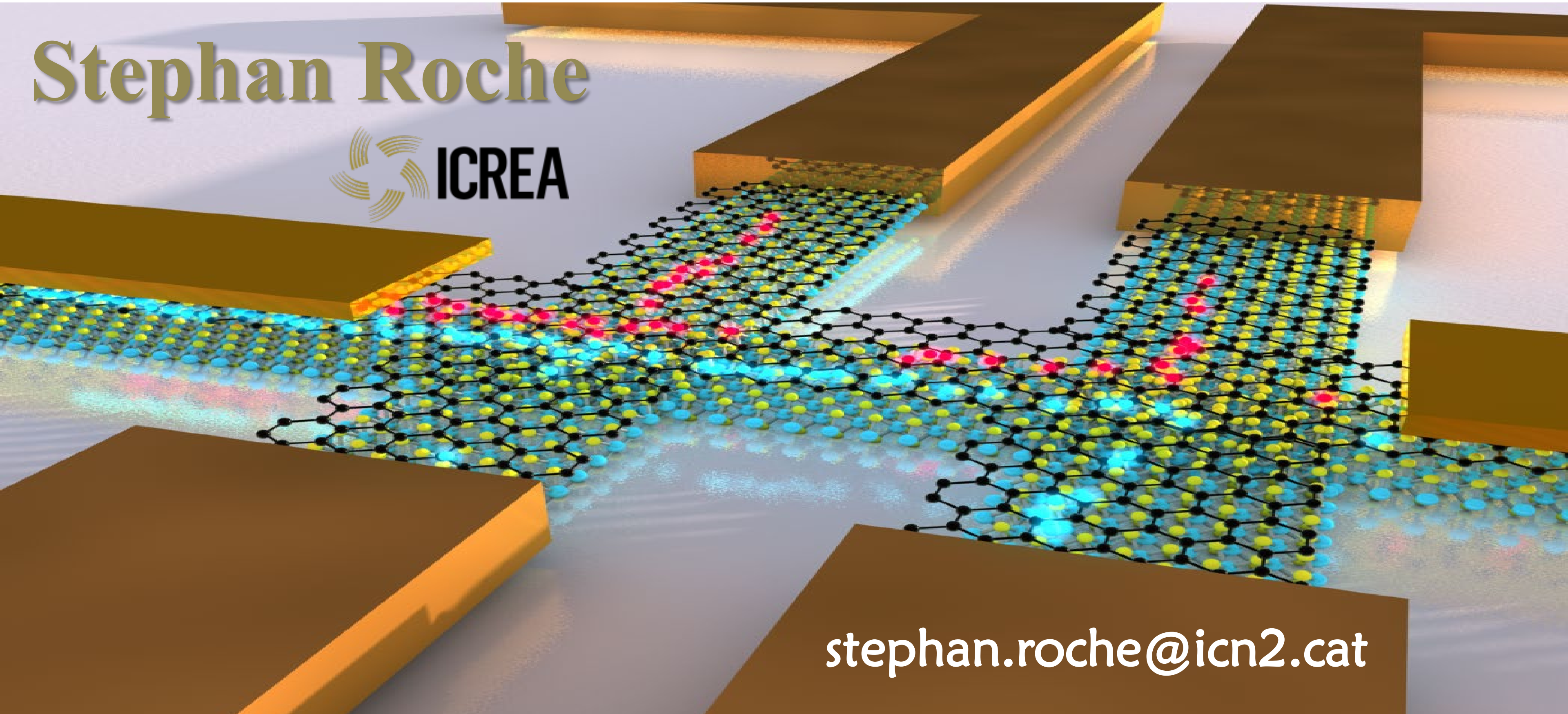
ICTP

ICN2 Institut Català de Nanociència i Nanotecnologia

EXCELENCIA SEVERO OCHOA

BIST Barcelona Institute of Science and Technology

Topological Spin Transport in *Quantum Materials & Entanglement Dynamics*



Stephan Roche

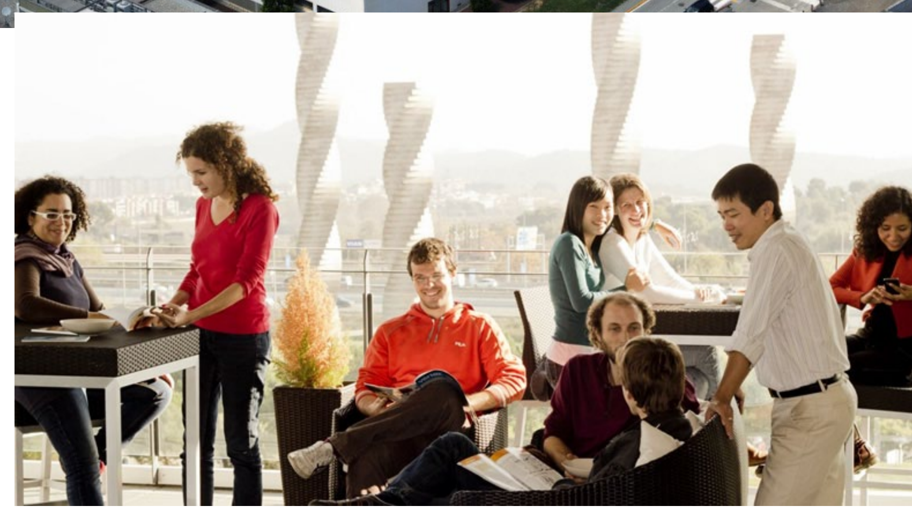
ICREA

stephan.roche@icn2.cat

Institute of Nanoscience & Nanotechnology

Barcelona Institute of Science & Technology

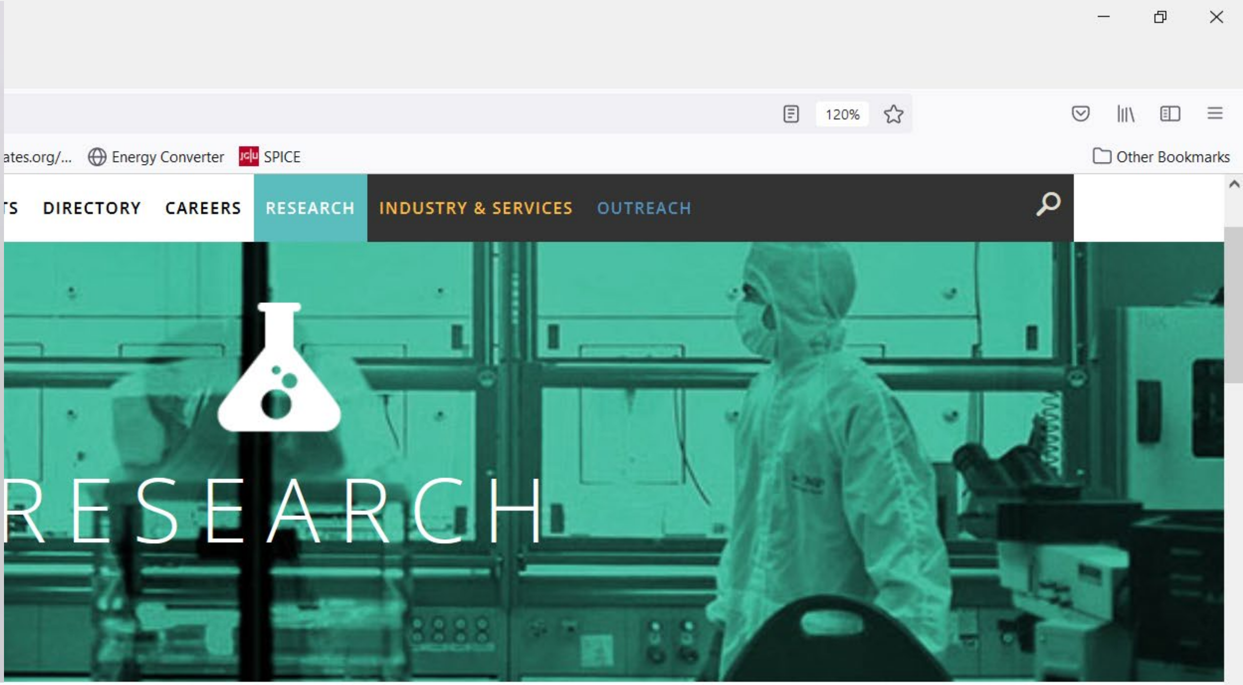
bist.eu

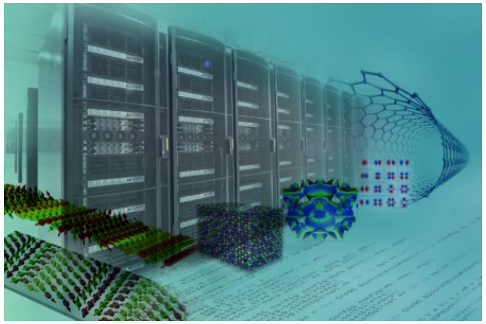


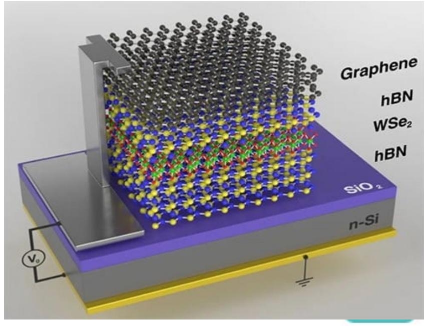
Quantum Materials @ICN2

www.icn2.cat

Sergio Valenzuela



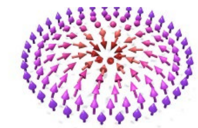




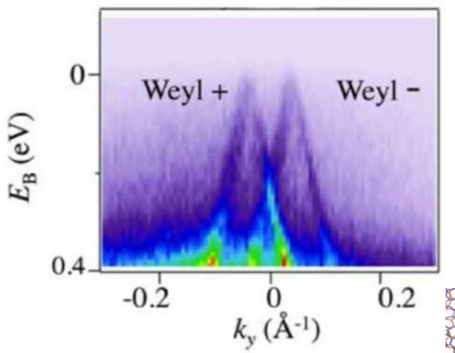
ROADMAP

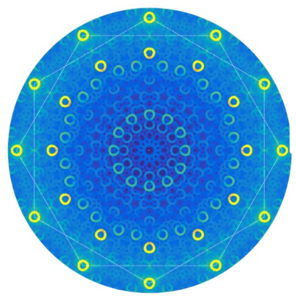
IOP Publishing

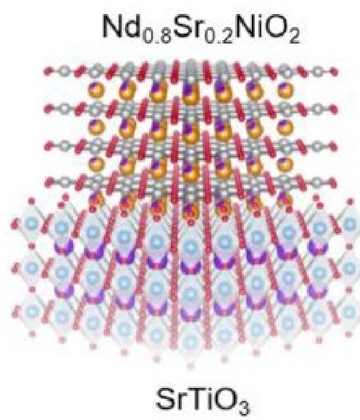
The 2021 quantum materials roadmap

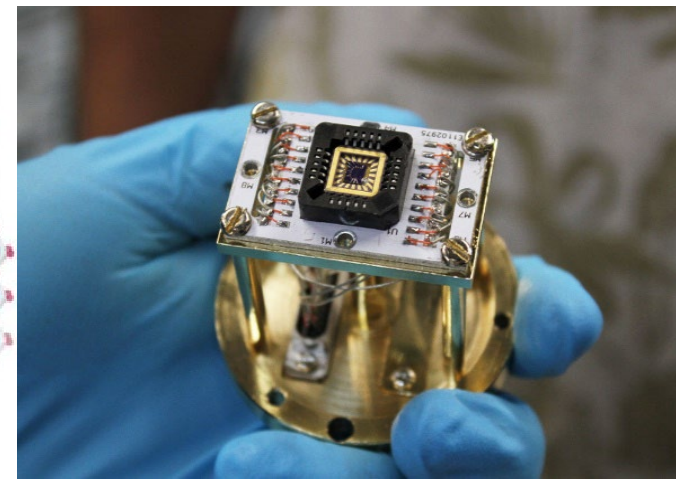


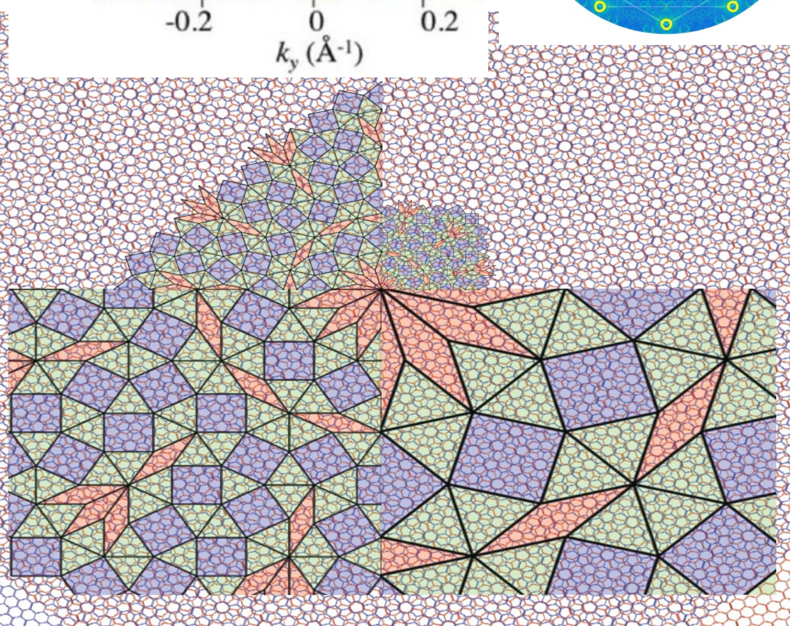
Feliciano Giustino[1,2], Jin Hong Lee[3], Felix Trier[3], Manuel Bibes[3], Stephen M Winter[4], Roser Valentí[4], Young-Woo Son[5], Louis Taillefer[6,7], Christoph Heil[8], Adriana I Figueroa[9], Bernard Plaçais[10], QuanSheng Wu[11], Oleg V Yazyev[11], Erik P A M Bakkers[12], Jesper Nygård[13], Pol 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]

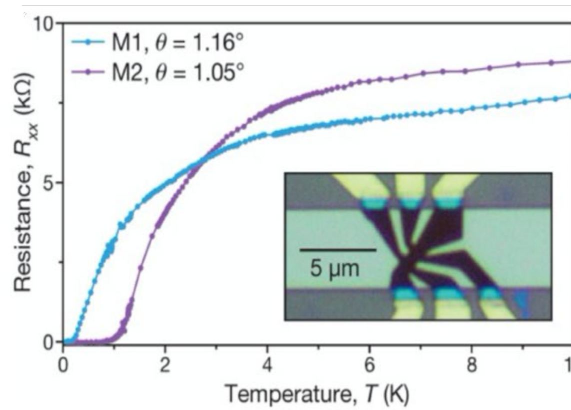


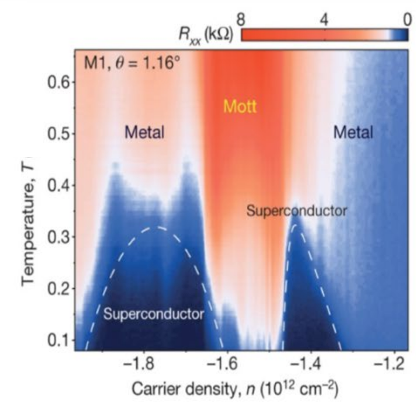












Theoretical & Computational Nanoscience

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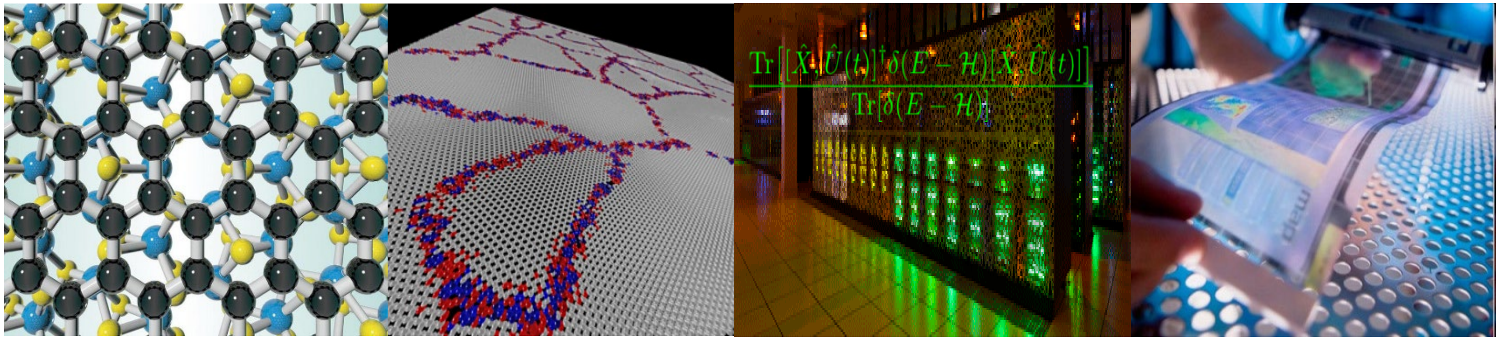

Members

Stephan Roche (head)
Aron W. Cummings (staff)
José H. Garcia (staff)
Thomas Galvani (Pdoc)
Isaac Alcón (Pdoc)
Luis Manuel Canonico (Pdoc)
Joaquin Medina Dueñas (PhD)
Onurcan Kaya (PhD)
Pedro Alcazar (PhD)
Jorge Ramírez and Jaime Garrido (Master students)

Past members

José-Eduardo Barrios
Bruna Gabrielly
Pablo Piskunow
Antonio Benitez
Aleandro Antidormi
Nicolas Leconte
Dinh Van Tuan
Frank Ortmann
David Soriano
Stephen Power

Topological Quantum Matter
Forefront Research

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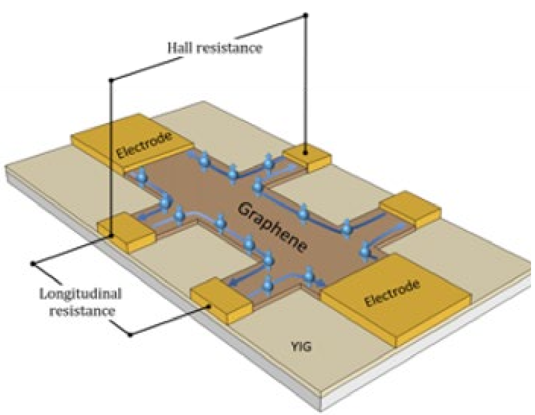
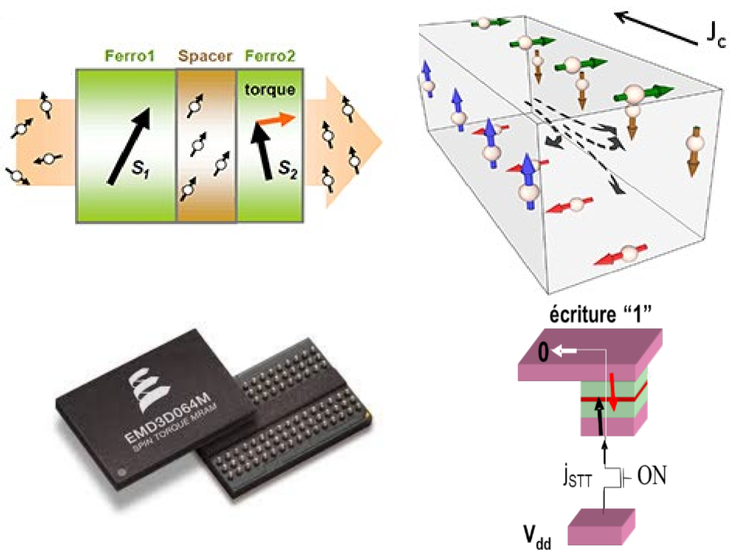
Topological Physics	**Spin Manipulation**	**Entanglement**
Fundamental	**Memory Techs**	**Quantum info manipulation**



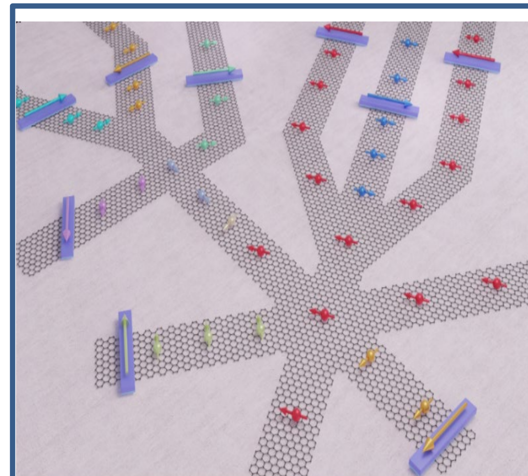
Non-local transport measurements

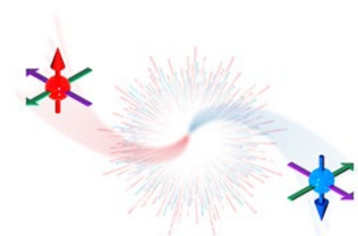
QHE (resistance standard)
QSHE (Topological insulators)
QAHE (magnetism/SOC)
...



Generation of spin current and Manipulation of magnets

Spin-orbit torque
(STT-MRAM and SOT-MRAM)





SYNOPSIS

"Quo Vadis 2D Spintronics?"

Linear scaling quantum tran... ...t methods

Low symmetry t... ...rials

– persistent...

"Spukhafte Fernwirkung!"

Multiple con...

Spin Hall E...

($MoTe_2$ monol...

Giant SHE

$\lambda_s \theta_{sH}^{\alpha} \sim 10 - 50\ \mathrm{nm}$

...uantum Spin Hall Effect

(WTe_2 monolayer)

Electrically tunable

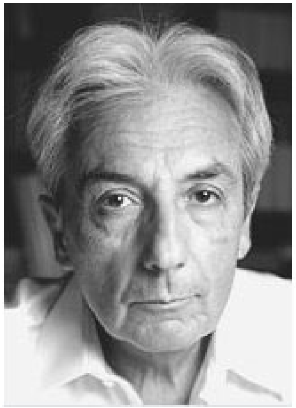
spin polarized topological currents

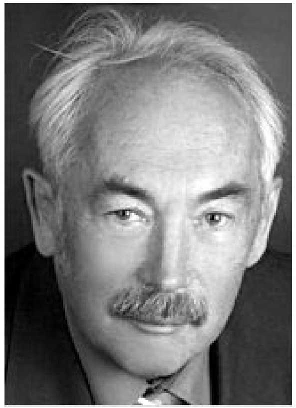
Higher resilience to disorder scattering (long spin lifetimes)
& to Rashba SOC (inversion symmetry breaking)

"Quo Vadis 2D Spintronics?"

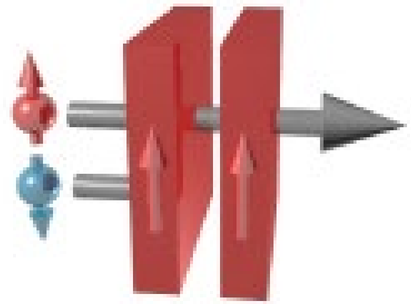
Spintronics and its industrial/Societal impact

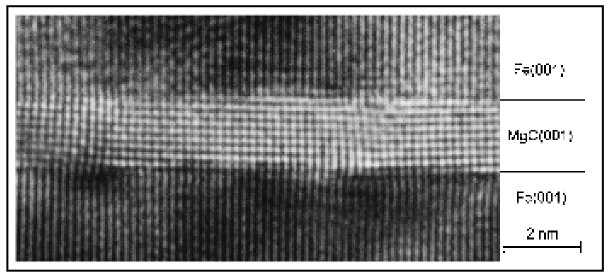
Albert Fert Peter Grünberg



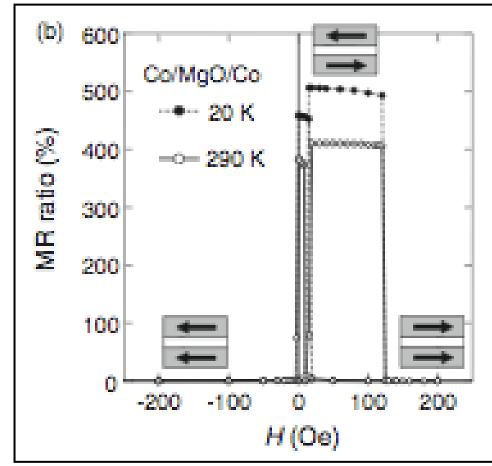


2007 Physics Nobel Laureates

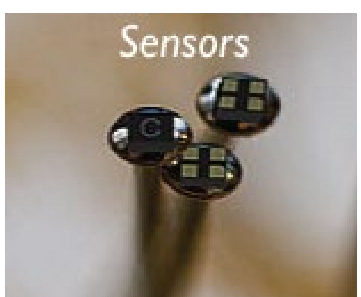


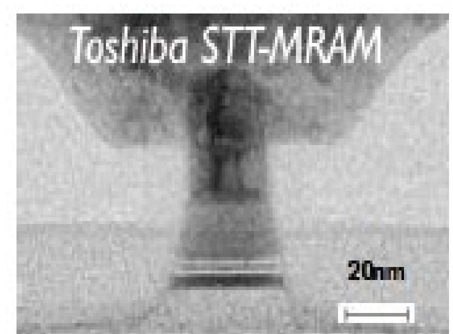


$$MR = \frac{R_{AP} - R_P}{R_P}$$



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





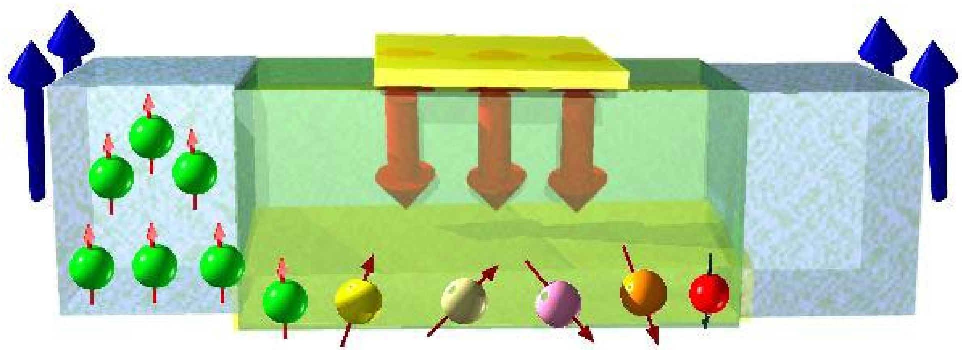
Spin-based information processing ?

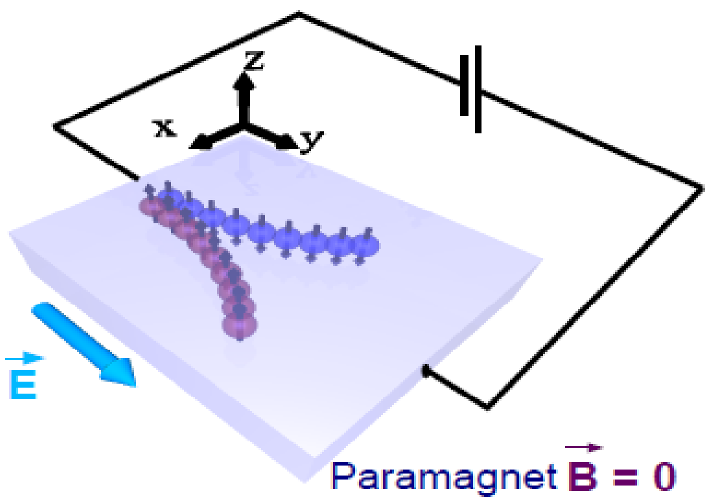
Need for spin information transport on long distance (room T)

Spin injection and detection (ferromagnets/nonmagnetic materials)

Active devices based on **Spin manipulation** ?

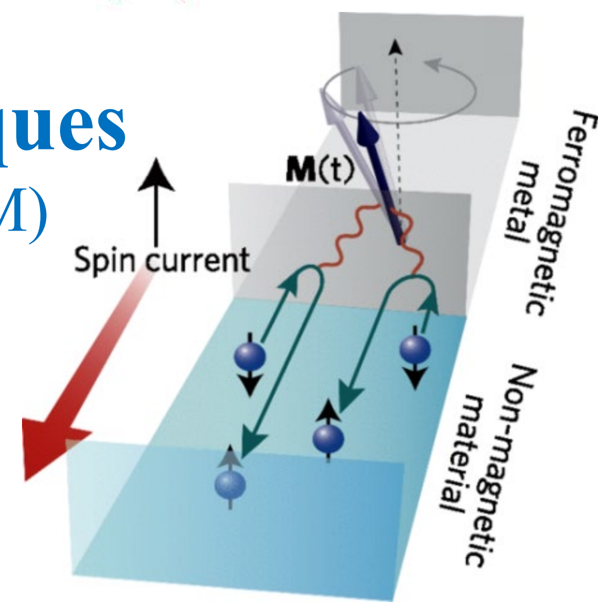
Datta-Das spin transistor





Spin torques

(SOT-MRAM)

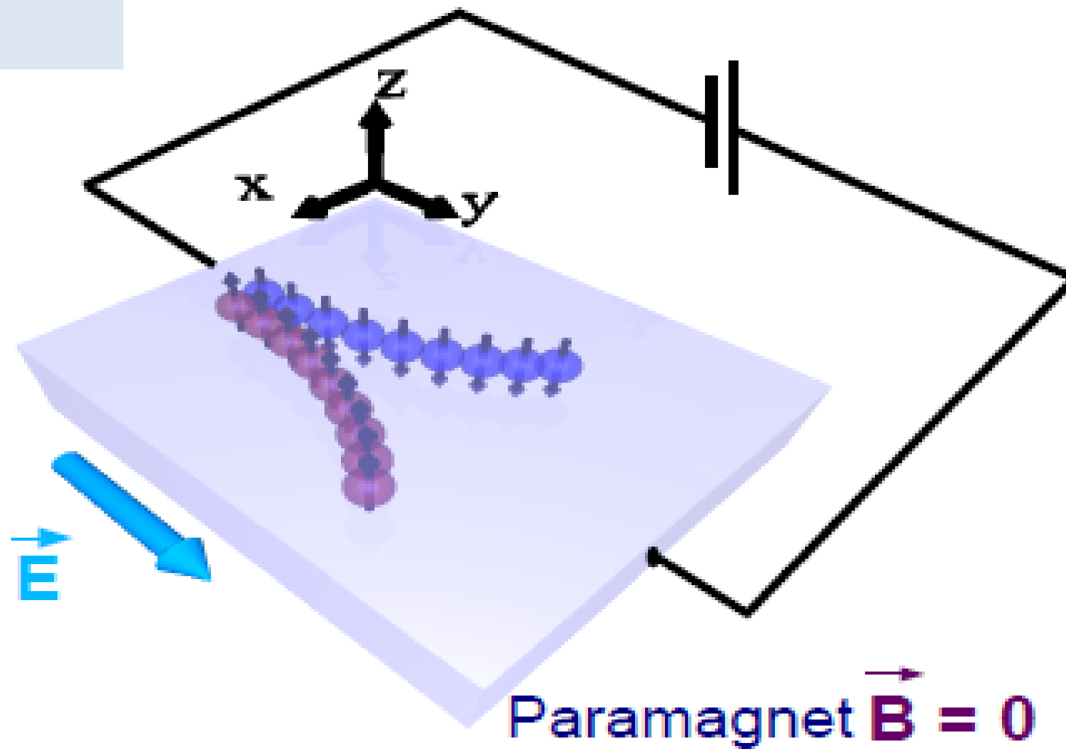


Spin Hall Effect

Spin Hall effect

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

(strong spin-orbit coupling materials)



Spin-orbit coupling fields
(effective magnetic field)
Generates (bulk) transversal spin current
(spin polarization ortogonal to both currents)

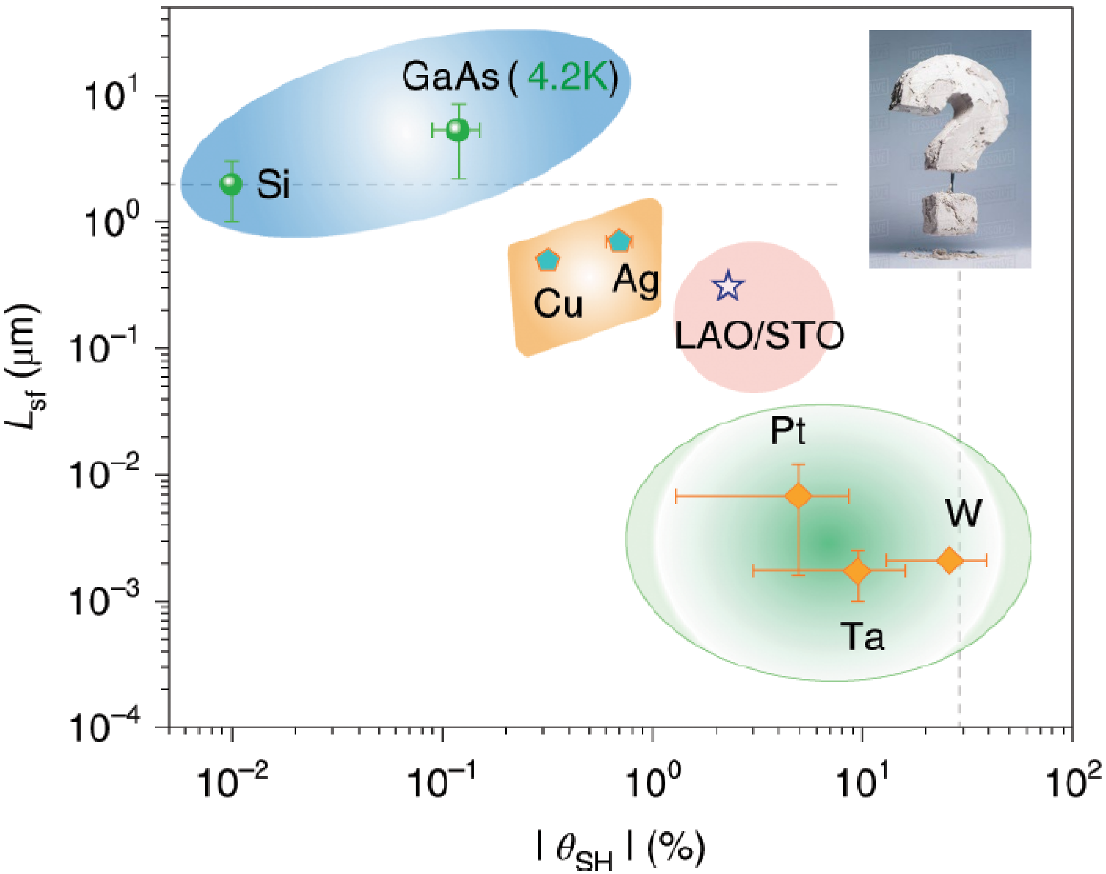
$$\vec{J}_s = \theta_{sH} \vec{\sigma} \wedge \bar{J}$$

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 ↗

θ_{sH} ↗

λ_s ↘

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

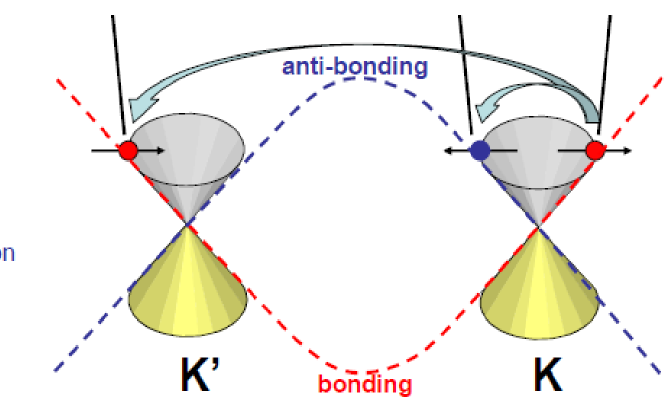
J. Sinova, S. O. Valenzuela et al. **Rev. Mod. Phys. 87, 1213 (2015)**

Could graphene solve such conundrum?

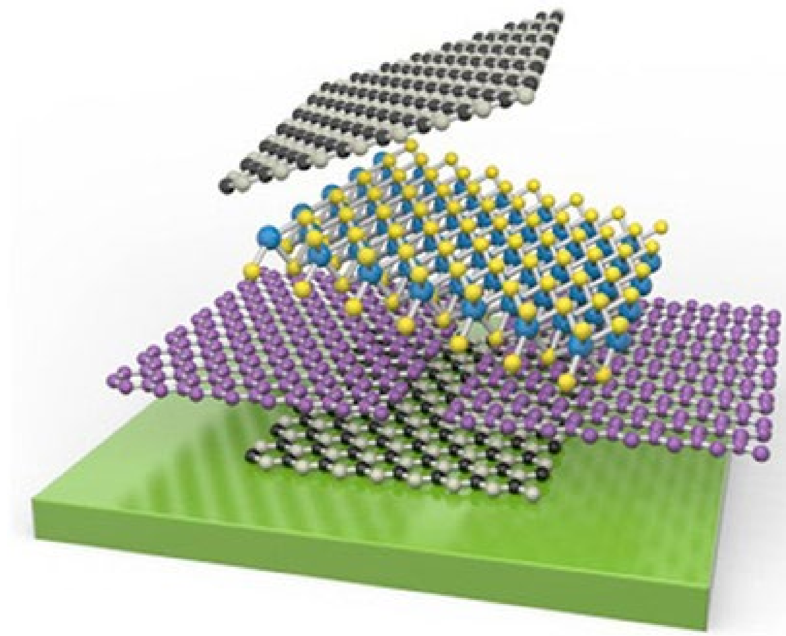
- Ambipolar/tuneable transport

- **Large mobilities**
(> 100k $cm^2/V.s$ at RT, 1M $cm^2/V.s$ at 4K)

- **Low spin-orbit interaction**



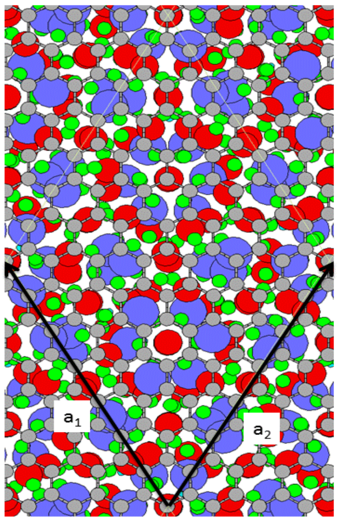
- Graphene properties can **be tailored by proximity effects**

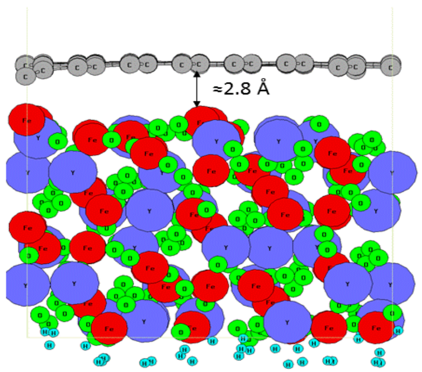


magnetizing graphene, generating spin currents, and fabricating "active spin devices, etc...

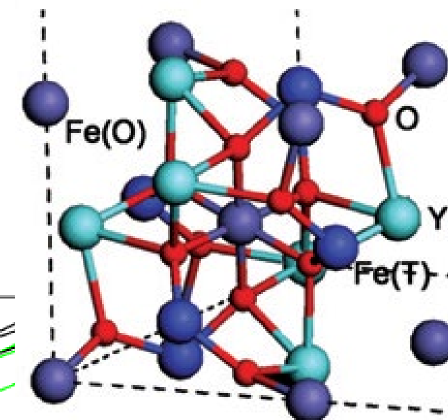
Graphene/Magnetic insulators

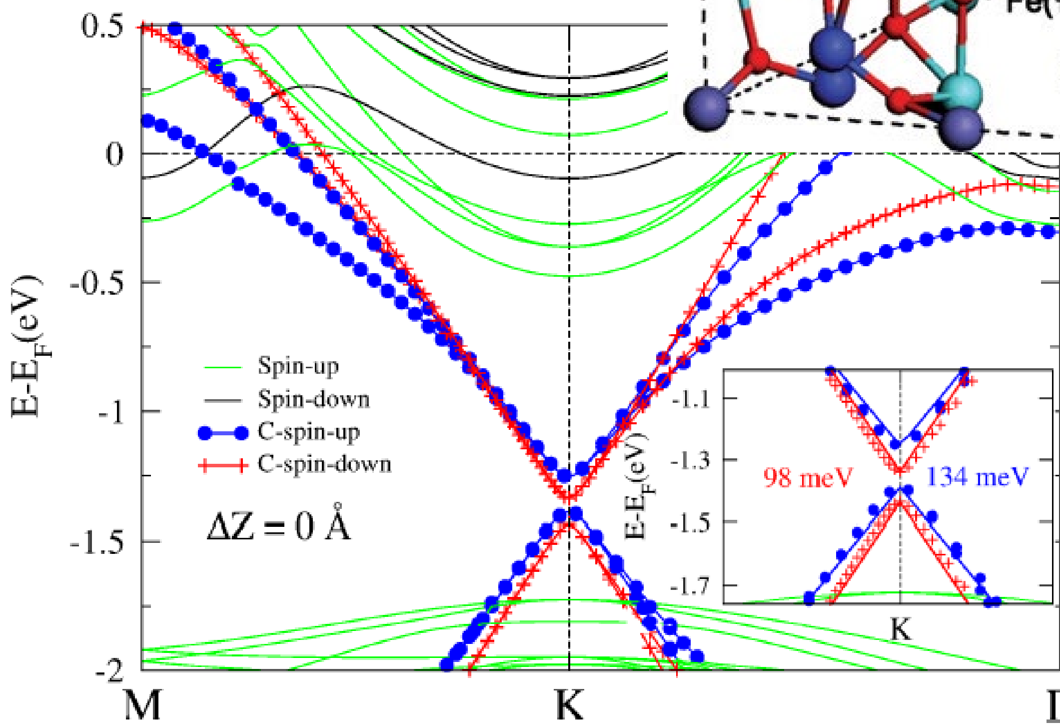
Graphene/EuO and Graphene/Y_3Fe_5O





Spin filtering and exchange splitting Gaps





Exchange splitting (G/YIG) = 40 meV

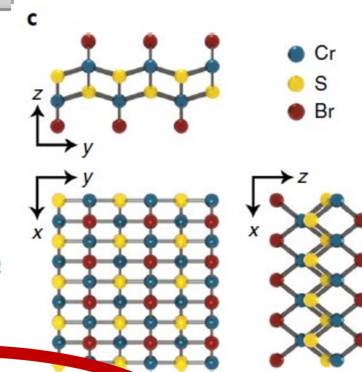
Yang, Hallal, Waintal, Roche, **M. Chshiev,** PRL 110, 046603 (2013)

Hallal et al. **M. Chshiev,** 2D materials 4 , 025074 (2017)

nature nanotechnology
university of groningen
ARTICLES
https://doi.org/10.1038/s41565-021-00887-3
Check for updates

Electrical and thermal generation of spin currents by magnetic bilayer graphene

Talieh S. Ghiasi[1], Alexey A. Kaverzin[1], Avalon H. Dismukes[2], Dennis K. de Wal[1], Xavier Roy[2] and Bart J. van Wees[1]

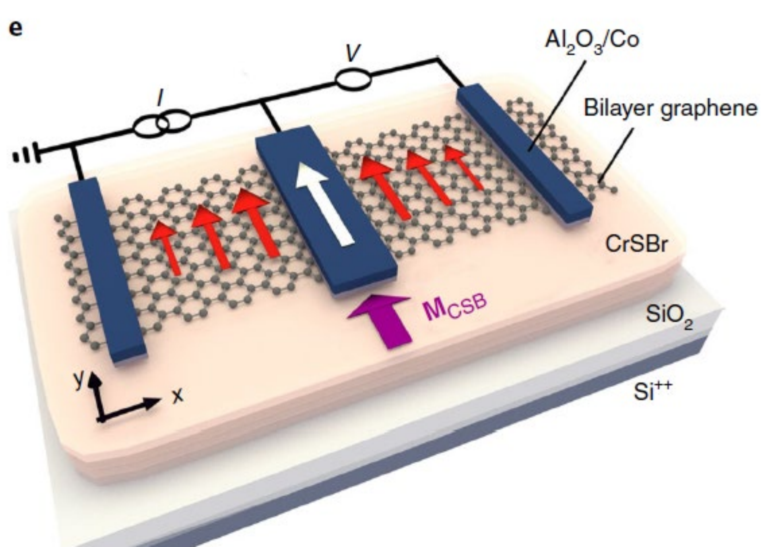


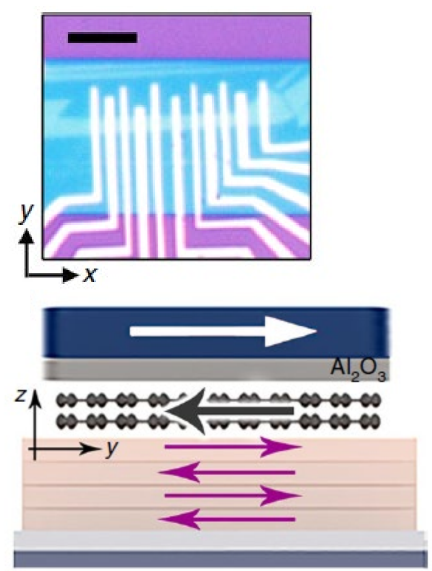
$P_{Gr} \approx 14\%$

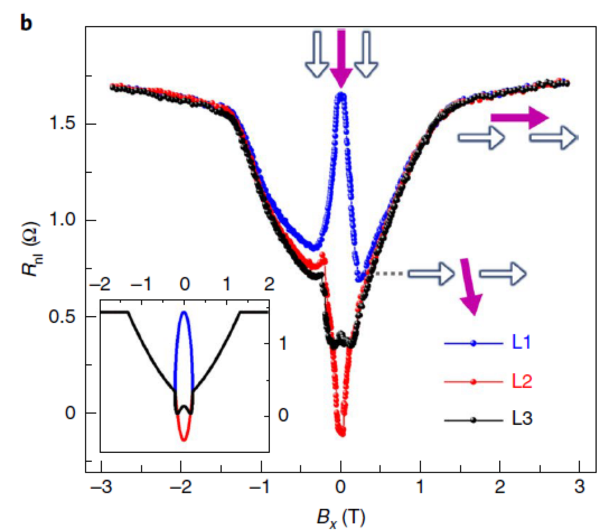
Exchange splitting to be $\Delta \approx 20$meV, which corresponds to **$B_{exch} \approx 170$ T**

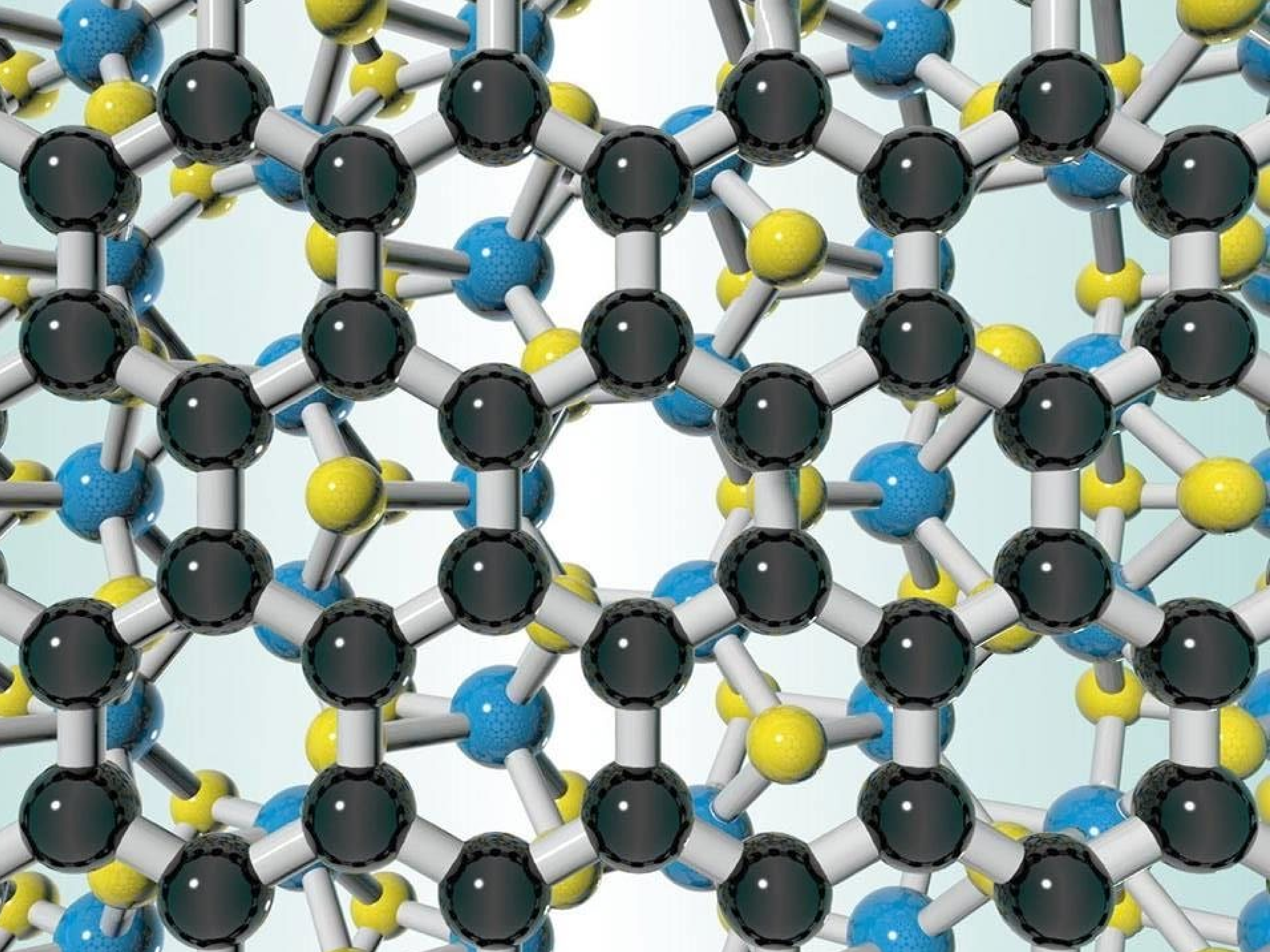
Generation of the spin currents by the magnetized graphene should persist up to the Néel temperature of **CrSBr** ($T_N \approx 132$ K) *interlayer antiferromagnet*

chromium sulfide bromide





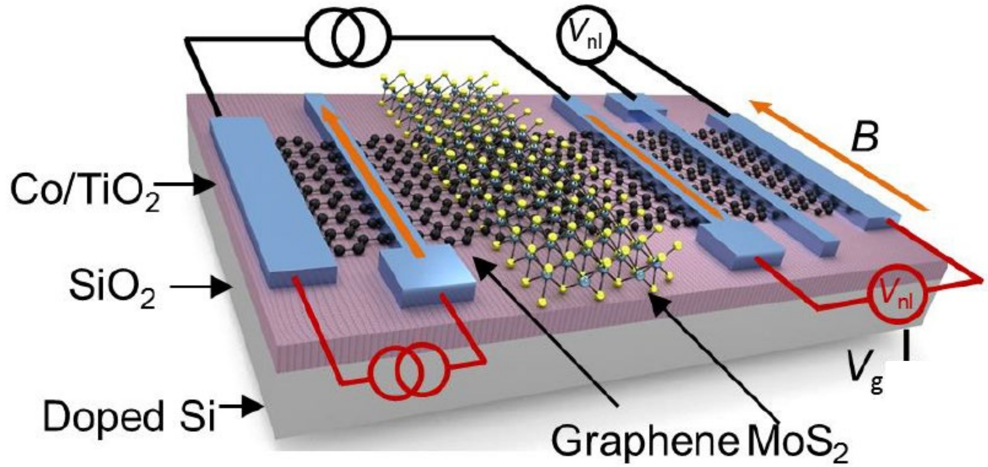


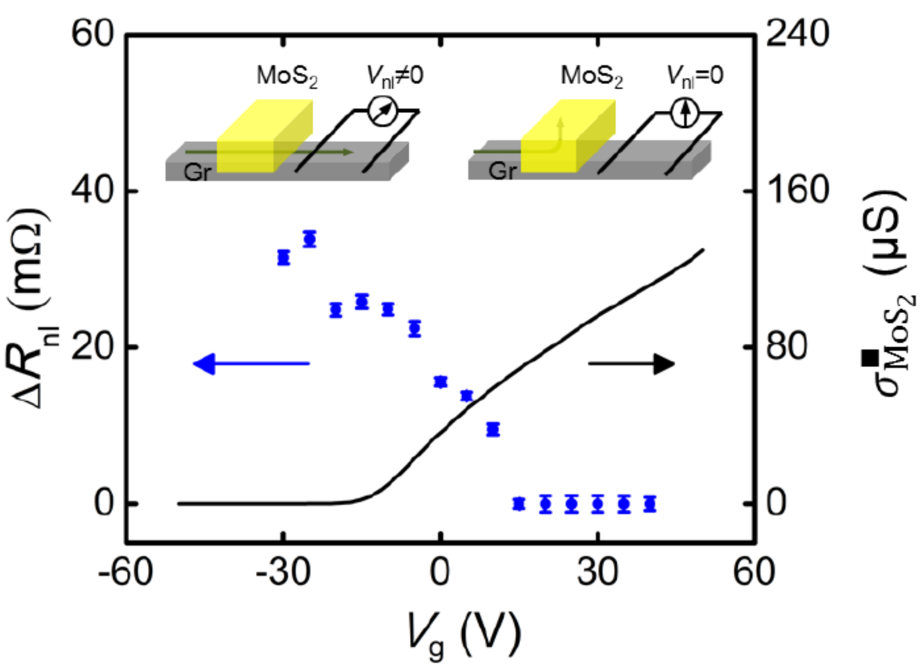


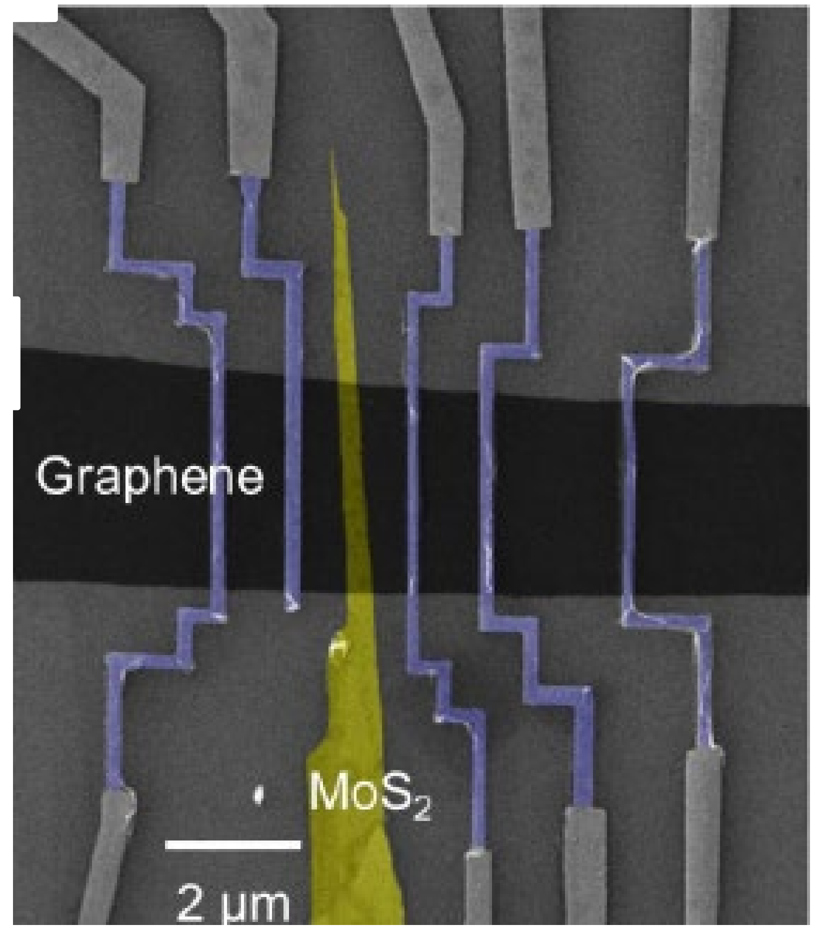
Two-dimensional spin field-effect switch

W. Yan, O. Txoperena, R. Llopis, H. Dery, **Luis E. Hueso** & **Felix Casanova**

Nature Comm. 7, 13372 (2016)



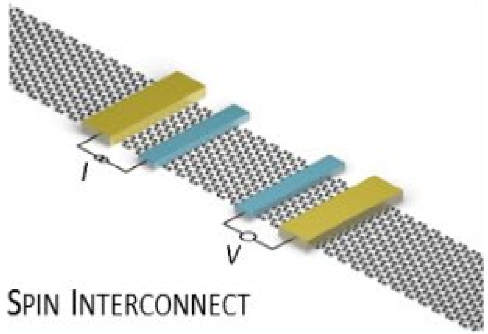




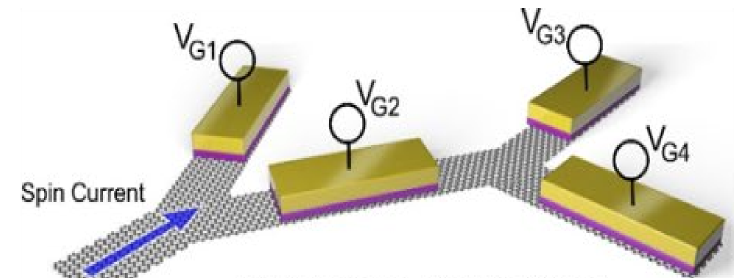
Spin Communication

Weak SOC

Xenes (multilayer) Graphene, black phosphorous...



Spin Interconnect



Spin Logics & Demultiplexer

Spin Injection & Detection

2D magnets, CSI, Optospintronics

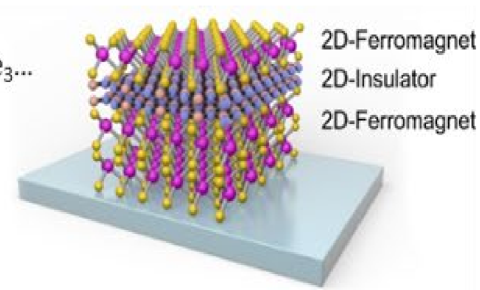
FM/AFM CrI_3, VSe_2, $CrSe_2$, $Cr_2Ge_2Te_6$, $MnPSe_3$...

Insulators hBN

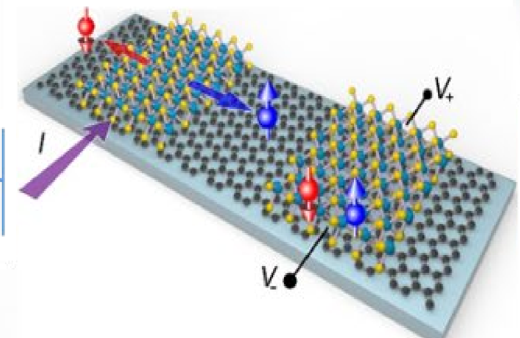
TMDCs MoS_2, $MoSe_2$, WTe_2...

Topological Insulators 2D: Heavy Xenes
3D: $(Bi,Sb)_2(Te,Se)_3$, α-Sn...

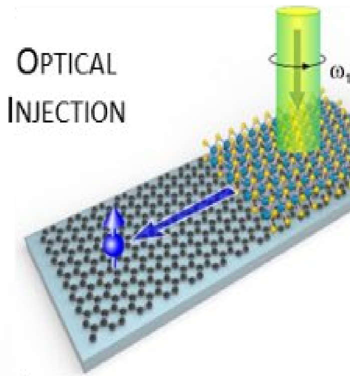
Magnetic Tunnel Junction



Charge-Spin Interconversion



Optical Injection



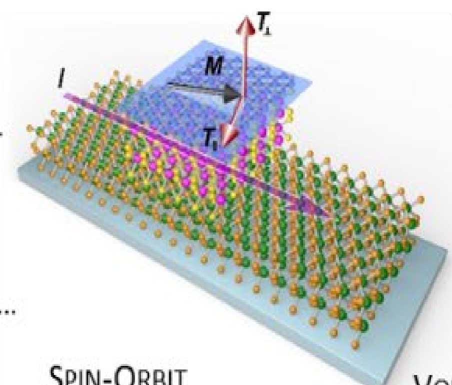
Spin Manipulation & Control

Strong SOC

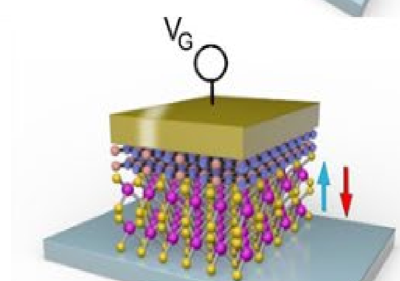
FM/AFM CrI_3, VSe_2, $CrSe_2$, $Cr_2Ge_2Te_6$, $MnPSe_3$...

TMDCs MoS_2, $MoSe_2$, WTe_2...

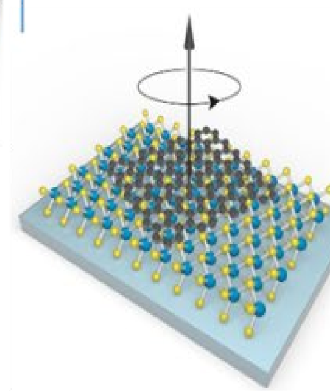
Topological Insulators 2D: Heavy Xenes
3D: $(Bi,Sb)_2(Te,Se)_3$, α-Sn...



Spin-Orbit Torque



Voltage Control of the Magnetization



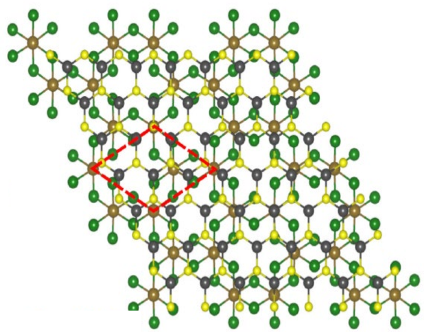
Twist Angle & Stacking

J.F. Sierra et al

Nature Nanotech. 16, 856–868 (2021)

“Race” to understand & tailor proximity effects

PHYSICAL REVIEW B **100**, 085128 (2019)

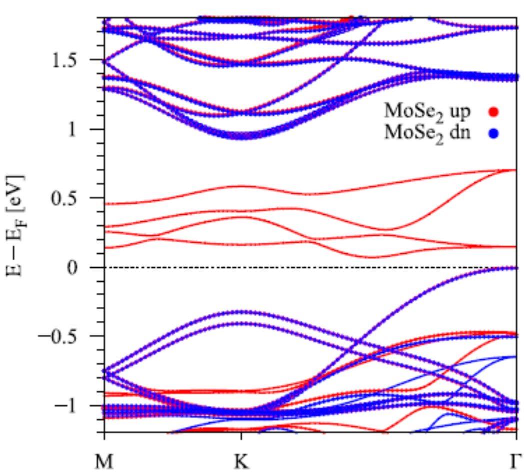


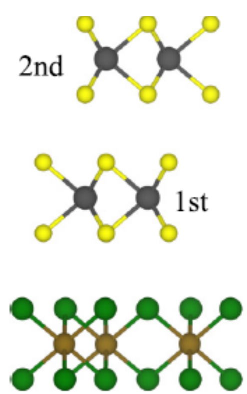
Editors' Suggestion

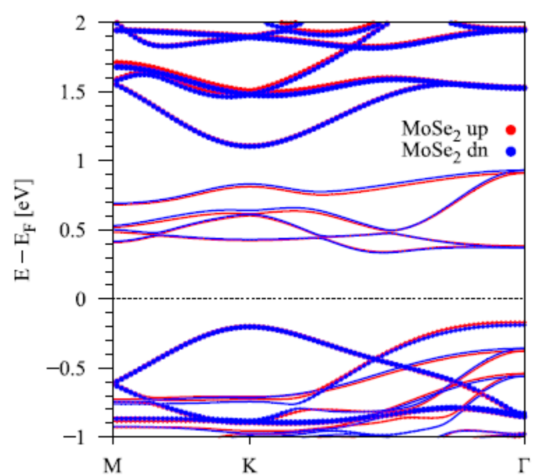
Proximity exchange effects in $MoSe_2$ and WSe_2 heterostructures with CrI_3: Twist angle, layer, and gate dependence

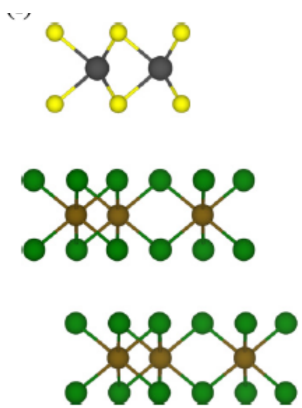
Klaus Zollner,* Paulo E. Faria Junior, and Jaroslav Fabian
Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

(Received 24 June 2019; revised manuscript received 1 August 2019; published 16 August 2019)









Roadmap of 2D-based spintronics

Perspective

Two-dimensional materials prospects for non-volatile spintronic memories

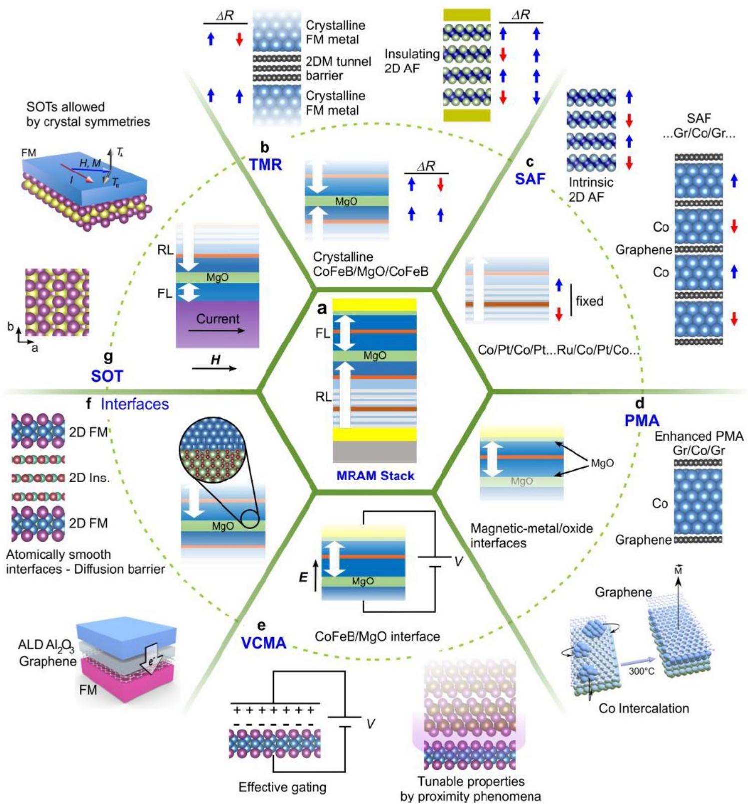
https://doi.org/10.1038/s41586-022-04768-0

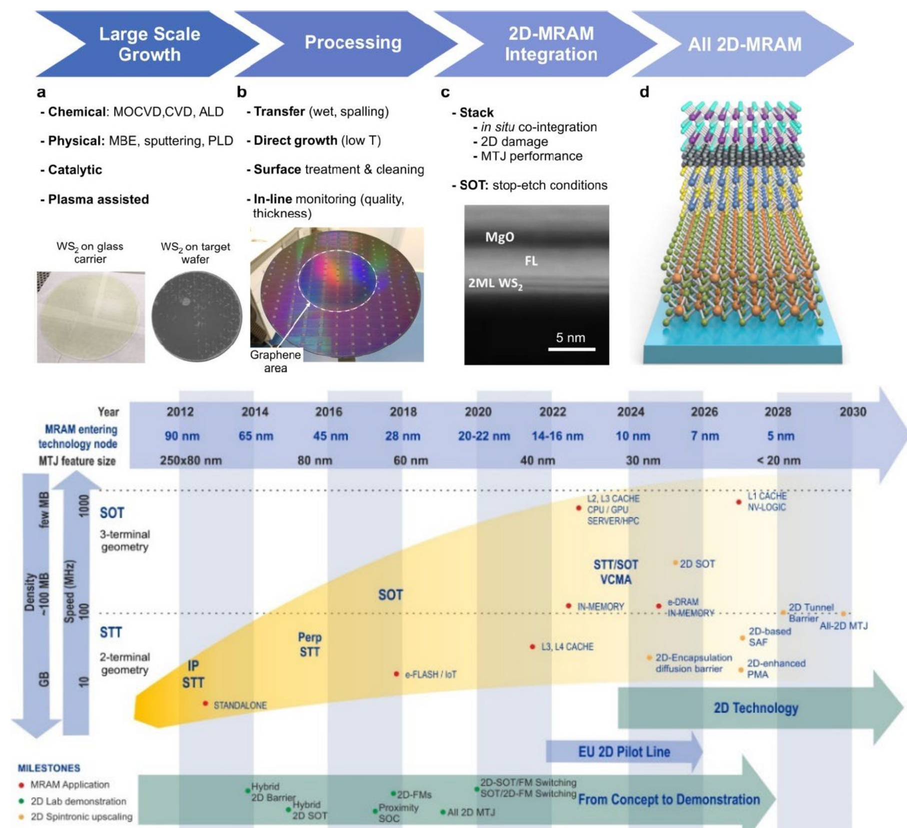
Received: 7 July 2020

Accepted: 19 April 2022

Hyunsoo Yang[1]✉, Sergio O. Valenzuela[2,3]✉, Mairbek Chshiev[4,5], Sébastien Couet[6], Bernard Dieny[4], Bruno Dlubak[7], Albert Fert[7], Kevin Garello[4,6], Matthieu Jamet[4], Dae-Eun Jeong[8], Kangho Lee[9], Taeyoung Lee[10], Marie-Blandine Martin[7,11], Gouri Sankar Kar[6], Pierre Sénéor[7], Hyeon-Jin Shin[12] & Stephan Roche[2,3]✉

Nature 606 (7915), 663-673 (2022)





Linear scaling quantum transport methods

Linear scaling quantum transport methods

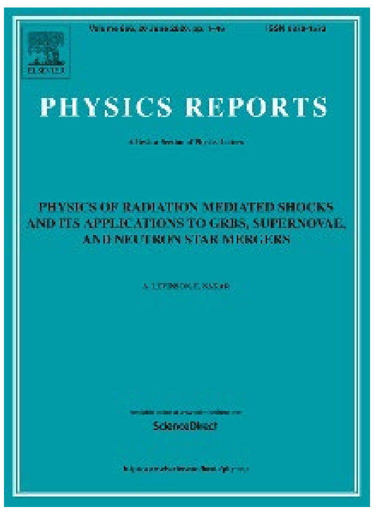
(Kubo, (Spin)-Hall Kubo, Landauer-Büttiker, spin dynamics)

Billion atoms scale / disordered models

Linear scaling quantum transport methodologies

Phys. Rep. *903, 1 (2021)*

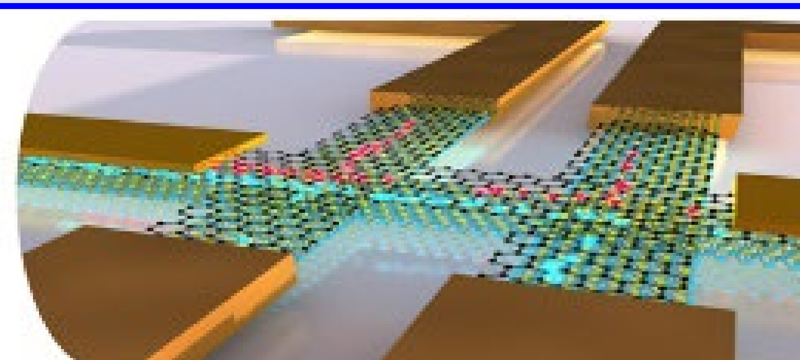
Zheyong Fan[a,b,1], José H. Garcia[c,1], Aron W. Cummings[c,1], Jose Eduardo Barrios-Vargas[d], Michel Panhans[e,f], Ari Harju[b], Frank Ortmann[e,f], Stephan Roche[c,g,*]



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

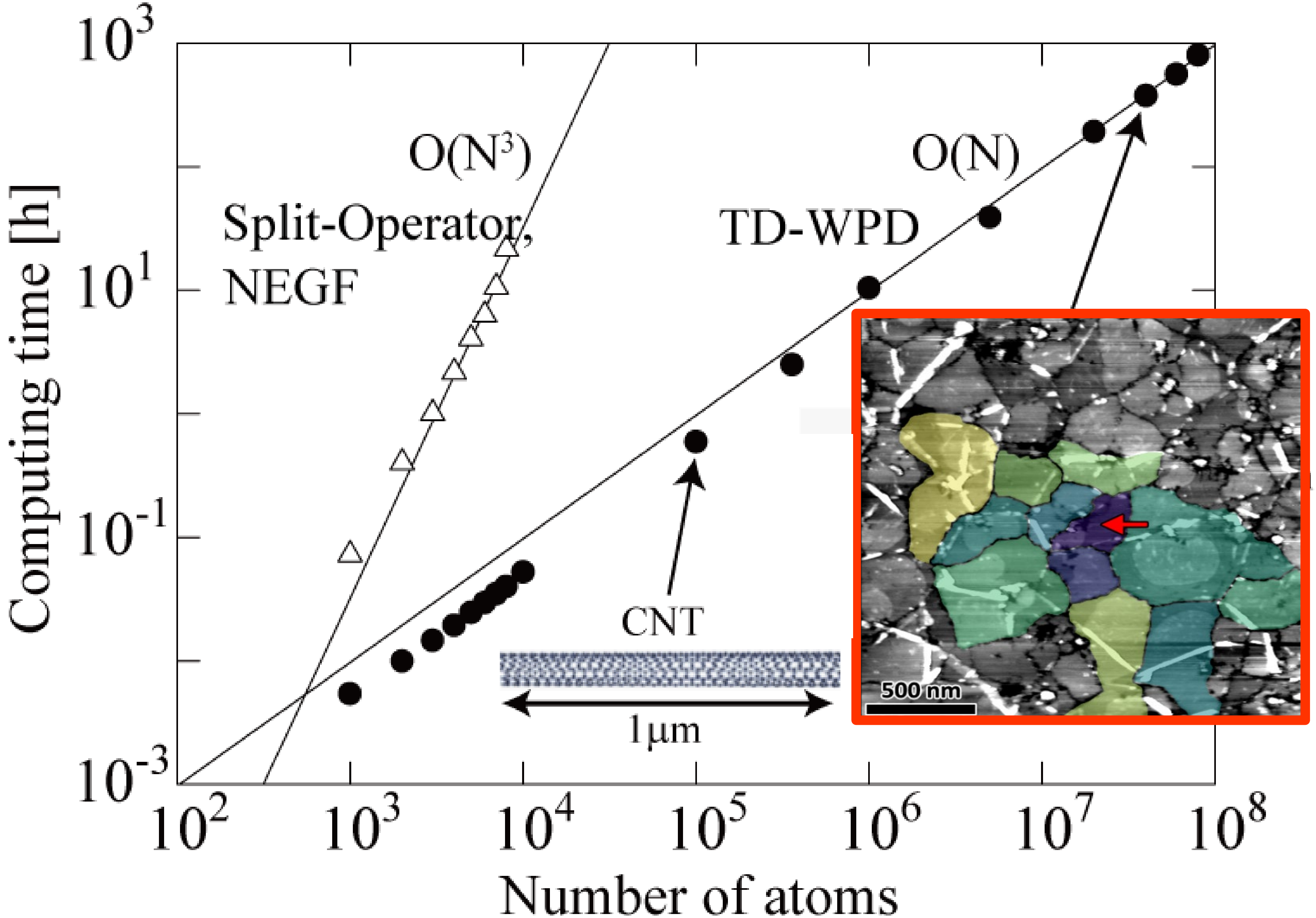
LSQUANT
LINEAR SCALING QUANTUM TRANSPORT

www.lsquant.org



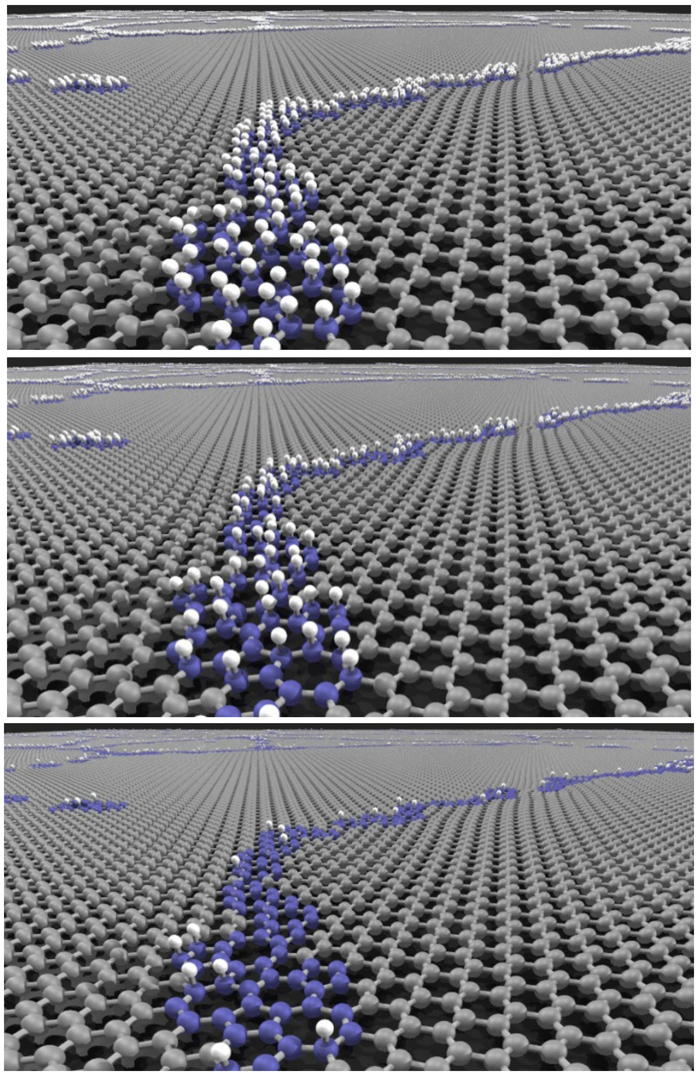
3 weeks versus 1 billion years....

"Advantage" of linear scaling quantum transport

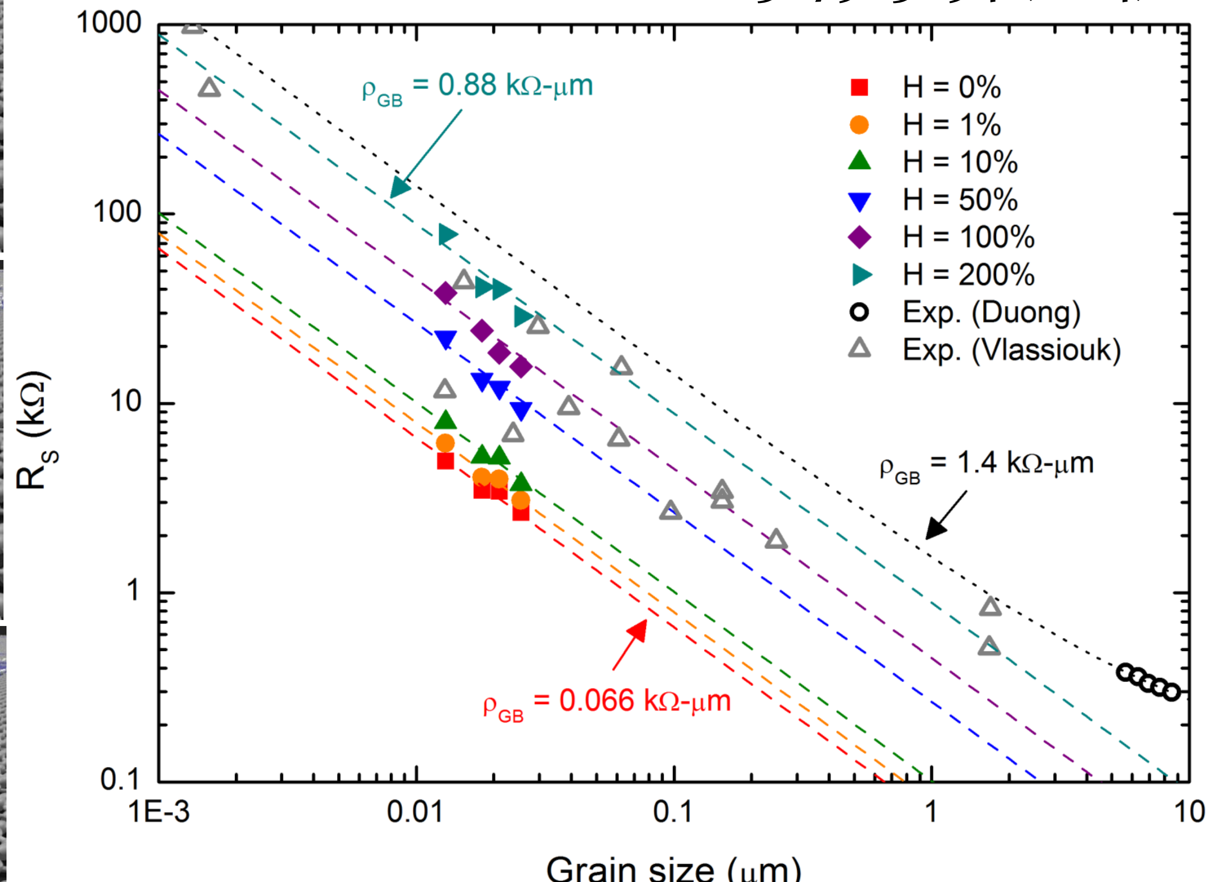


Sheet resistance scaling law

***Sheet resistance** vs. grain size in chemically disordered CVD graphene*



A. Cummings et al,
Advanced Materials 26, 5079–5094 (2014)



Significant increase in R_S with GB adsorbates

Kubo-Greenwood formula
for quantum conductivity

$$\Re e \sigma(\omega) = \frac{2\pi e^2 \hbar}{\Omega} \int_{-\infty}^{+\infty} dE \frac{f(E) - f(E + \hbar\omega)}{\hbar\omega} \mathrm{Tr}[\hat{V}_x \delta(E - \hat{\mathcal{H}}) \hat{V}_x \delta(E - \hat{\mathcal{H}})]$$

R Kubo, **Rep. Prog. Phys. 29 255-284 (1966)**

Linear Response - Non-interacting electrons

Treat all multiple scattering phenomena

Give access to semiclassical transport

(Mean free path, charge mobility)

Non-perturbative regimes (disorder + B,...)

Beyond usual treatment semi-classical Bloch-Boltzmann

Weak localization/strong localization

Generalization to Hall effects (topological physics)

$$\Re e\sigma_{xx}(\omega) = \frac{2\pi e^2\hbar}{\Omega}\int_{-\infty}^{+\infty} dE\,\frac{f(E)-f(E+\hbar\omega)}{\hbar\omega}\mathrm{Tr}[\hat{V}_x\delta(E-\hat{\mathcal{H}})\hat{V}_x\delta(E-\hat{\mathcal{H}})]$$

$$\sigma_{dc} = e^2 n(E_F)\lim_{t\to\infty}\frac{d}{dt}\Delta X^2(E_F,t) = e^2 n(E_F)\lim_{t\to\infty} D(t)$$

Linear scaling algorithm

$$D(t) = \frac{\mathrm{Tr}\left[[\hat{X},\hat{U}(t)]^\dagger\delta(E-\mathcal{H})[\hat{X},\hat{U}(t)]\right]}{\mathrm{Tr}[\delta(E-\mathcal{H})]}$$

$$\downarrow$$

$$\frac{\langle\widetilde{\varphi}_{RP}(t)|\delta(E-\mathcal{H})|\widetilde{\varphi}_{RP}(t)\rangle}{\langle\varphi_{RP}|\delta(E-\mathcal{H})|\varphi_{RP}\rangle}$$

$$|\tilde{\varphi}_{RP}(T)\rangle = [\hat{X},\hat{U}(t)]|\varphi_{RP}\rangle \simeq \sum_{n=0}^{N} c_n(T)[\hat{X},P_n(H)]|\varphi_{RP}\rangle$$

$$\langle\varphi_{RP}|\delta(E-\hat{\mathcal{H}})|\varphi_{RP}\rangle = -\frac{1}{\pi}\lim_{\eta\to 0}\Im m\langle\varphi_{RP}|\frac{1}{E+i\eta-\hat{\mathcal{H}}}|\varphi_{RP}\rangle,$$

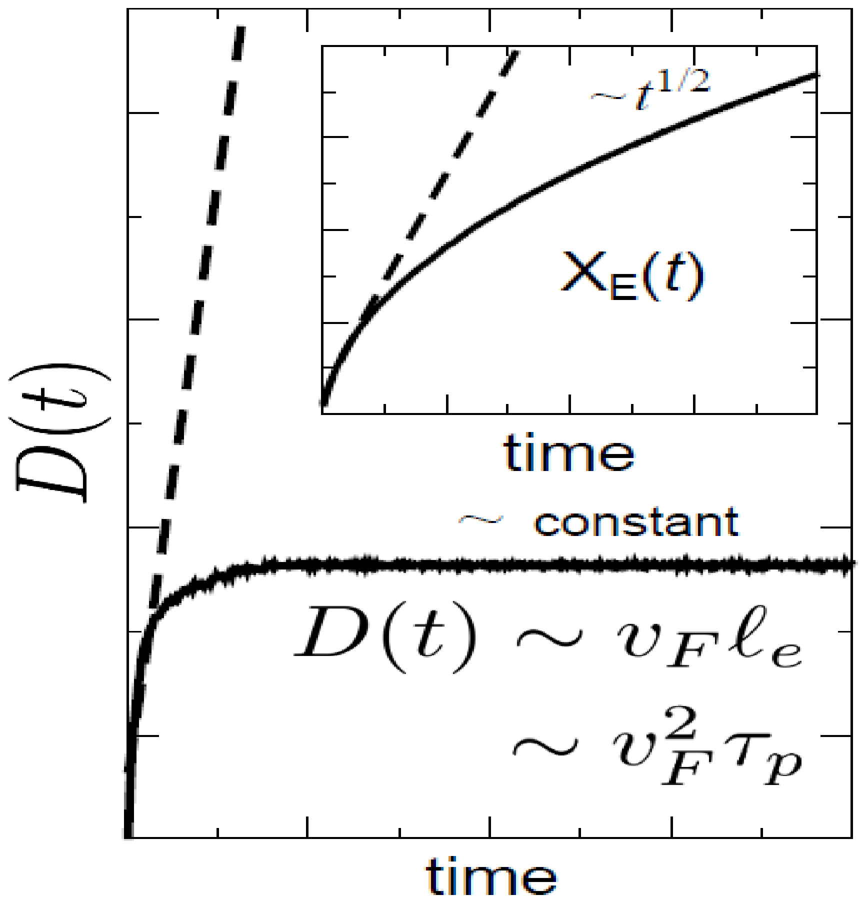
No matrix inversion

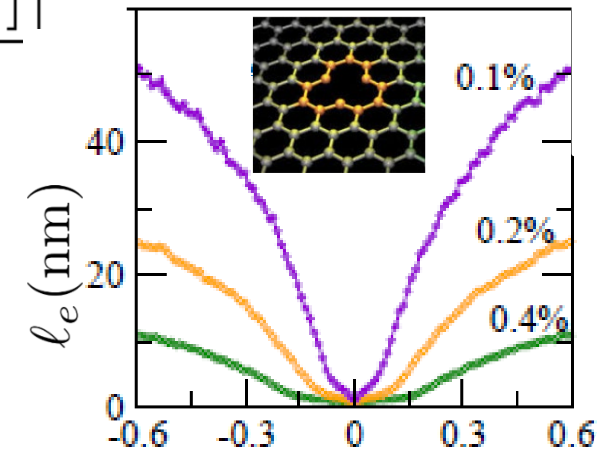
$$\cfrac{1}{E+i\eta-a_1-\cfrac{b_1^2}{E+i\eta-a_2-\cfrac{b_2^2}{\ddots\;\cfrac{}{E+i\eta-a_N-b_N^2\Sigma(\omega)}}}}$$

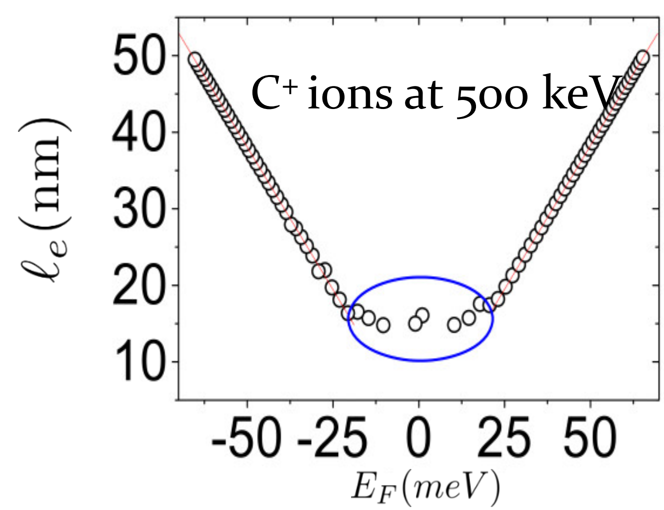
S. Roche & D Mayou **Phys. Rev. Lett. (1997)**
S. Roche **Phys. Rev. B (1999)**

Quantum dynamics & scaling analysis

$$D(t) = \frac{\mathrm{Tr}\left[[\hat{X},\hat{U}(t)]^\dagger \delta(E-\mathcal{H})[\hat{X},\hat{U}(t)]\right]}{\mathrm{Tr}[\delta(E-\mathcal{H})]}$$





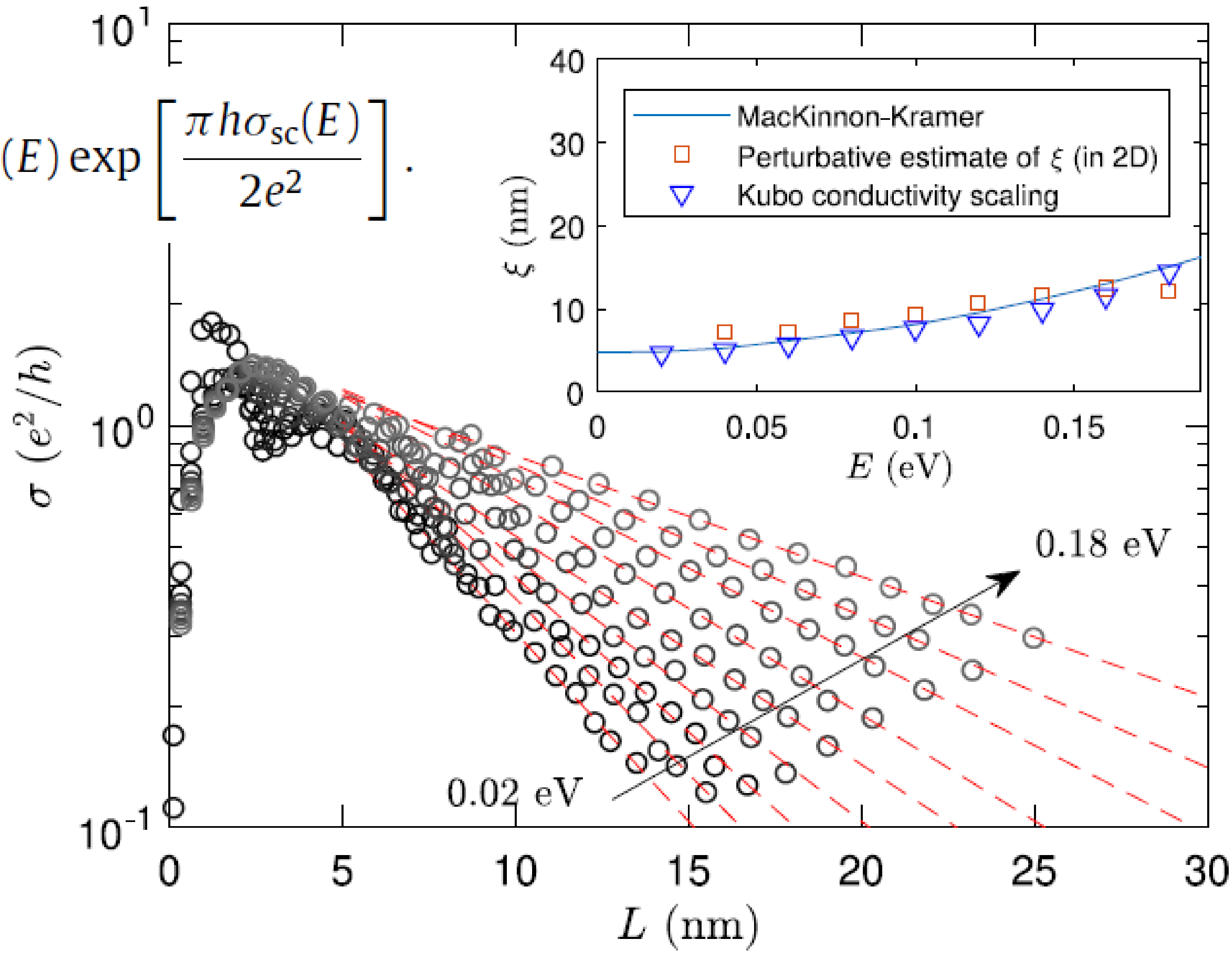


F. Giannazzo et al,
Nanoscale Res.Lett.6, 109 (2011)

From weak to strong (Anderson) localization

disordered graphene lattice (lattice vacancies)

$$\xi(E) = l_{sc}(E)\exp\left[\frac{\pi h \sigma_{sc}(E)}{2e^2}\right].$$



Hall Kubo-Streda formalism

Hall Kubo formula for real space implementation

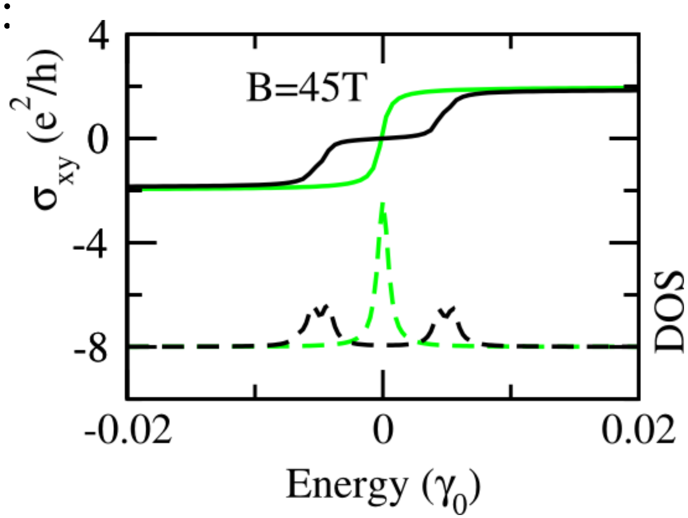
(10^6 atoms- disorder – B=1mT- 60T)

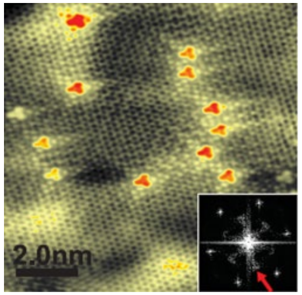
$$\sigma_{xy}(E) = -\frac{2}{\Omega}\int_0^{+\infty} dt e^{-\eta t/\hbar}\int_{-\infty}^{+\infty} dE' f(E'-E)$$
$$\times \Re e\left[\langle\varphi_{RP}|\delta(E'-\hat{\mathcal{H}})\hat{J}_y \frac{1}{E'-\hat{\mathcal{H}}+i\eta}\hat{J}_x(t)|\varphi_{RP}\rangle\right]$$

Magnetic field modeled by Peierls' phase:

$$\gamma_{ij} = \gamma_0 e^{i\Phi_{ij}}$$

$$\Phi_{ij} = \frac{e}{\hbar}\int_i^j d\mathbf{s}\mathbf{A}(\mathbf{s})$$





F. Ortmann & S. Roche
Phys. Rev. Lett 110, 086602 (2013)
F. Ortmann, N. Leconte, S. Roche
Phys. Rev. B 91, 165117 (2015)

L. Zhao *et al.*
Science 333, 999 (2011)

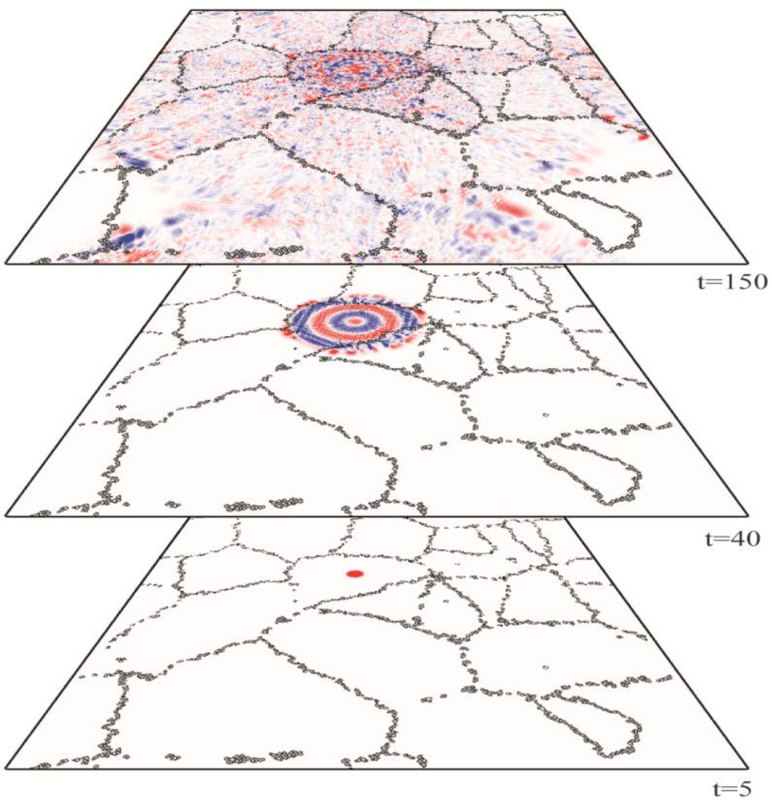
Spin dynamics of propagating wavepacket

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

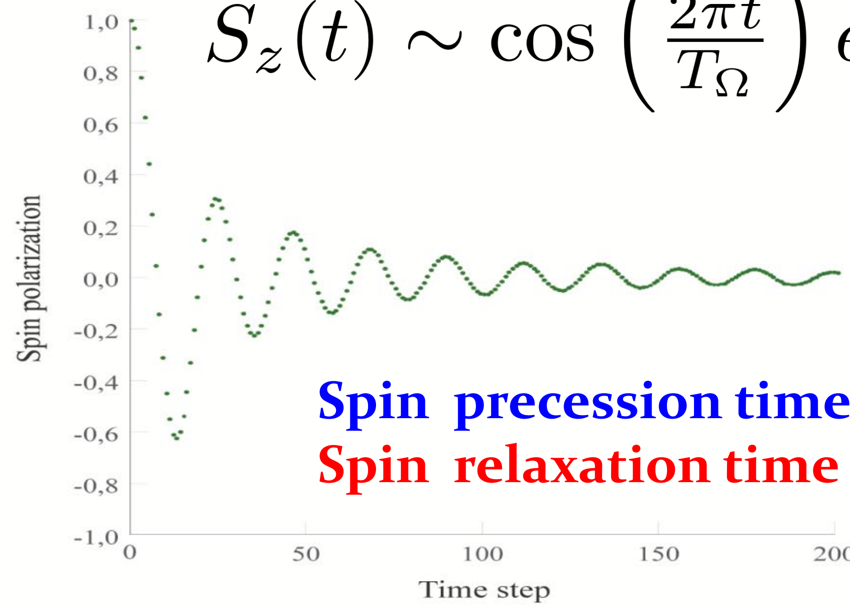
$$s_i(t) = |\Psi_i^{\uparrow}(t)|^2 - |\Psi_i^{\downarrow}(t)|^2$$

(time-dependent)
Local spin density in real space

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



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

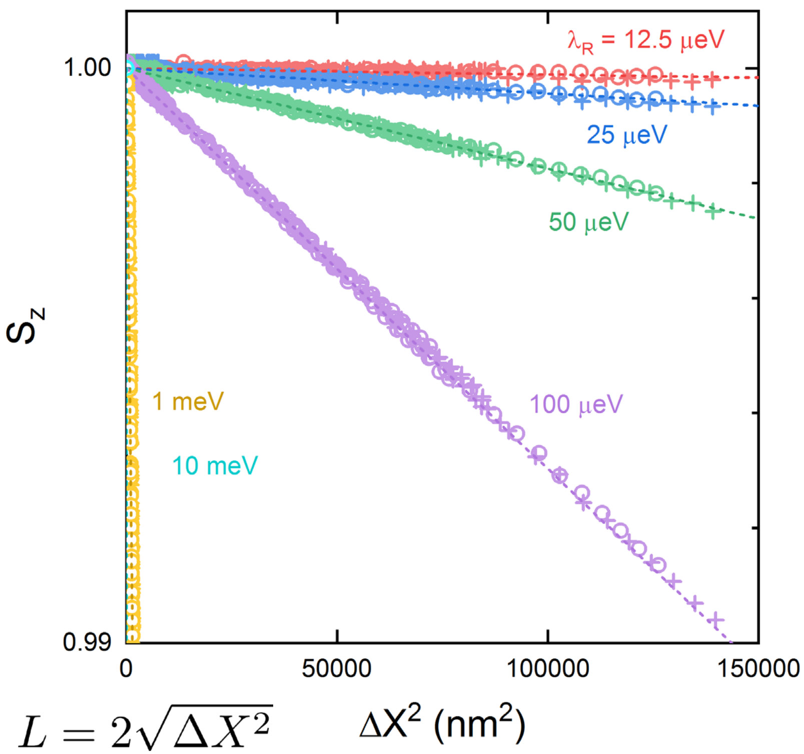


Spin precession time T_Ω
Spin relaxation time τ_s

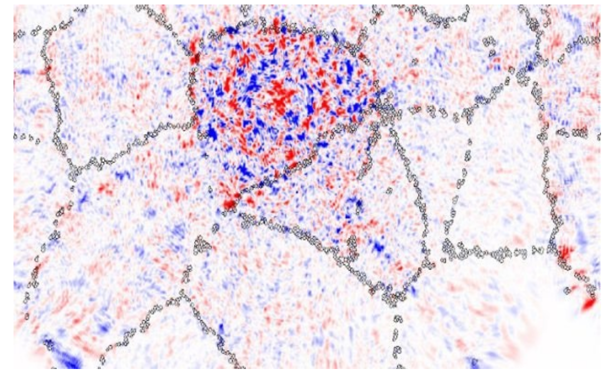
Universal spin diffusion length

ICN2
GRAPHENE FLAGSHIP
UCL Université catholique de Louvain

AW Cummings et al **Nano lett. 19, 7418 (2019)**



$L = 2\sqrt{\Delta X^2}$



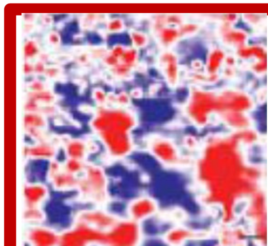
Spin polarization vs mean square displacement

$$s_z(X) = \exp\left(-\Delta X^2 / L_s^2\right)$$

No dependence on grain size (!!!)

10 nm or 100 microns

$$L_s = \frac{\hbar v_F}{2\lambda_R}$$



Rashba SOC = 25μeV

$$L_s = 10\mu m$$

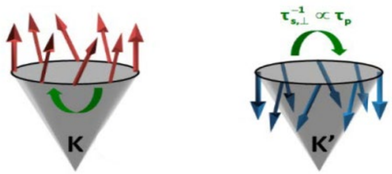
Rashba SOC = 5μeV

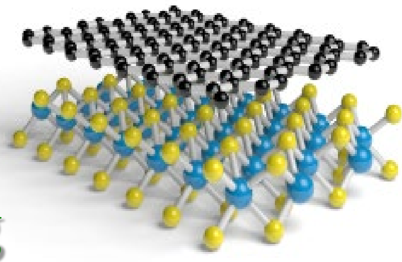
$$L_s = 50\mu m$$

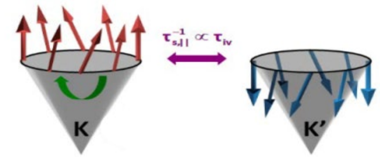
Giant Spin lifetimes Anisotropy

AW Cummings, JH Garcia, J Fabian, S Roche
Phys. Rev. Lett. 119 (20), 206601 (2017)

$$\frac{\tau_{s,\perp}}{\tau_{s,\parallel}} = 10 - 100$$

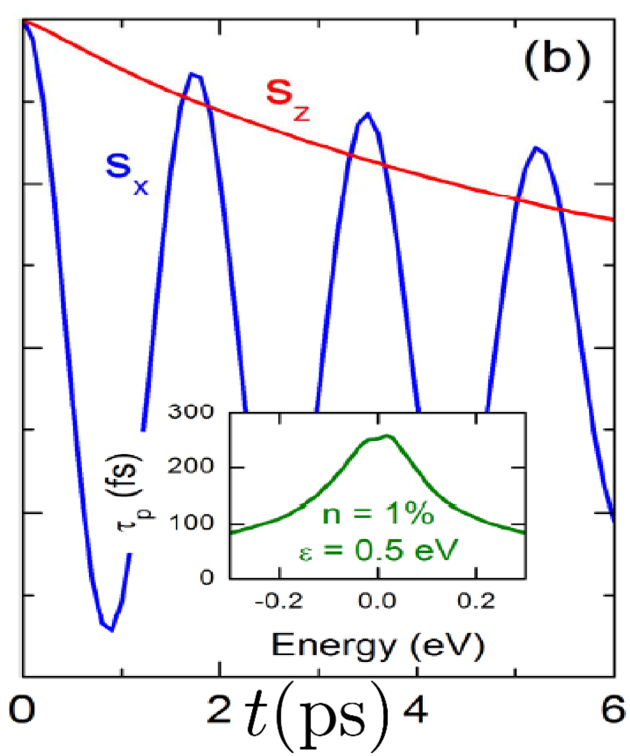


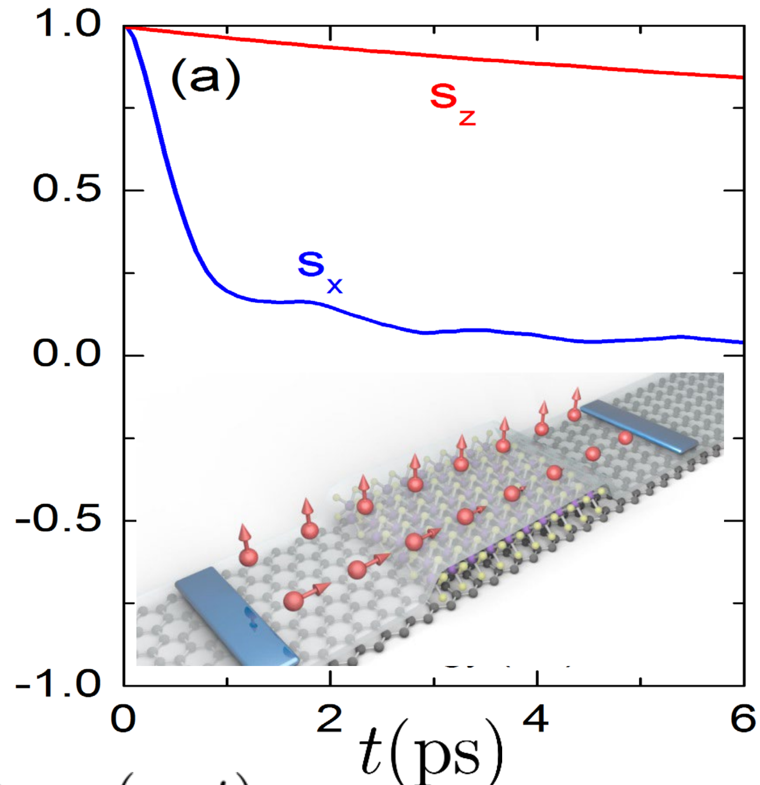




Intravalley scattering

Strong valley mixing





$$S_\alpha \simeq \exp(-t/\tau_{s,\alpha})\cos(\omega_z t)$$

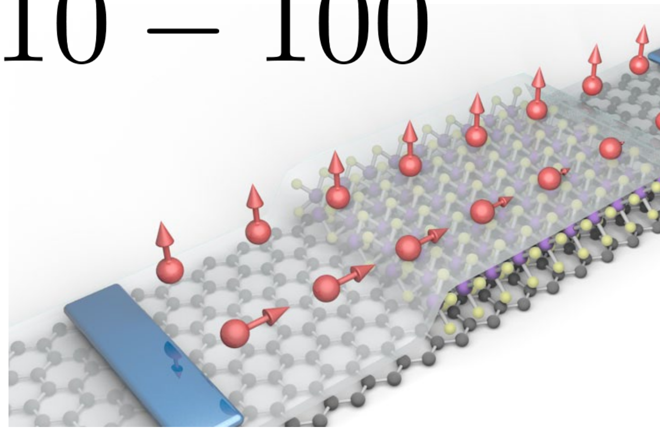
GRAPHENE FLAGSHIP

Experimental confirmation

university of groningen

ICN2

$$\frac{\tau_{s,\perp}}{\tau_{s,\parallel}} = 10 - 100$$



NANO LETTERS Cite This: Nano Lett. XXXX, XXX, XXX−XXX

Large Proximity-Induced Spin Lifetime Anisotropy in Transition-Metal Dichalcogenide/Graphene Heterostructures

Talieh S. Ghiasi,* Josep Ingla-Aynés, Alexey A. Kaverzin, and Bart J. van Wees

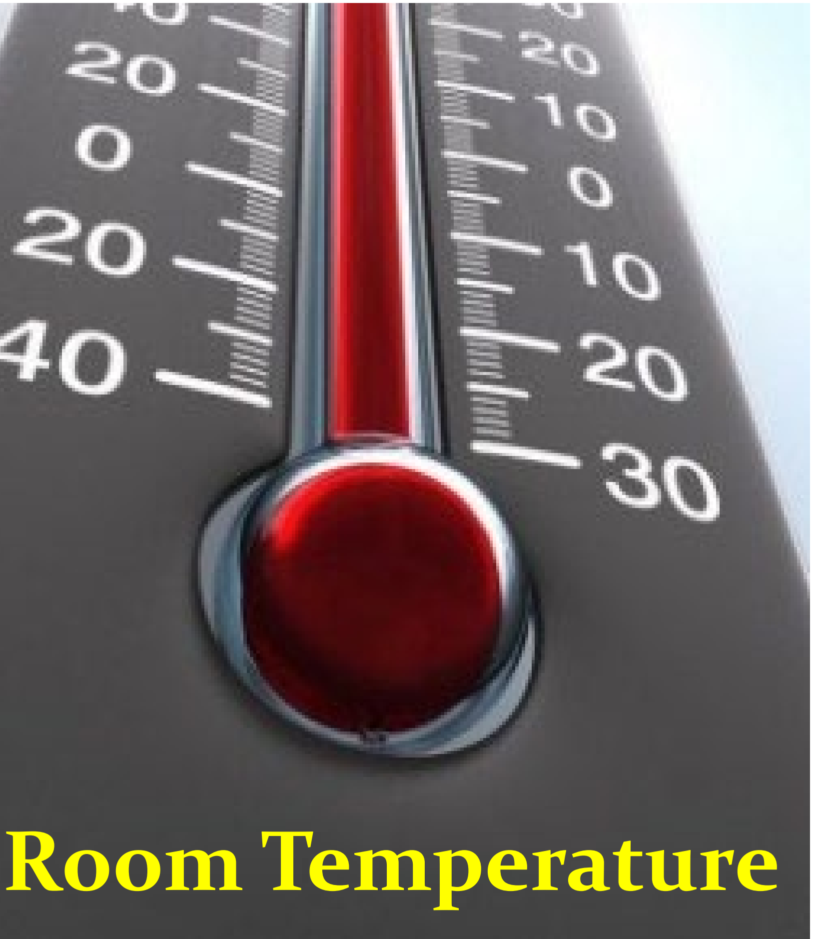
Physics of Nanodevices, Zernike Institute for Advanced Materials, University of Groningen, Groningen, 9747 A

nature physics

https://doi.org/10.1(

Strongly anisotropic spin relaxation in graphene–transition metal dichalcogenide heterostructures at room temperature

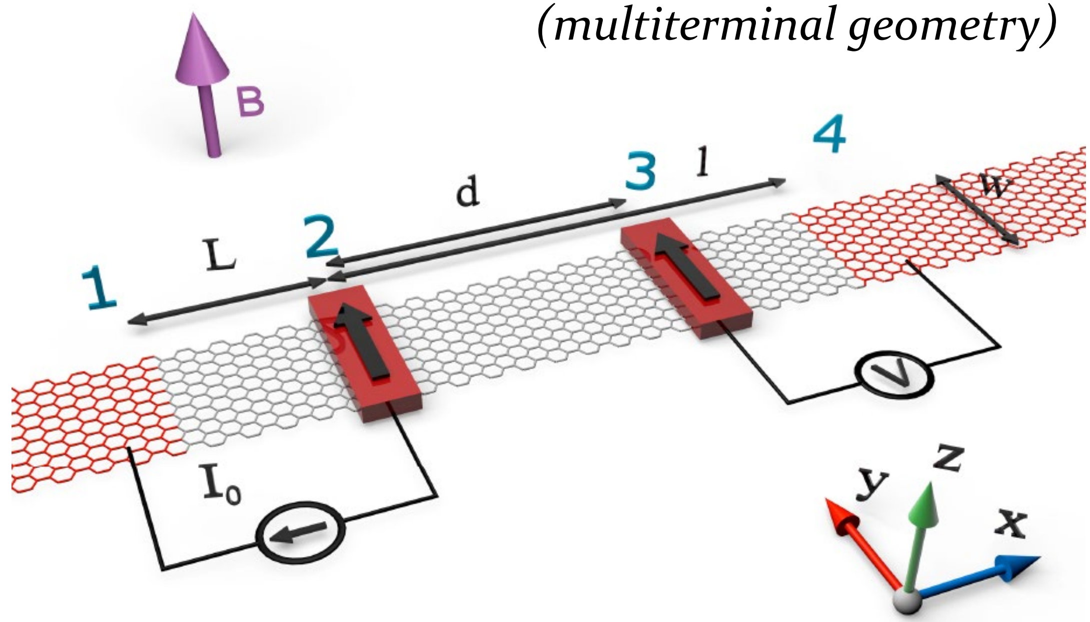
L. Antonio Benítez[1,2*], Juan F. Sierra[1], Williams Savero Torres[1], Aloïs Arrighi[1,2], Frédéric Bonell[1], Marius V. Costache[1] and Sergio O. Valenzuela[1,3*]



Nonlocal spin transport

(multiterminal geometry)

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



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

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

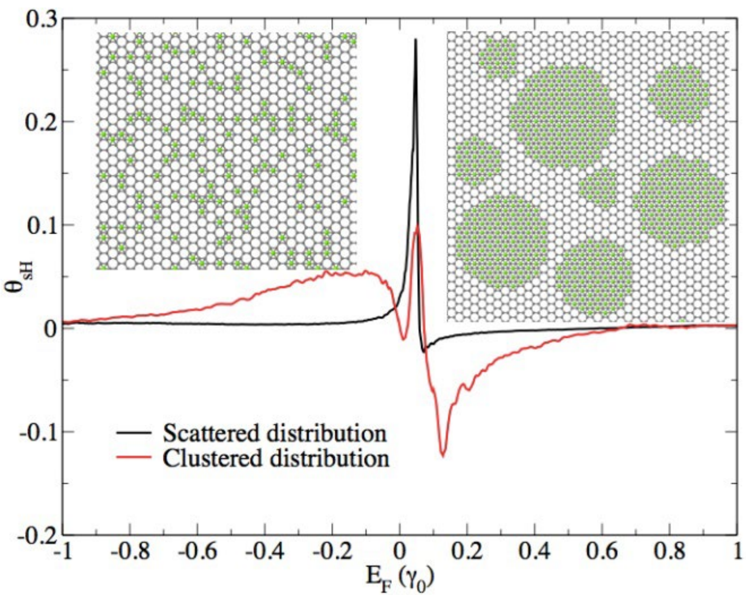
$$I_p^{s_\alpha} \quad G_{pq}^{s_\alpha} = \frac{e^2}{h} \int dE \, \mathrm{Tr}[s_\alpha \mathbf{t}_{pq}\mathbf{t}_{pq}^\dagger](-\partial f/\partial E) \qquad \theta_{sH} = \frac{I^{s_z}}{I_0}$$

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

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

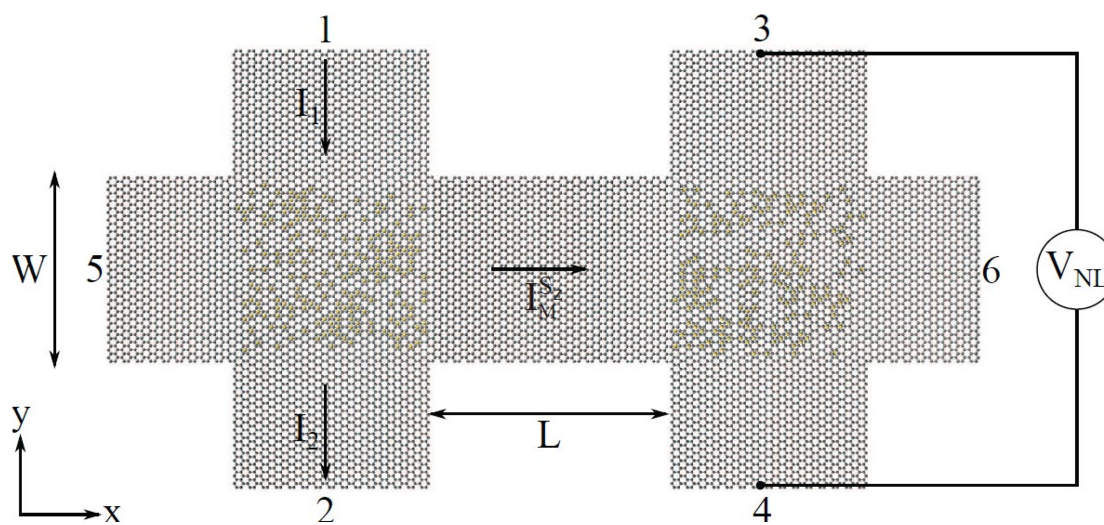
D. Van Tuan,[1,2] J. M. Marmolejo-Tejada,[3,4] X. Waintal,[5] B. K. Nikolić,[3,*] S. O. Valenzuela,[1,6] and S. Roche[1,6,†]
[1]Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and The Barcelona Institute of Science and Technology, Campus UAB, Bellaterra, 08193 Barcelona, Spain
[2]Department of Electrical and Computer Engineering, University of Rochester, Rochester, New York 14627, USA
[3]Department of Physics and Astronomy, University of Delaware, Newark, Delaware 19716-2570, USA
[4]School of Electrical and Electronics Engineering, Universidad del Valle, Cali AA 25360, Colombia
[5]Univ. Grenoble Alpes, INAC-PHELIQS, F-38000 Grenoble, France and CEA, INAC-PHELIQS, F-38000 Grenoble, France
[6]ICREA—Institució Catalana de Recerca i Estudis Avançats, 08010 Barcelona, Spain
(Received 19 February 2016; published 20 October 2016)

Kubo formalism
(dissipative & Hall conductivities)



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

Multiterminal landauer-Büttiker formalism

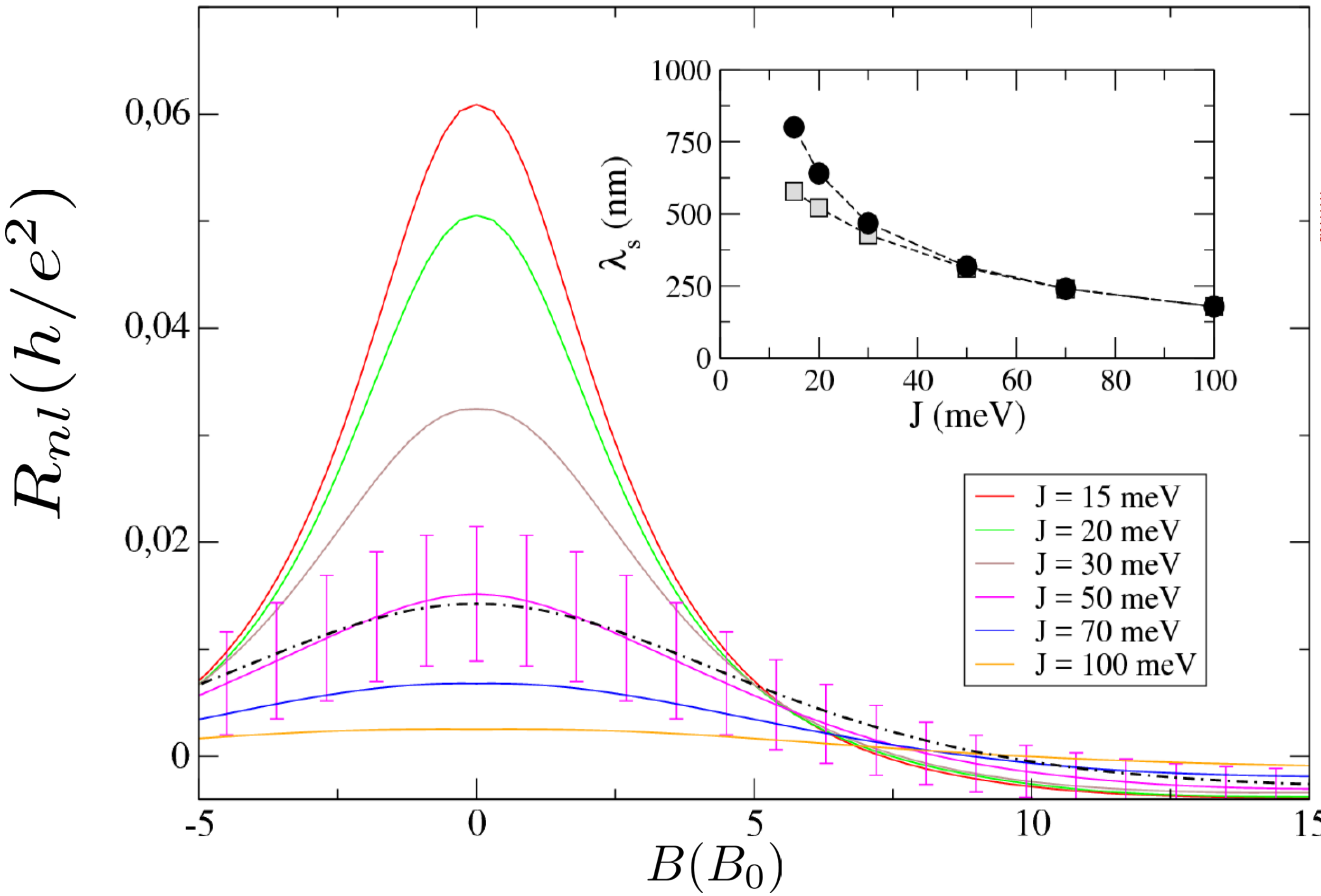


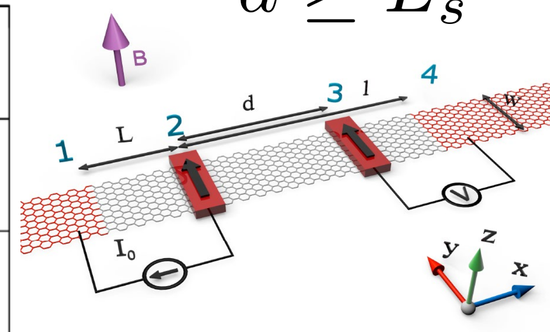
$$\theta_{\rm sH} = I_5^{s_z}/I_1$$

Hanle spin precession simulations

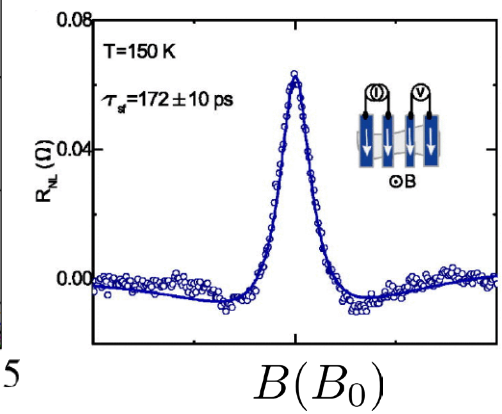
Graphene with random magnetic impurities

$d \geq L_s$



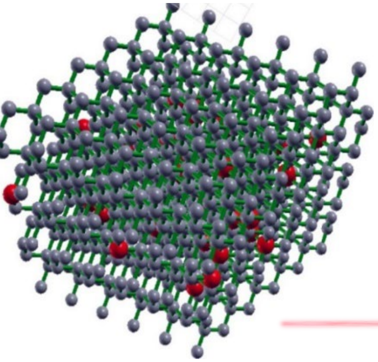


Consistent extrapolation of spin diffusion length



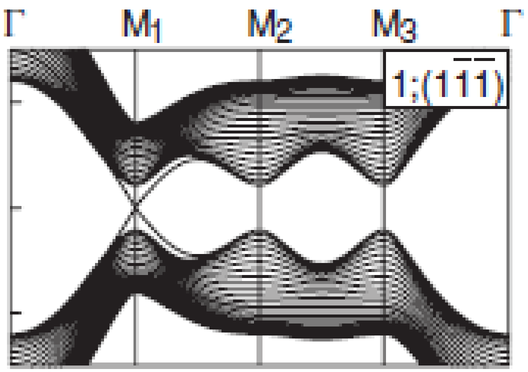
M. Vila, J.H. Garcia, A.W. Cummings, S. Power, C. Groth, X. Waintal, S. Roche

Physical Review Letters 124 (19), 196602 (2020)



Transport properties in *High-dimensionality, disordered* topological materials

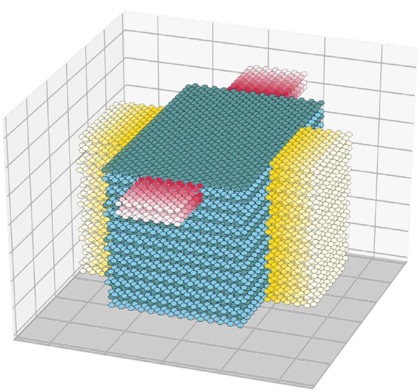
Pablo Piskunow

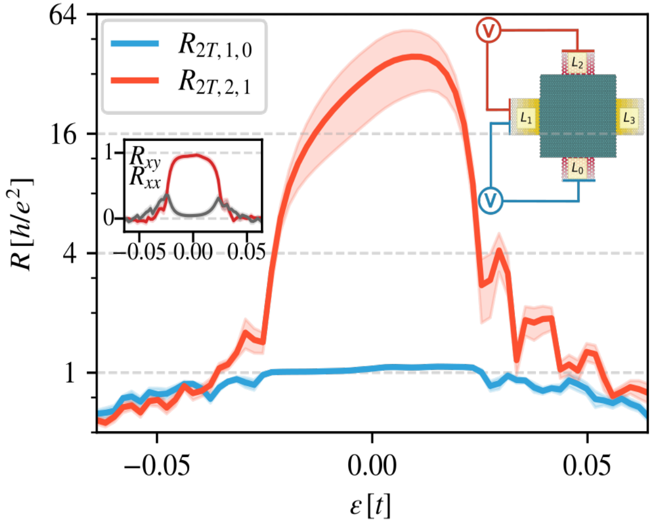


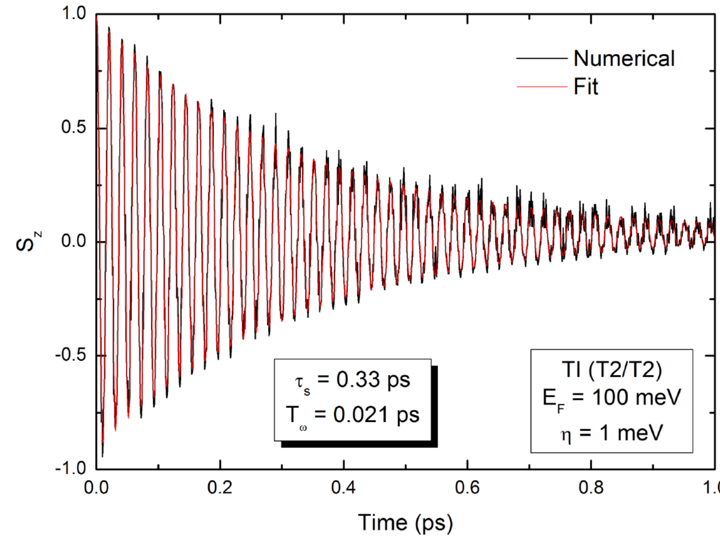
3D Fu-Kane-Mele Hamiltonian for topological insulators
With magnetic impurities (proximity effects)

$$\mathcal{H} = \sum_{\langle ij \rangle} t_{ij} c_i^\dagger c_j + i(4\hbar\lambda_{SO}/a^2) \sum_{\langle\langle ij \rangle\rangle} c_i^\dagger \sigma.(\mathbf{d}_{ij}^1 \times \mathbf{d}_{ij}^2) c_j$$

$$\mathcal{H}_Z = \sum_{i,\alpha,\beta} c_{i,\alpha}^\dagger \left[(m_i + \delta m_i) \hat{\boldsymbol{z}} \cdot \boldsymbol{s} \right]_{\alpha,\beta} c_{i,\beta}$$







PM Perez-Piskunow & S Roche, **Phys. Rev. Lett. 126, 167701 (2021)**

Low symmetry topological materials

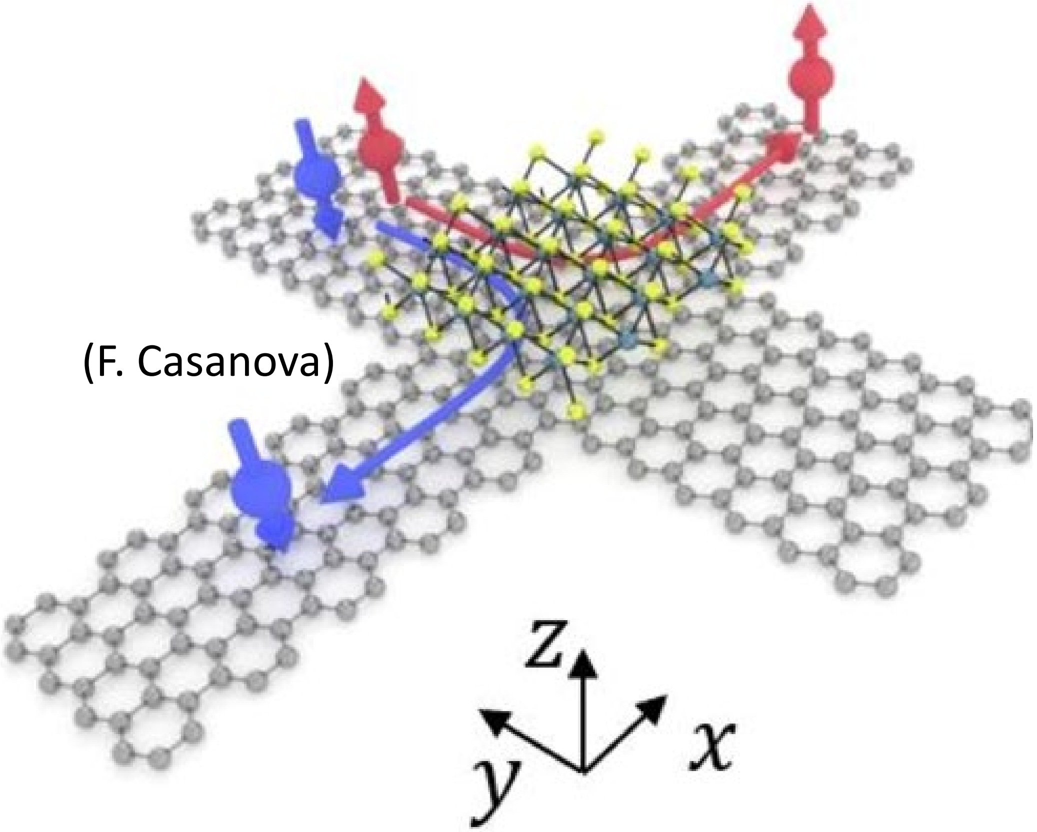
Multiple components

Spin Hall Effect

($MoTe_2$ monolayer)

M. Vila et al. **Physical Review Research** 3 (4), 043230 (2021)

"Spin currents by proximity effect"



Using strong SOC
Spin Hall Effect

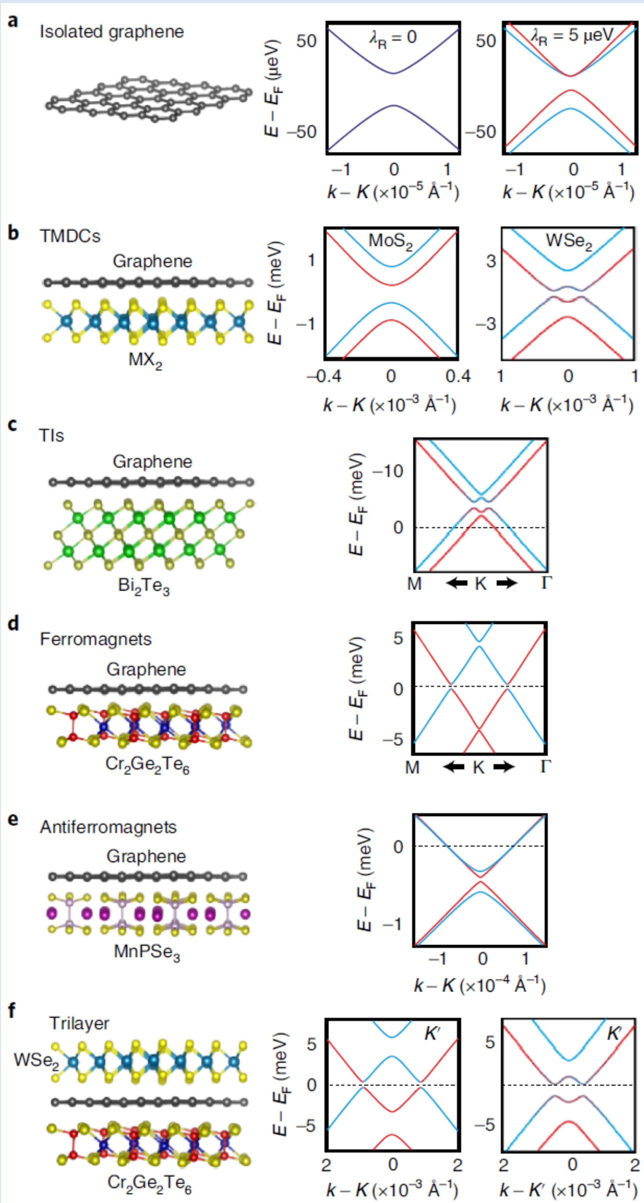
$$\theta_{sH} = \frac{|J_s^z|}{|J_c|}$$

Spin Hall angle

efficiency of ***converting charge current to spin current***

Can we use proximity effects to generate and control spin currents?

Emergent Hamiltonian in proximitized graphene



$$H = H_0 + H_\Delta + H_\mathrm{I} + H_\mathrm{VZ} + H_\mathrm{R} + H_\mathrm{PIA} + H_\mathrm{EX}$$

$$H_0 = \hbar v_F \left(\tau k_x \sigma_x + k_y \sigma_y\right)$$

$$H_\mathrm{I} = \lambda_\mathrm{I} \tau \sigma_z s_z$$

$$H_\mathrm{R} = \lambda_\mathrm{R} (\tau \sigma_x s_y - \sigma_y s_x$$

$$H_\mathrm{VZ} = \lambda_\mathrm{VZ} \tau \sigma_0 s_z$$

$$H_\mathrm{PIA} = \alpha(\lambda_\mathrm{PIA} \sigma_z + \Delta_\mathrm{PIA})(k_x s_y - k_y s_x)$$

$$H_\mathrm{EX} = \lambda_\mathrm{EX} s_z + \lambda_\mathrm{EX}^\mathrm{AF} \sigma_z s_z$$

J.F. Sierra, J. Fabian, R Kawakami, S. Roche, SO Valenzuela

Nature Nanotech. 16 (8), 856-868 (2021)

Spin Hall Kubo conductivity

(SHE in dissipative regime)

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

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

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

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

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

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

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

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

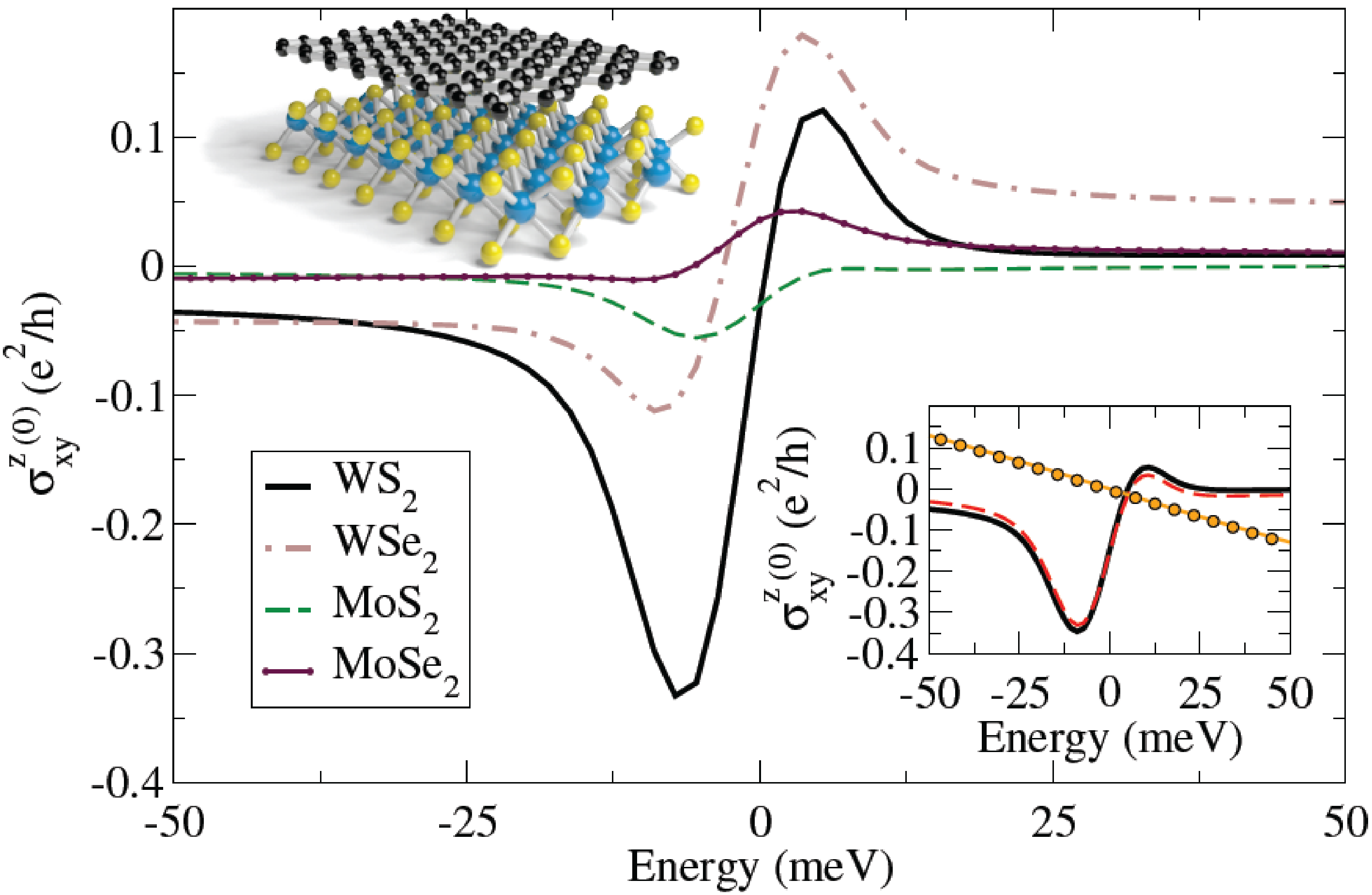
$$\sigma_{xx} = \frac{2\hbar e^2}{\pi \Omega} \sum_{m,n=0}^{M} \mathcal{I}m[g_m(\epsilon + i\eta)] \mathcal{I}m[g_n(\epsilon + i\eta)] \mu_{mn}$$

dc-Kubo conductivity

JH Garcia et al. **Phys. Rev. Lett. 114, 6602 (2015)**

Spin Hall Kubo conductivity

in clean graphene/TMDC interfaces



Dissipative SHE

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

Clean case :

"intrinsic SHE"

WS_2 leads to larger Spin Hall conductivity (larger SHA)

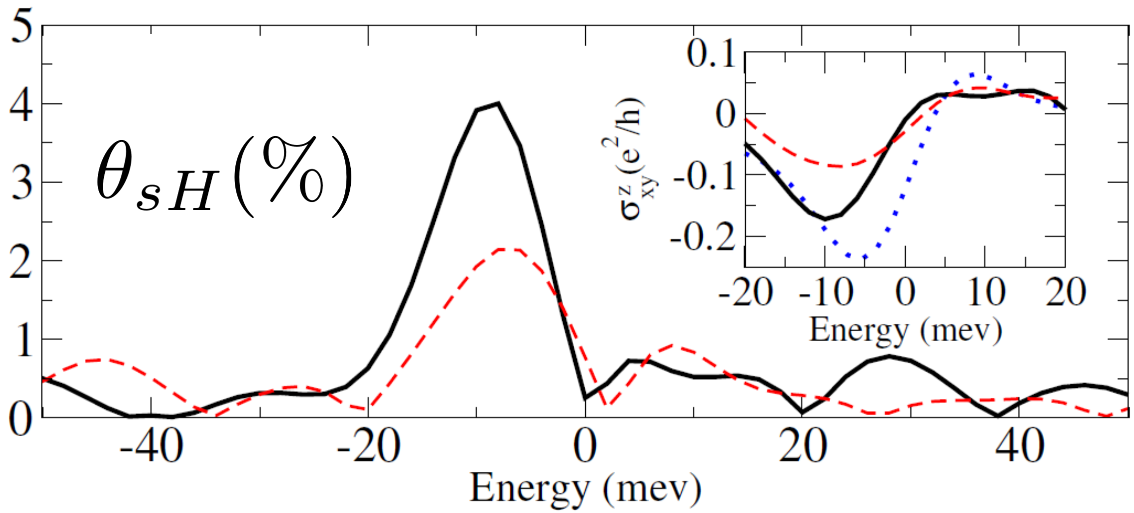
"extrinsic SHE"

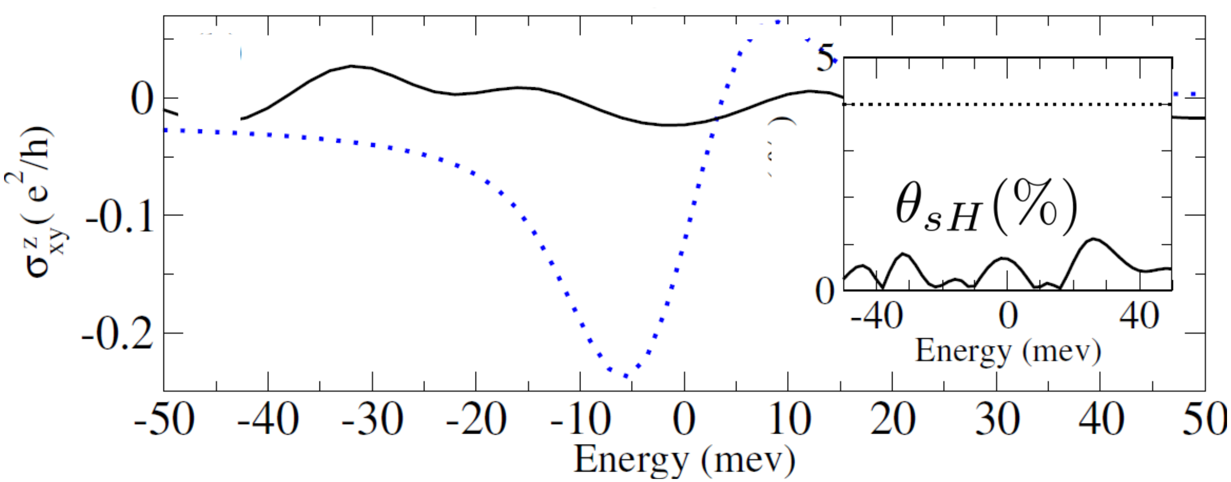
To be continued !

JH Garcia et al. **Nano Lett. 17, 5078-5083 (2017)**

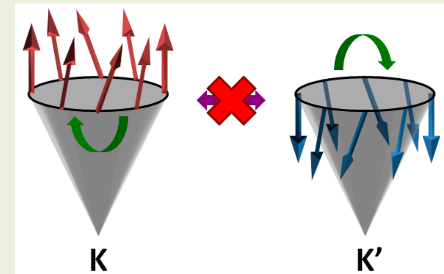
Upper limit Spin Hall Effect

in disordered graphene/TMDC interfaces



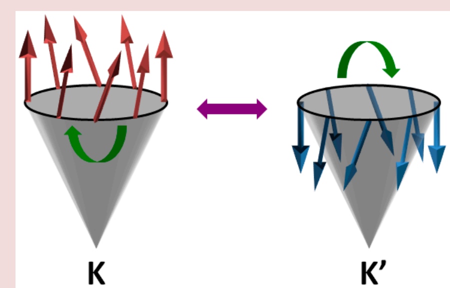


$\theta_{sH}(\%) \simeq 4\%$



Intravalley scattering

$\theta_{sH}(\%) \ll 1\%$



Intervalley scattering

JH Garcia et al. **Nano Letters 17 (8), 5078 (2017)**

nature materials

ARTICLES

https://doi.org/10.1038/s41563-019-0575-1

Nature Materials 19 (2), 170-175 (2020)

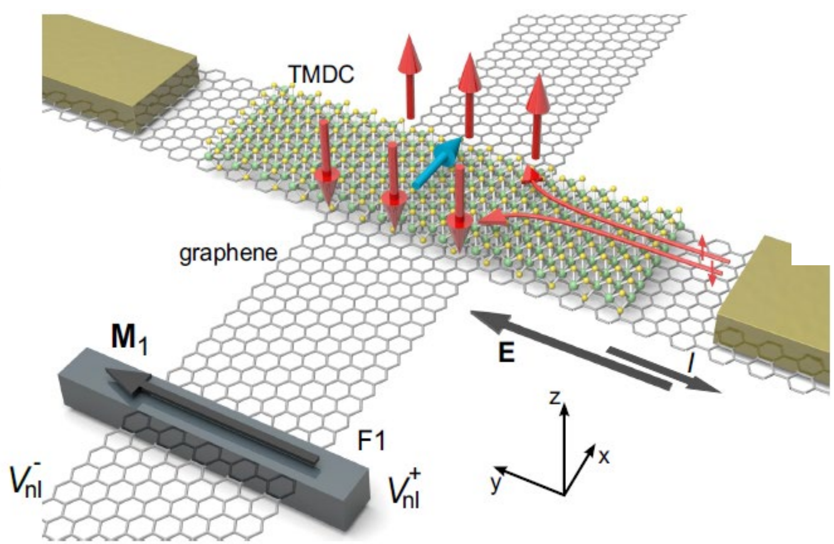
Tunable room-temperature spin galvanic and spin Hall effects in van der Waals heterostructures

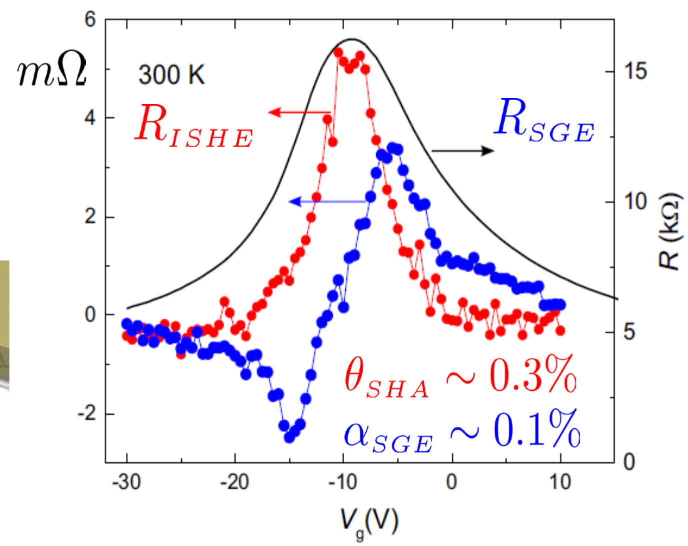
L. Antonio Benítez[1,2,4*], Williams Savero Torres[1,4*], Juan F. Sierra[1], Matias Timmermans[1,2], Jose H. Garcia[1], Stephan Roche[1,3], Marius V. Costache[1] and Sergio O. Valenzuela[1,3*]

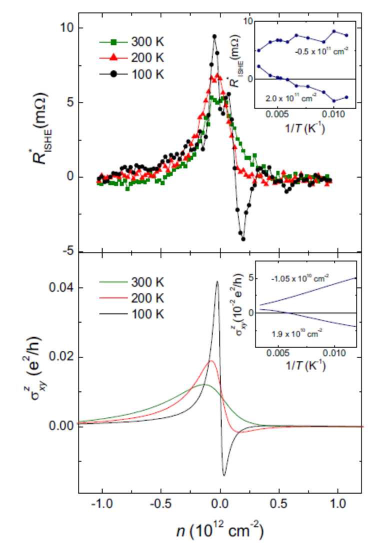
GRAPHENE FLAGSHIP

$$\lambda_s \theta_{sH}^{\alpha} \sim 5 - 10 \text{ nm}$$

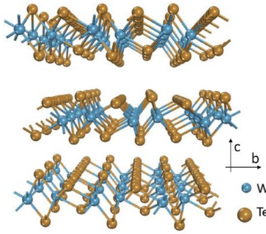
ICN2







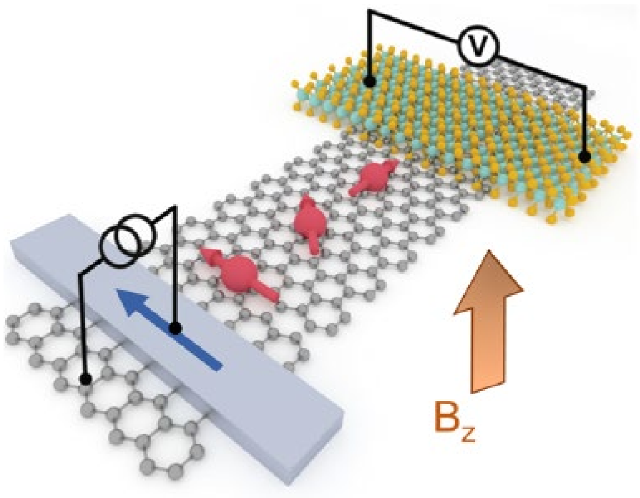
SHE in Low-symmetry multilayers TMDs

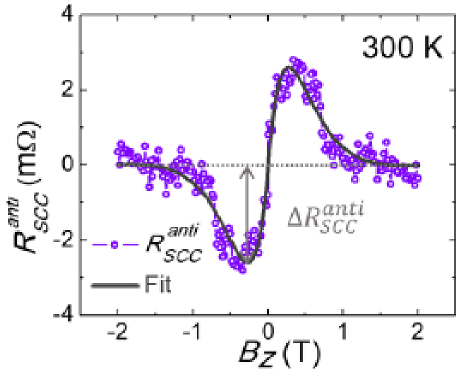


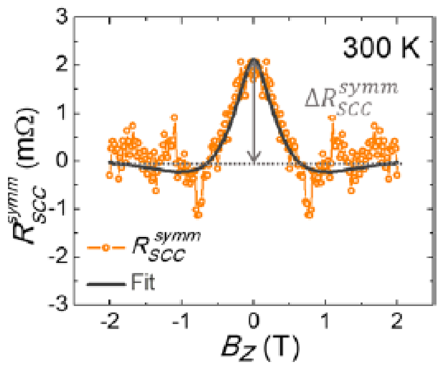
C. K. Safeer, et al. Nano Letters **19** (12), 8758-8766 (2019)

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

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







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

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

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

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

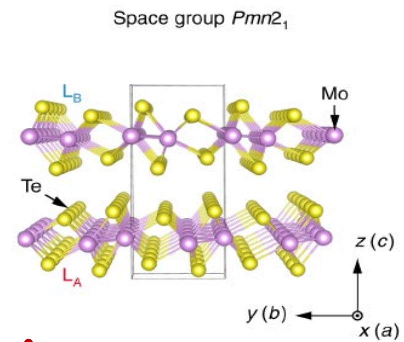
$$\lambda_s . \theta_{sH} \sim 300\text{nm !!}$$

4-band symmetry-based model TMD-1T_d

Centre for Advanced 2D Materials

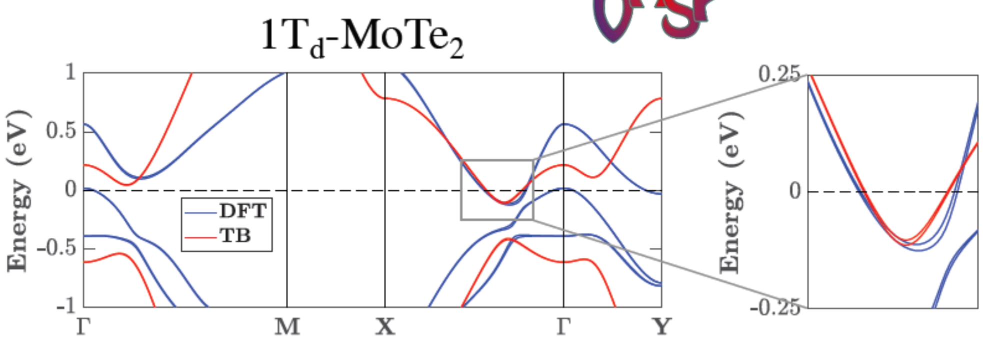
Bulk crystal structure of 1T_d-TMD

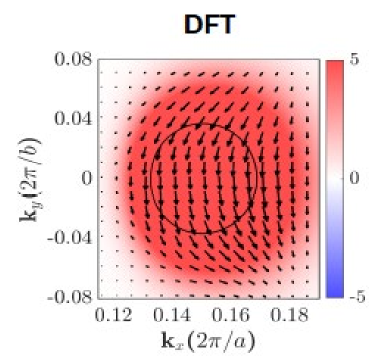
(mirror symmetry in the yz plane (M_x) & a glide mirror symmetry (M_y) along the perpendicular z direction)



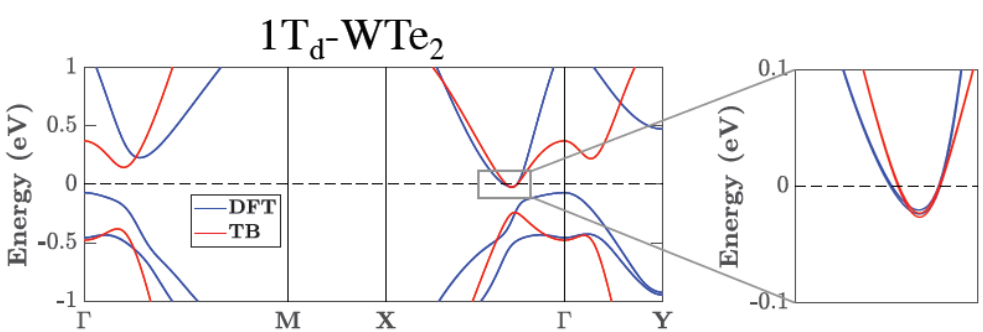
Monolayer 1T_d-TMD: *Lowering symmetry*

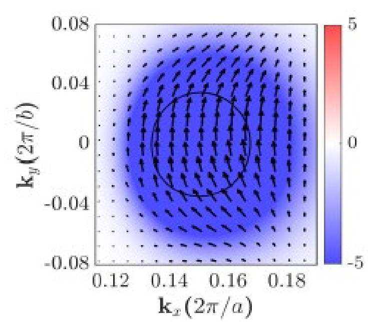
2D structure loses translational symmetry along the z direction





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





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

4-band symmetry-based model TMD-1T_d

NUS National University of Singapore

Centre for Advanced 2D Materials

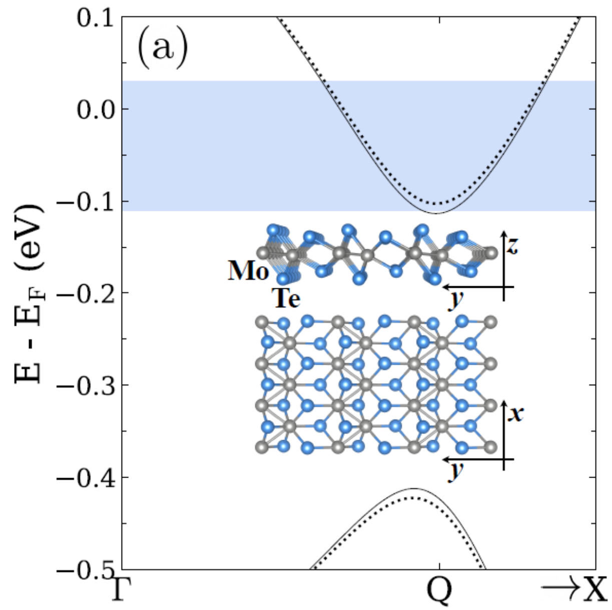
4-band real space tight binding model (*interpolated in Wannier basis (Wanier90)*)
generated by two orbitals (plus spin) / unit cell – p_y of the chalcogens and d_{yz} of the metal ions

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

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*

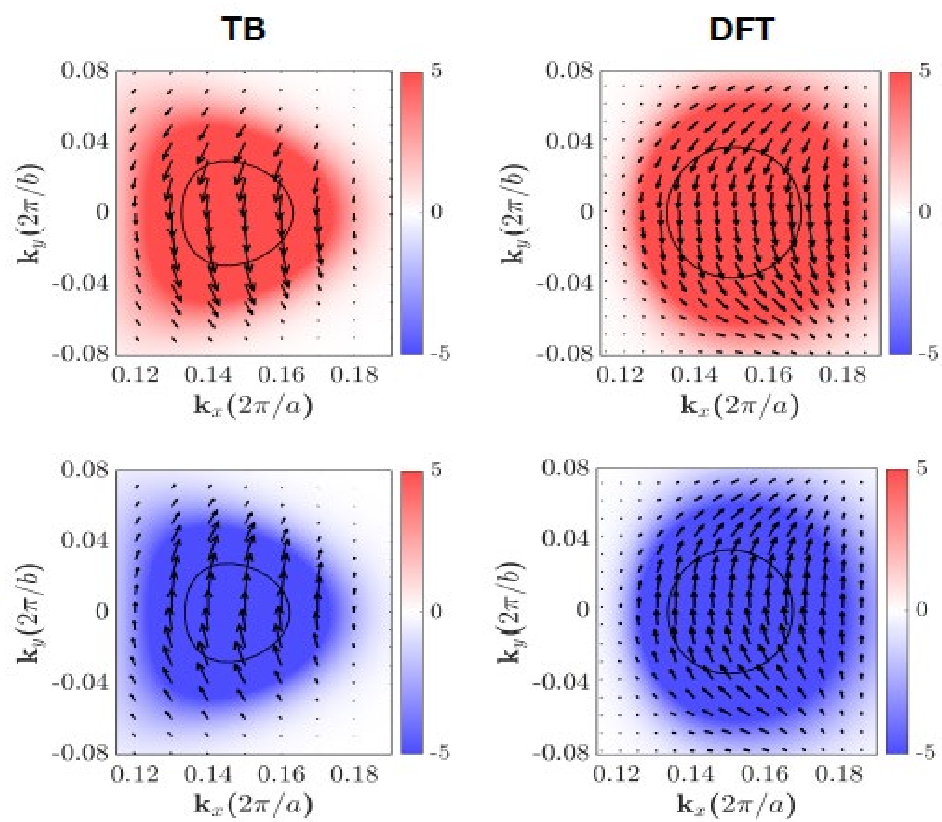


CB1

$MoTe_2$

CB2

WTe_2



Anisotropic spin dynamics in $MoTe_2$

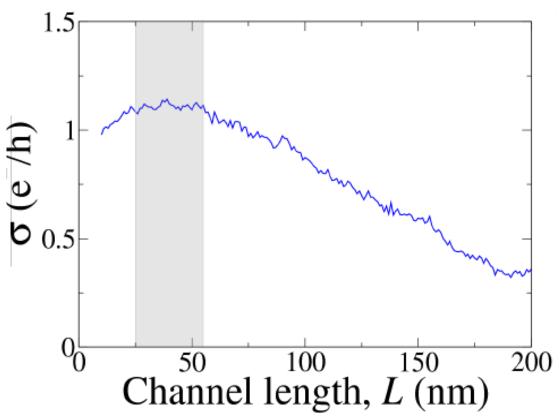
Study of the nonlocal resistance versus channel length to extract spin diffusion length

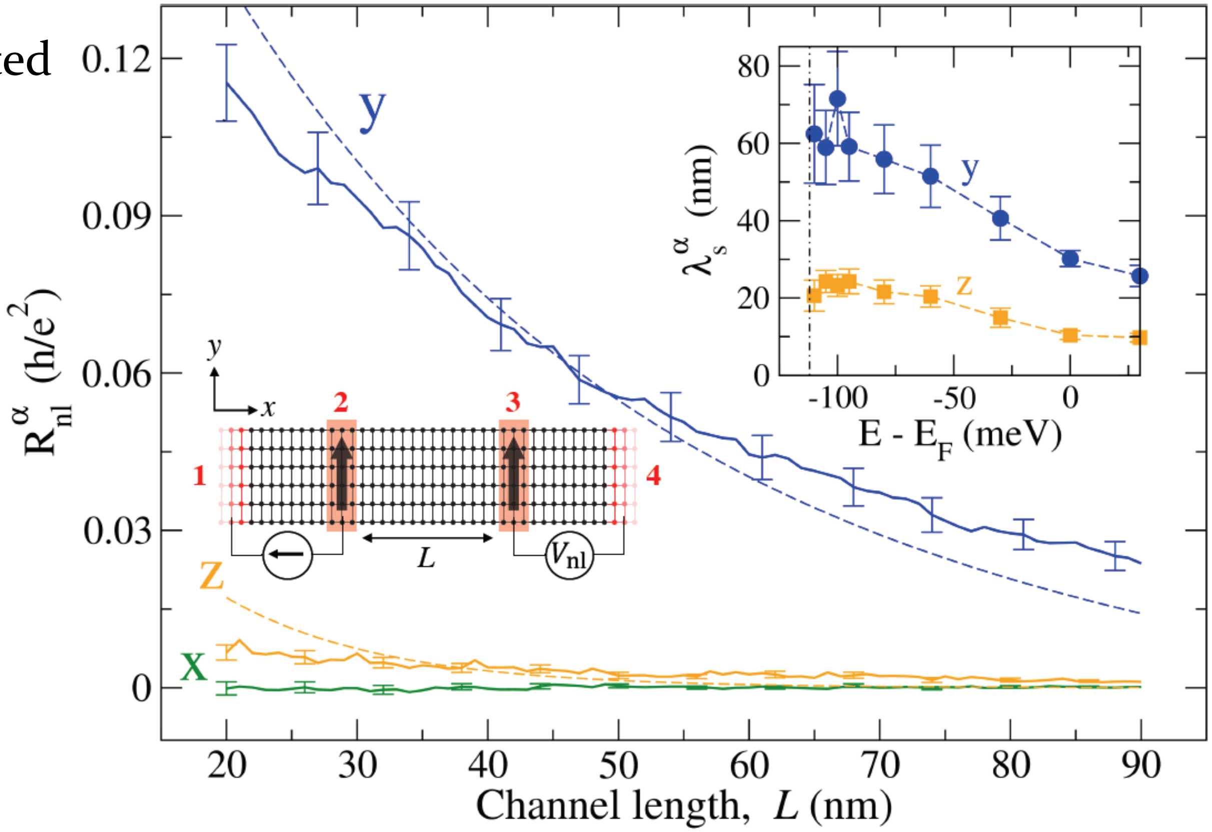
$$I_0^\alpha \quad \alpha \in \{x, y, z\}$$

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

$$\lambda_{\rm S}^y > \lambda_{\rm S}^z \gg \lambda_{\rm S}^x$$

M. Vila et al. **Phys. Rev. Res.** 3, 043230 (2021)

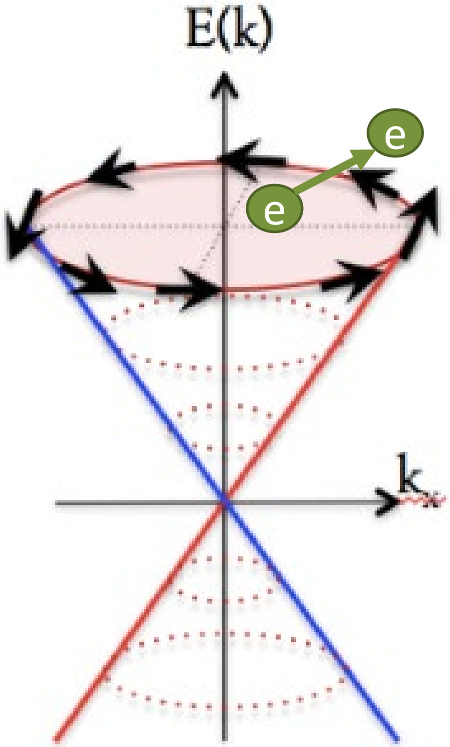
Anisotropic spin dynamics in $MoTe_2$

In 2D Rashba SOC materials

Spin-momentum locking

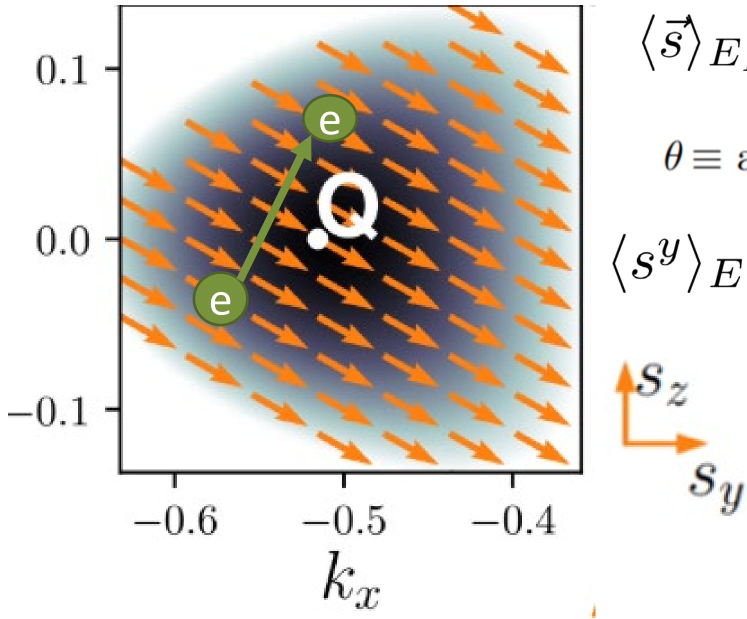
scattering changes effective (in-plane) magnetic field randomly

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



In 2D Weyl semimetal TMD

Persistent (canted) spin texture



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

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

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

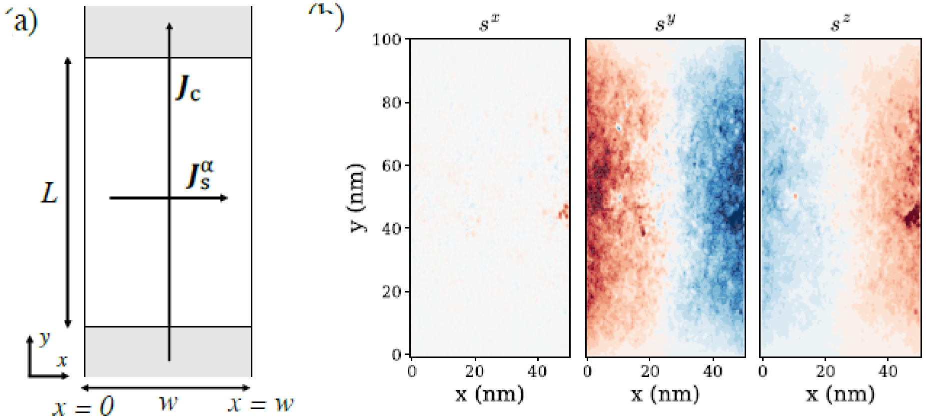
Effective magnetic field is fixed (**pointing in the yz plane**)

x-polarized spins precess much faster- shorter spin diffusion

z-polarized spins precess faster than y-polarized

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

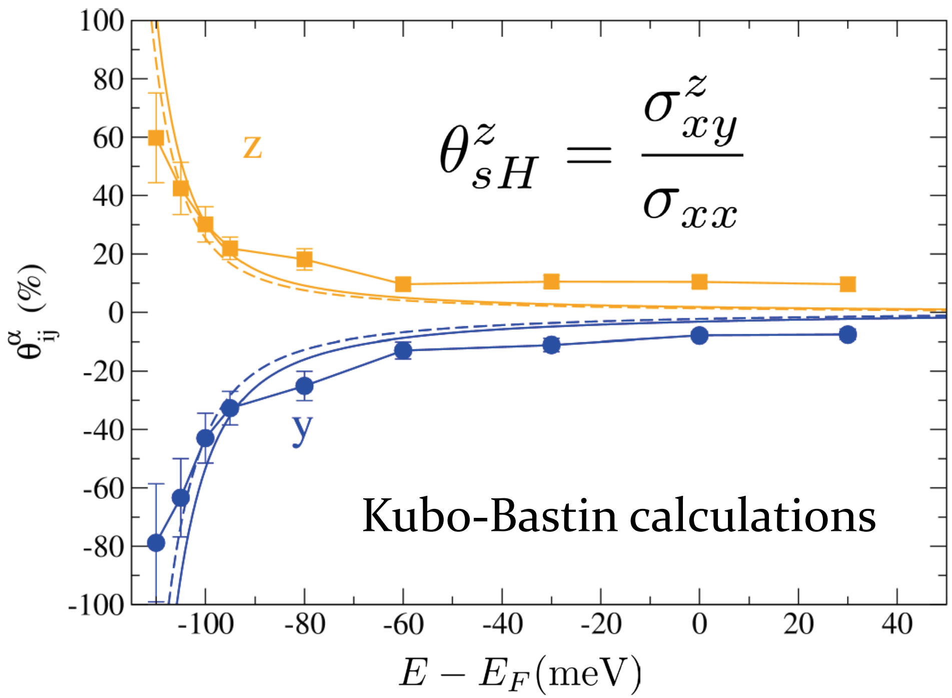
Spin accumulation & (Giant) Spin Hall angle

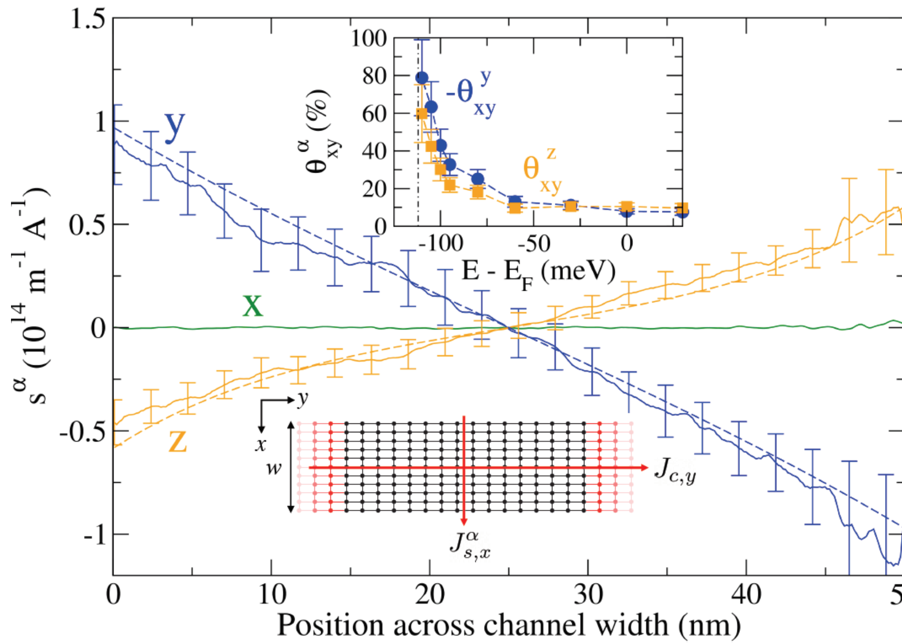


Extract the spin accumulation across the channel

Fitting the results with solution of the *Spin drift-diffusion equation*

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





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

M. Vila et al. **Phys. Rev. Res.** 3, 043230 (2021)

Experimental fingerprints (Hanle)

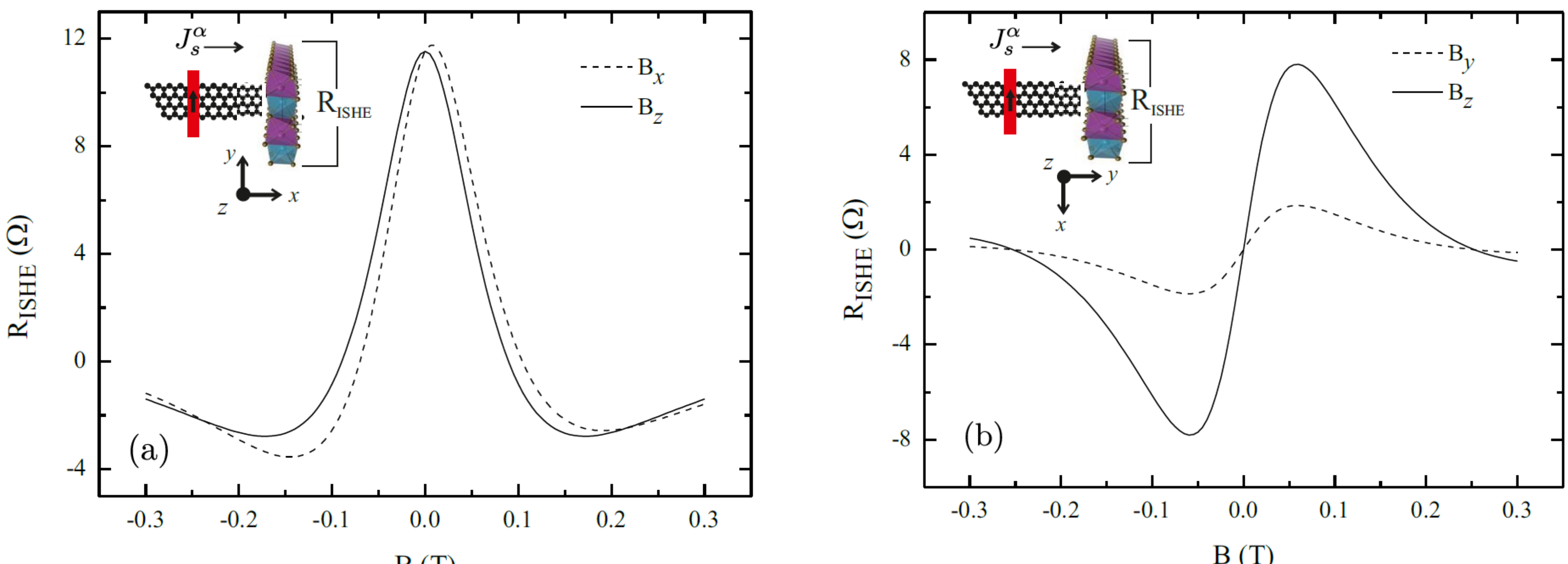
Simulated response of the inverse SHE (R_{ISHE})
to spin precession for two orientations of the TMD crystal (full absorption limit)

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

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

Anisotropic spin diffusion

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



M. Vila et al. Phys. Rev. Res. 3, 043230 (2021)

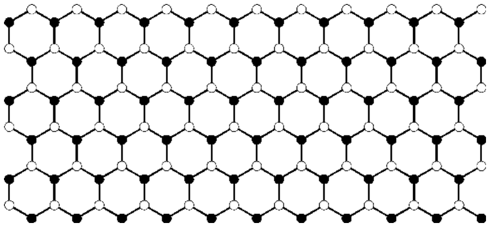
Low symmetry topological materials

Canted Quantum Spin Hall Effect

(WTe_2 monolayer)

J.H. Garcia et al. **Phys. Rev. Lett.** 125, 256603 (2020)
J.H. Garcia et al. **Phys. Rev. B** 106 (16), L161410 (2022)

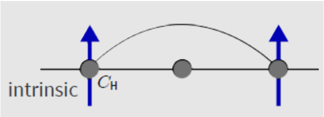
Quantum Spin Hall Effect

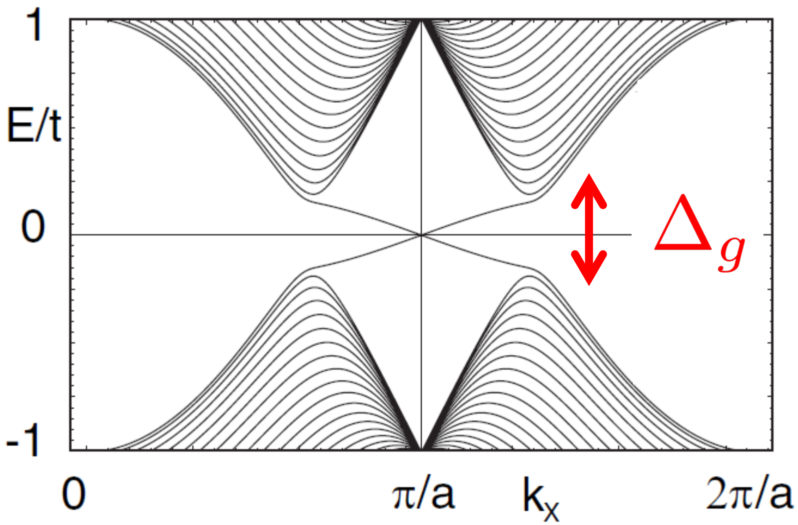


C.L. Kane and E. J. Mele,
Phys. Rev. Lett. 95, 26801 (2005)

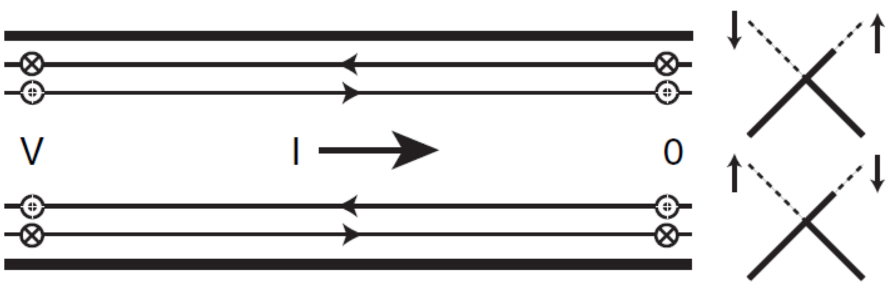
Zigzag graphene ribbon with intrinsic SOC

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





Gapless helical edge states
States with opposite spins counterpropagate at the edges



"QHE" in absence of magnetic field
Towards dissipation current **(TRS invariant)....**

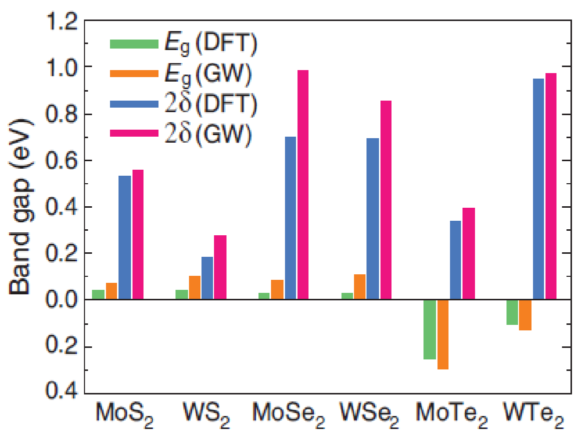
$\Delta_g \sim 0.1\text{meV}$

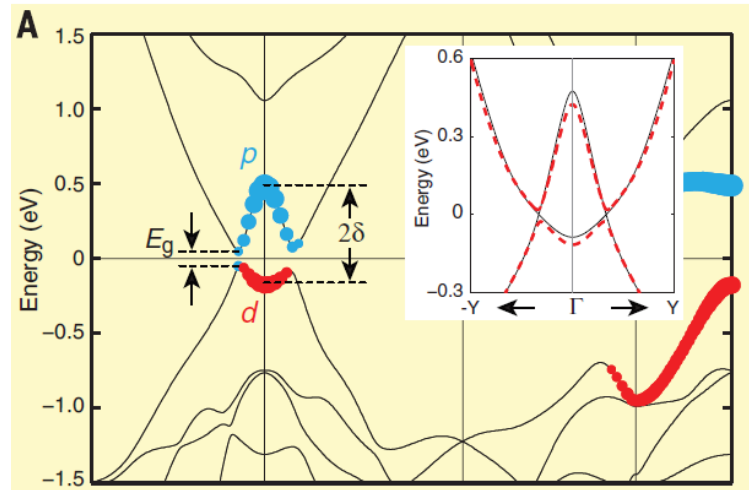
1T′-TMD monolayer as QSH insulators

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**)*

Prediction in 2014

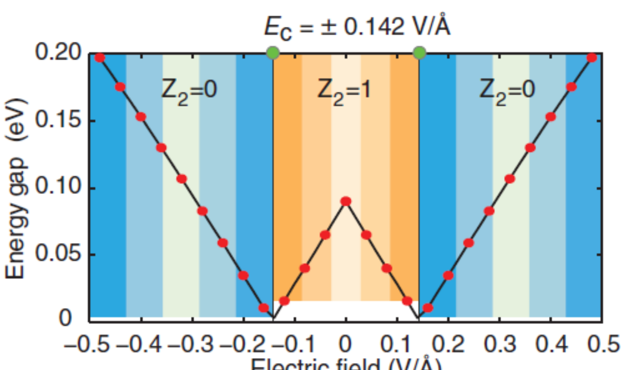


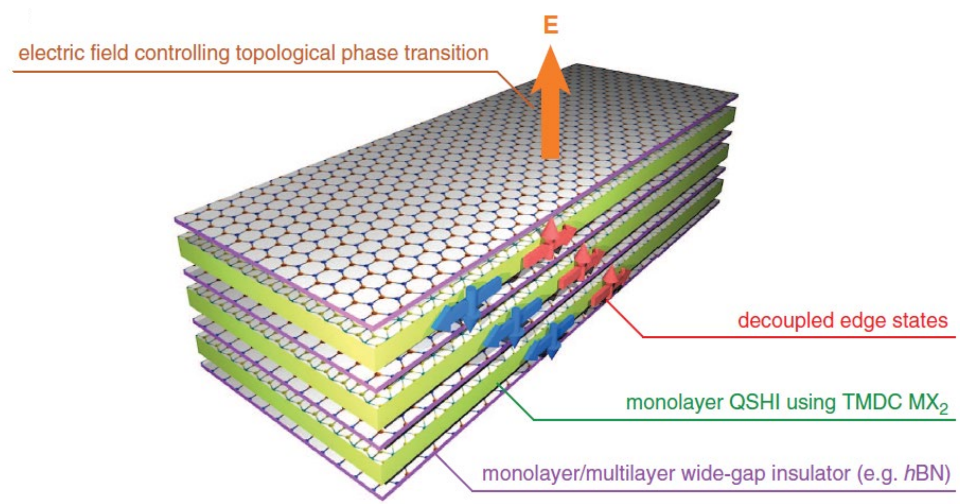


1T′-MoS_2

Topological field effect transistor

(low-power quantum electronics)





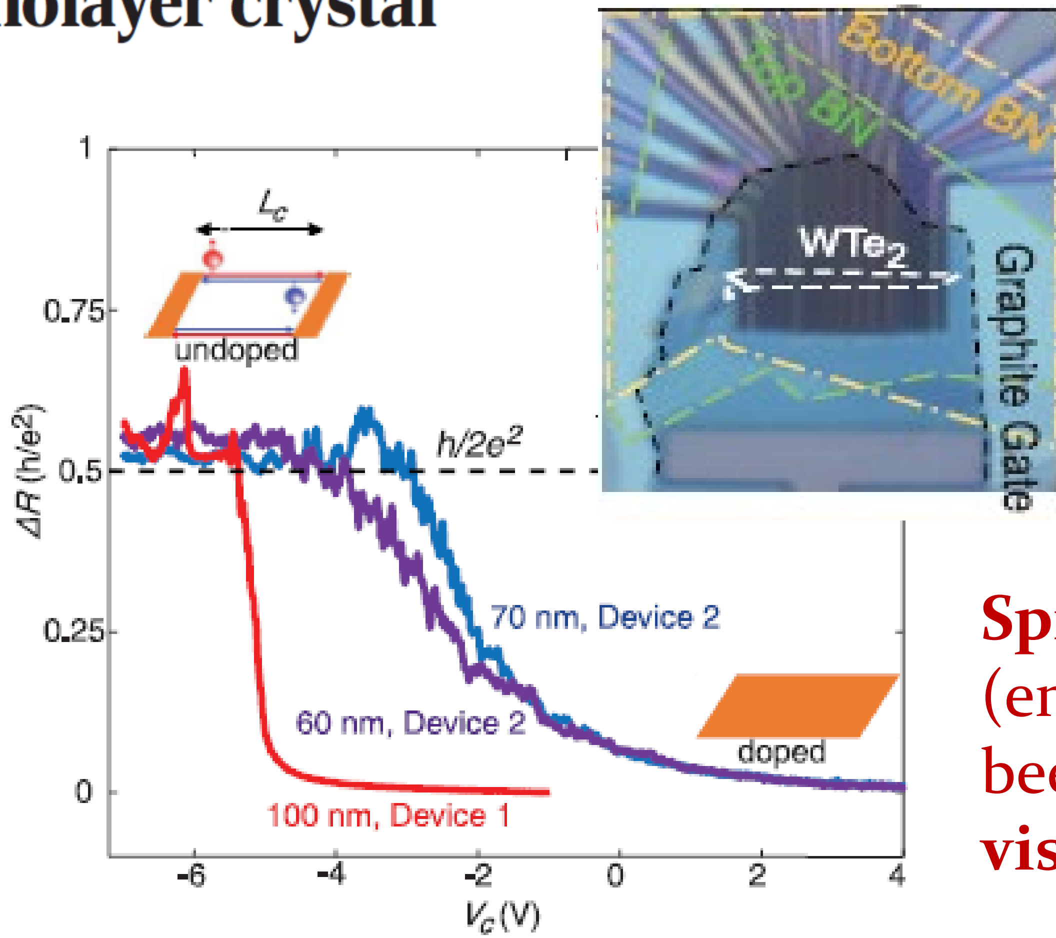
1T-WTe_2 as Quantum Spin Hall insulator

TOPOLOGICAL MATTER

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

Wu et al.

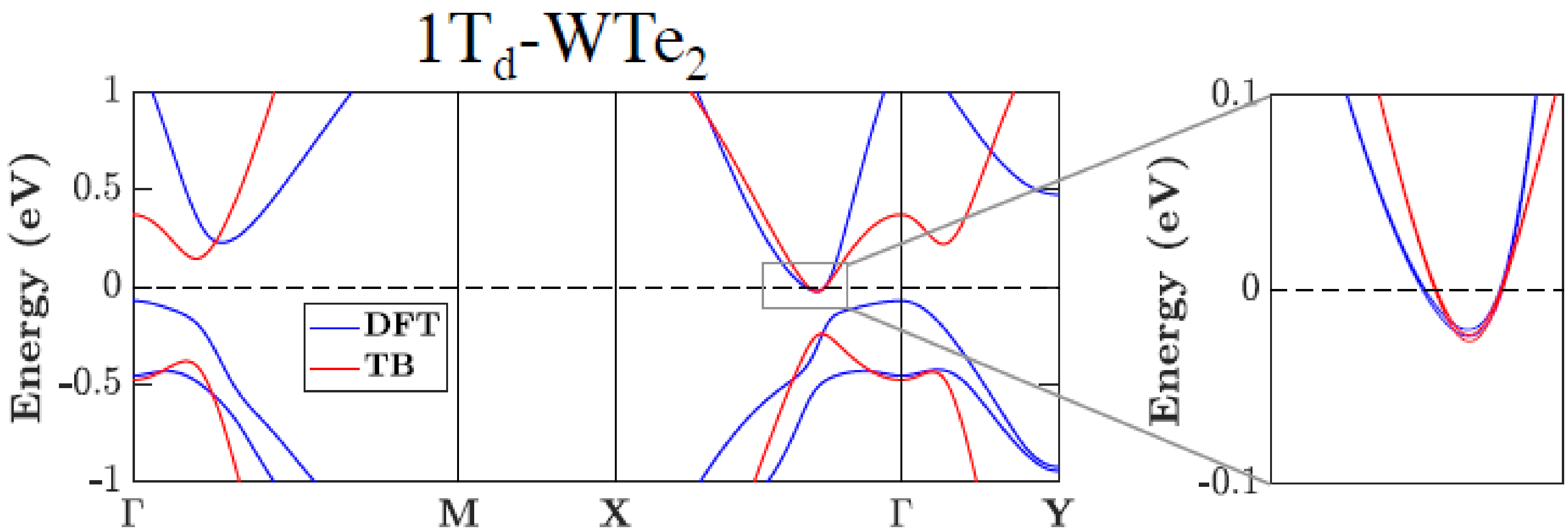
Science 359, 76-79 (2018)



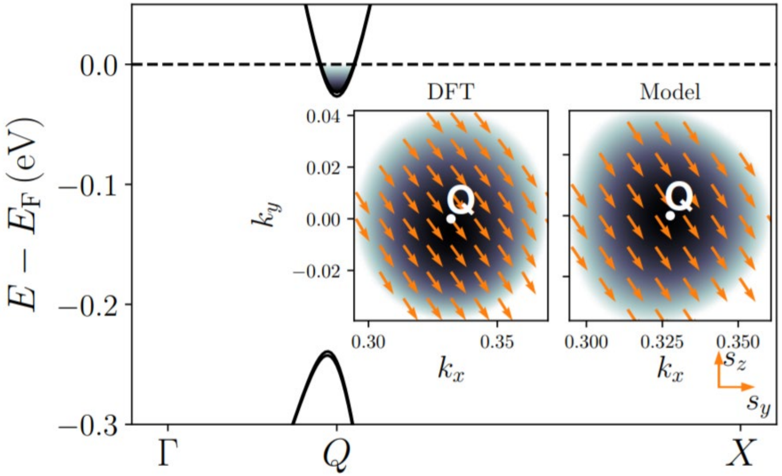
Purely electrical measurements

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

QSHE in WTe_2



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



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

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

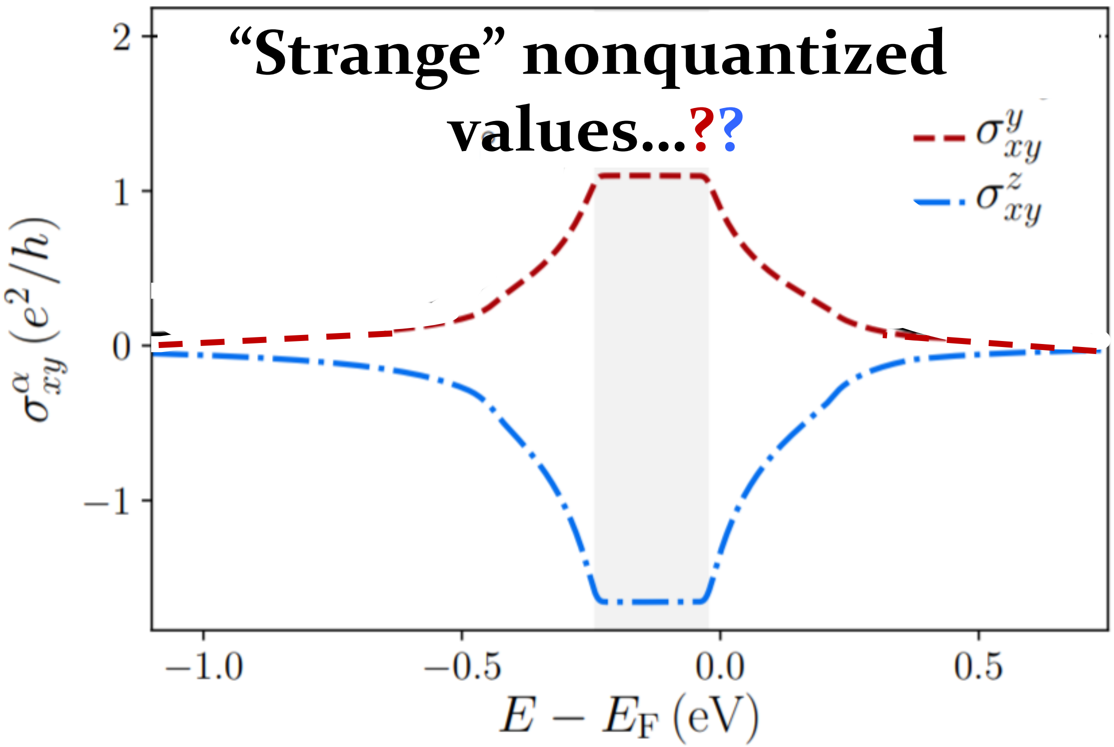
Spin Hall conductivity for WTe_2

Spin Hall conductivity tensor
(Kubo-Bastin formula)

$$\sigma_{ij}^{\alpha}, \alpha = x, y, z$$

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

measures of the spin projection onto α



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

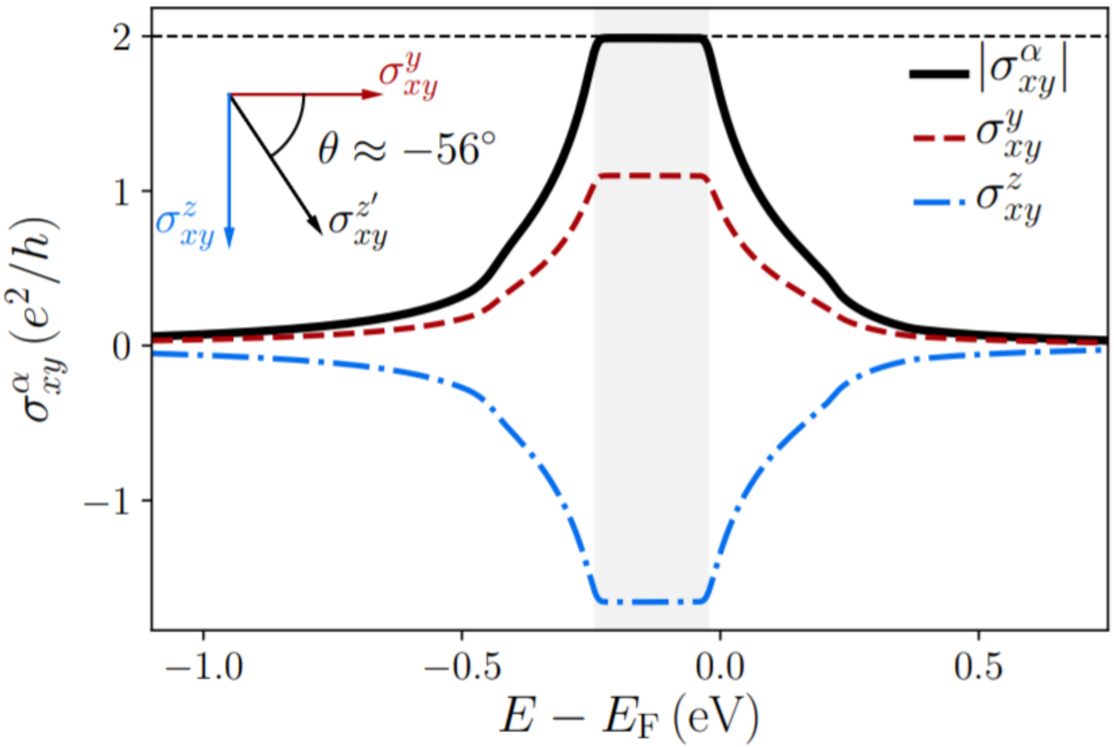
Spin Hall conductivity for WTe_2

Spin Hall conductivity tensor
(Kubo-Bastin formula)

$$\sigma_{ij}^{\alpha}, \alpha = x, y, z$$

measures of the spin projection onto α

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



In the gap, a combination of SHC in y and z directions

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

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

Two spin-canted topological states
sustaining QSHE in WTe_2

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

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

Spin quantization axis

$$[\mathcal{H}', \sigma_{z'}] \approx 0$$

(spin preserved along z′)

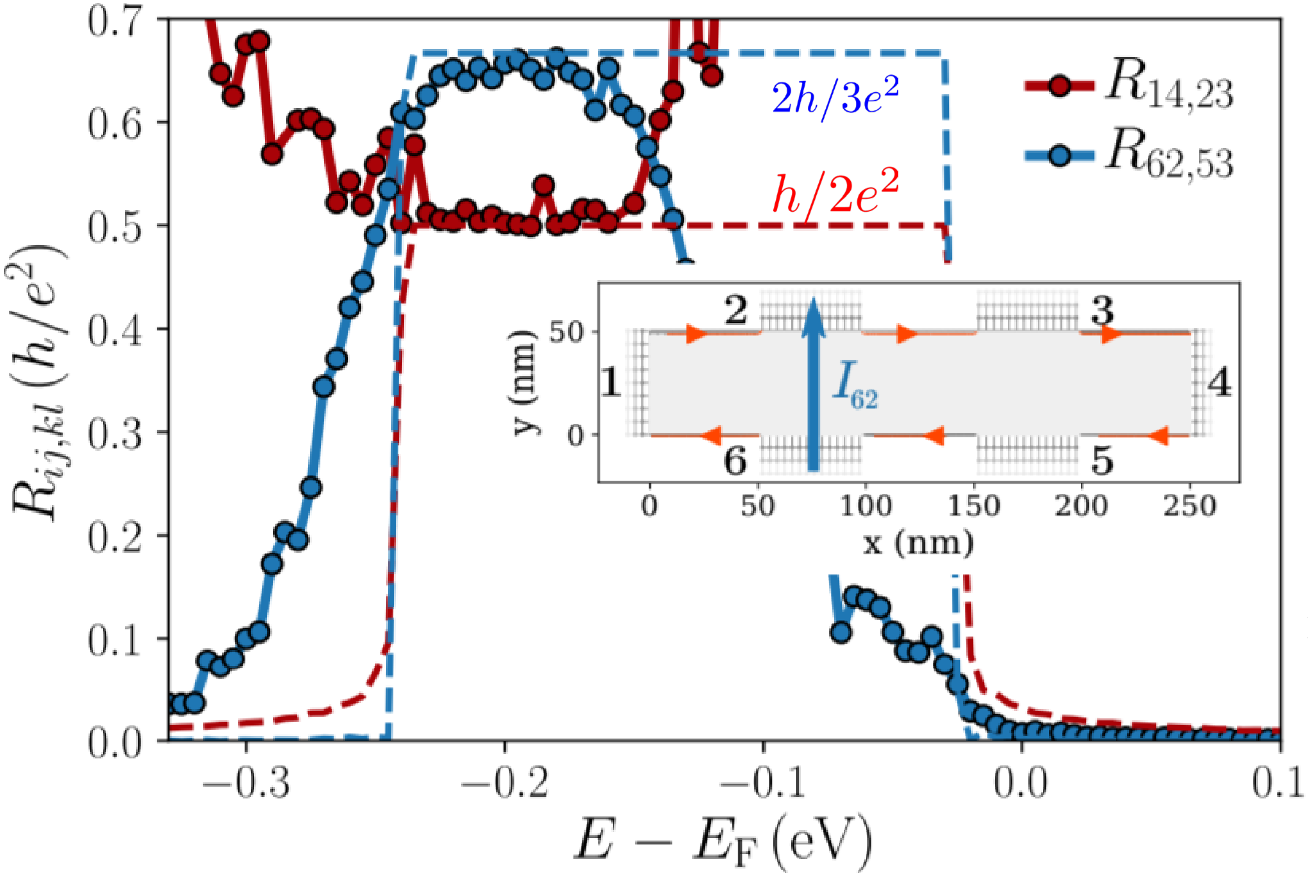
Nonlocal resistance calculations

Topologically protected edge-states

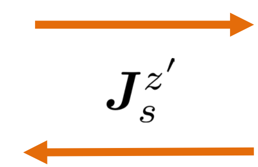
Quantized two-terminal resistance (2 channels) $h/2e^2$

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**



$J_s^{z'}$

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

$J_s^{y'}$

“vanishing contribution”

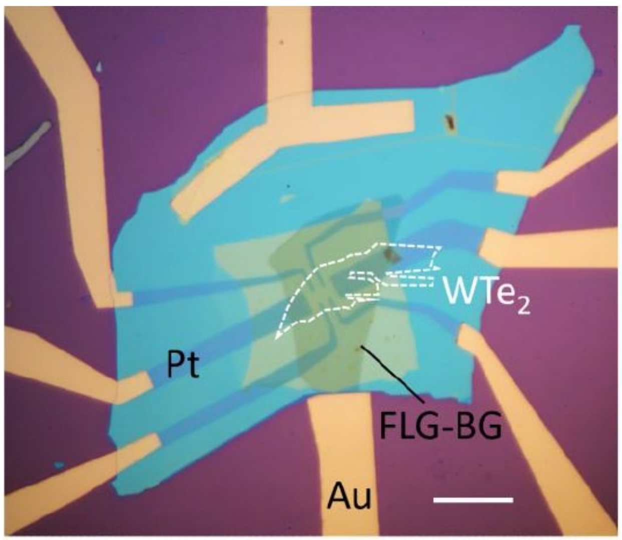
J.H. Garcia et al. Phys. Rev. Lett. 125, 256603 (2020)

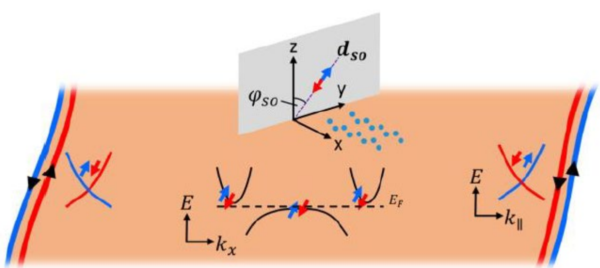
Determination of the helical edge and bulk spin axis in quantum spin Hall insulator WTe_2

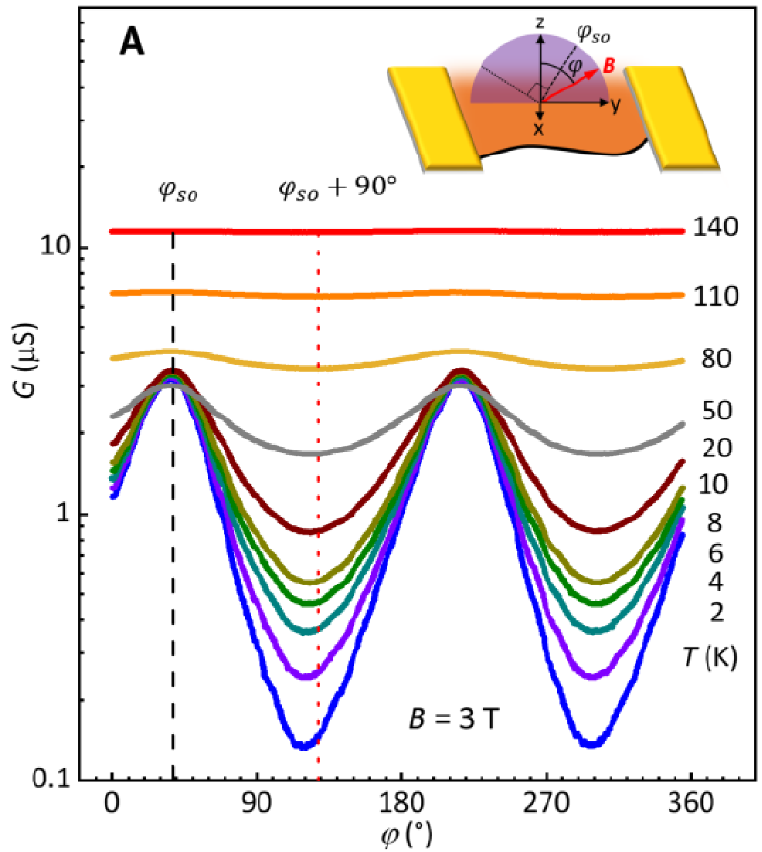
Wenjin Zhao[1]†, Elliott Runburg[1]†, Zaiyao Fei[1], Joshua Mutch[1], Paul Malinowski[1], Bosong Sun[1], Xiong Huang[2,3], Dmytro Pesin[4], Yong-Tao Cui[2,3], Xiaodong Xu[1,5], Jiun-Haw Chu[1], David H. Cobden[1]*

[1]Department of Physics, University of Washington, Seattle WA 98195, USA
[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

Phys. Rev. X 11, 041034 (2021)







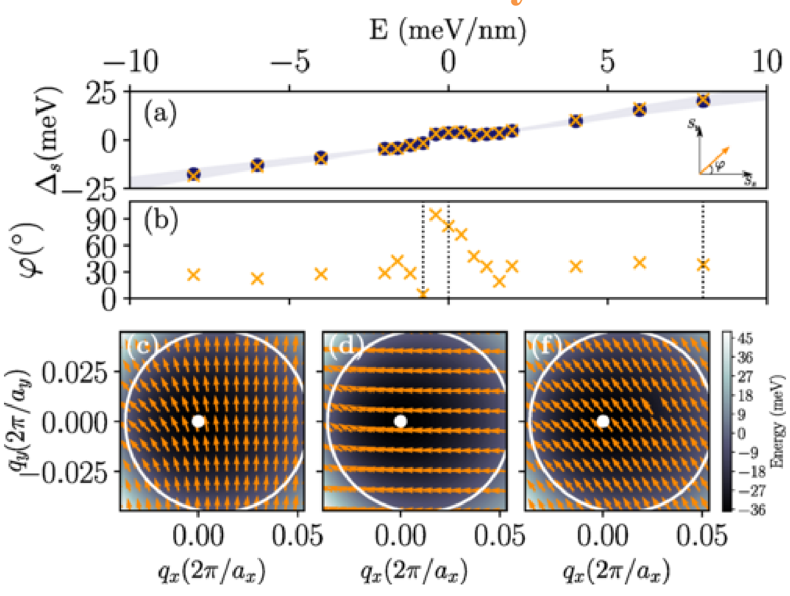
Electrical control of spin-polarized topological currents in monolayer WTe_2

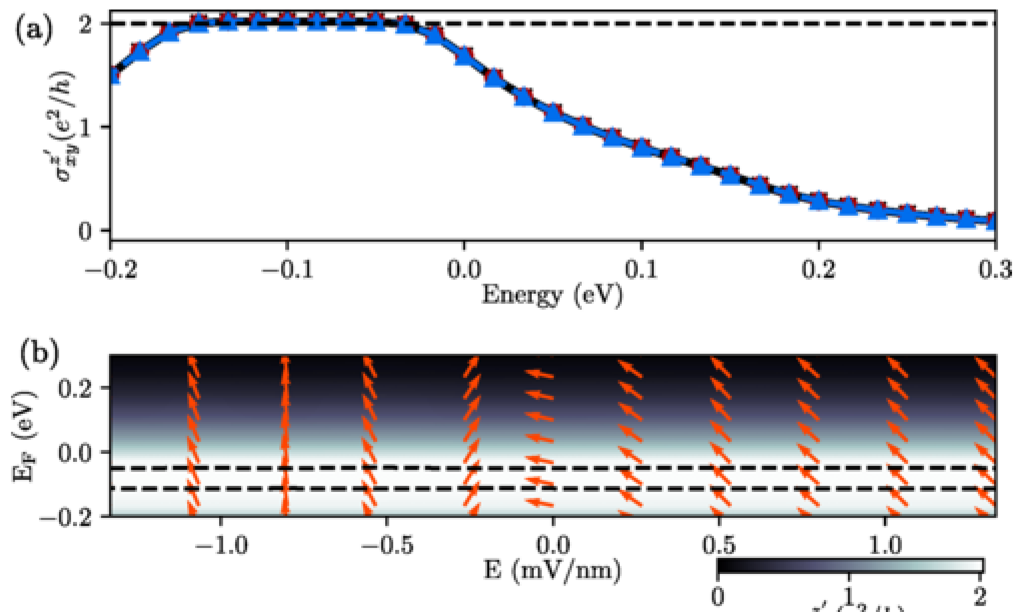
Jose H. Garcia,[1] Jinxuan You,[1,2] Mónica García-Mota,[2] Peter Koval,[2] Pablo Ordejón,[1]
Ramón Cuadrado,[1] Matthieu J. Verstraete,[3] Zeila Zanolli,[4,1] and Stephan Roche[1,5]
[1] *Catalan Institute of Nanoscience and Nanotechnology - ICN2, (CSIC and BIST), Campus UAB, Bellaterra, 08193 Barcelona, Spain*
[2] *Simune Atomistics S.L., Tolosa Hiribidea, 76, 20018 Donostia-San Sebastian, Spain*
[3] *nanomat/QMAT/CESAM and European Theoretical Spectroscopy Facility Universite de Liege, Allee du 6 Aout 19 (B5a), 4000 Liege, Belgium*
[4] *Dept. of Chemistry, Debye Institute for Nanomaterials Science, and ETSF, Utrecht University, The Nethe*
[5] *ICREA–Institució Catalana de Recerca i Estudis Avançats, 08010 Barcelona, Spain*

(Dated: May 25, 2022)

We evidence the possibility for coherent electrical manipulation of the spin orientation of topologically protected edge states in a low-symmetry quantum spin Hall insulator. By using a combination of *ab-initio* simulations, symmetry-based modeling, and large-scale calculations of the spin Hall conductivity, it is shown that small electric fields can efficiently vary the spin textures of edge currents in monolayer 1T'-WTe_2 by up to a 90-degree spin rotation, without jeopardizing their topological character. These findings suggest a new kind of gate-controllable spin-based device, topologically protected against disorder and of relevance for the development of topological spintronics.

Physical Review B 106 (16), L161410 (2022)



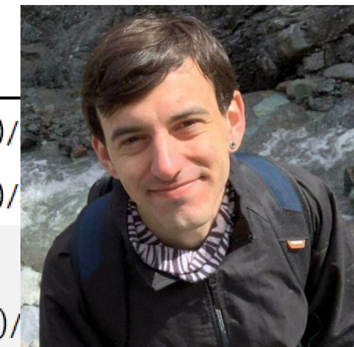


Increasing the variety of ***spin-orbit torque components***
By lowering the symmetry of the crystals
*& heterostructures (**twist degree of freedom..**)*

José Garcia

nature REVIEWS PHYSICS

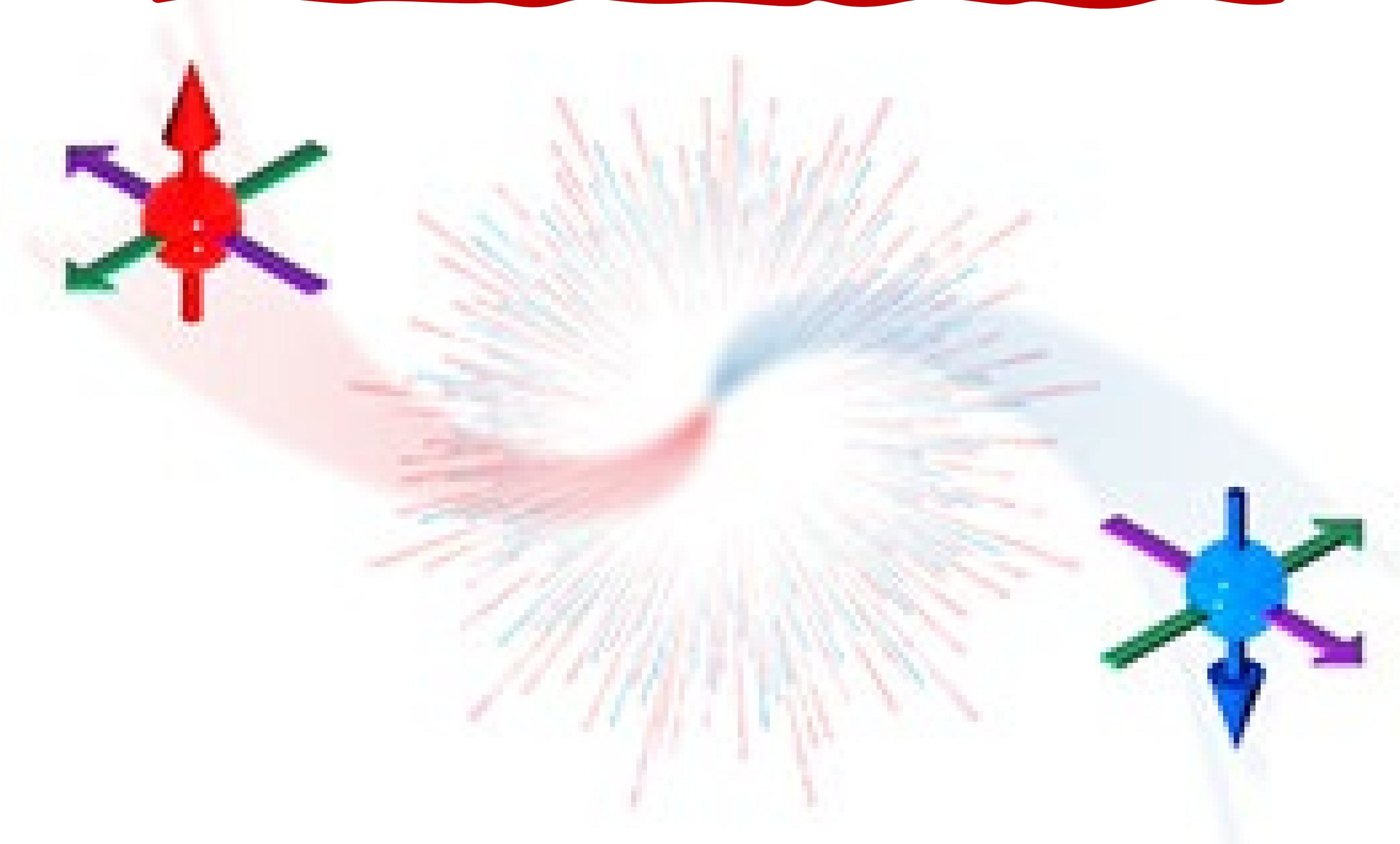
H. Kurebayashi, **J. H. Garcia**, S Khan, J. Sinova & S. Roche



Joaquin medina

Repr. Mat.	Space Group	Crystal System	$\mathbf{H^e}$	$\mathbf{H^o}$
MX_3*	$P\bar{6}2m$ (189)	Hexagonal	$\tau_{FL}\,\mathbf{J}\times\hat{\mathbf{z}}$	$\tau_{DL}\,\mathbf{m}\times(\mathbf{J}\times\hat{\mathbf{z}})+\tau_z m_z\,\mathbf{J}+\tau_{ani}\nabla_{\mathbf{m}}[\,J_y\,m_x m_y+J_x(m_y^2-m_x^2)/$
Fe_3GeTe_2*	$P\bar{6}m2$ (187)			$\tau_{DL}\,\mathbf{m}\times(\mathbf{J}\times\hat{\mathbf{z}})+\tau_z m_z\,\mathbf{J}+\tau_{ani}\nabla_{\mathbf{m}}[\,J_x\,m_x m_y+J_y(m_x^2-m_y^2)/$
$MnBi_2Te_2$	$P\bar{3}m1$ (164)	Trigonal	$\tau_{FL}\,\mathbf{J}\times\hat{\mathbf{z}}$	
MXY †	$P3m1$ (156)			$\tau_{DL}\,\mathbf{m}\times(\mathbf{J}\times\hat{\mathbf{z}})+\tau_z m_z\,\mathbf{J}+\tau_{ani}\nabla_{\mathbf{m}}[\,J_x\,m_x m_y+J_y(m_x^2-m_y^2)/$
Fe_5GeTe_2	$R\bar{3}m$ (147)			
CrI_3	$P\bar{3}1m$ (162)			$\tau_{DL}\,\mathbf{m}\times(\mathbf{J}\times\hat{\mathbf{z}})+\tau_z m_z\,\mathbf{J}+\tau_{ani}\nabla_{\mathbf{m}}[\,J_y\,m_x m_y+J_x(m_y^2-m_x^2)/2]$
$CrGeTe_3$	$P\bar{3}$ (147)	Trigonal	$\tau_{FL}^{I}\,\mathbf{J}\times\hat{\mathbf{z}}+\tau_F^{II}\,\mathbf{J}$	$\tau_{DL}^{I}\,\mathbf{m}\times(\mathbf{J}\times\hat{\mathbf{z}})+\tau_z m_z\,\mathbf{J}+\tau_{ani}^{I}\nabla_{\mathbf{m}}\left[J_y\,m_x m_y+\frac{J_x(m_x^2-m_y^2)}{2}\right]+\tau_{ani}^{II}\nabla_{\mathbf{m}}\left[J_y\,m_x m_y+\frac{J_x(m_x^2-m_y^2)}{2}\right]+\tau_o^{II}[(\mathbf{J}\times\boldsymbol{m})\cdot\hat{\mathbf{z}}]\hat{\mathbf{z}}$
FeTe †	$P4/nmm$ (129)	Tetragonal	$\tau_{FL}\,\mathbf{J}\times\hat{\mathbf{z}}$	$\tau_o\,\mathbf{m}\times(\mathbf{J}\times\hat{\mathbf{z}})+\tau_z m_z\,\mathbf{J}$
CrI_2	$P\bar{4}m2$ (115)	Orthorhombic	$\begin{pmatrix}0 & \tau_{FL}^{xy}\\ \tau_{FL}^{yx} & 0\end{pmatrix}\mathbf{J}$	$(\mathbf{M}\cdot\hat{\mathbf{z}})\begin{pmatrix}\tau_z^x & 0\\ 0 & \tau_z^y\end{pmatrix}\mathbf{J}+\mathbf{M}\cdot\begin{pmatrix}\tau_o^x & 0\\ 0 & \tau_o^y\end{pmatrix}\mathbf{J}\ \hat{\mathbf{z}}$
CrSBr	Pnmm (59)	Orthorhombic	$\begin{pmatrix}0 & \tau_{FL}^{xy}\\ \tau_{FL}^{yx} & 0\end{pmatrix}\mathbf{J}$	$(\mathbf{M}\cdot\hat{\mathbf{z}})\begin{pmatrix}\tau_z^x & 0\\ 0 & \tau_z^y\end{pmatrix}\mathbf{J}+\mathbf{M}\cdot\begin{pmatrix}\tau_o^x & 0\\ 0 & \tau_o^y\end{pmatrix}\mathbf{J}\ \hat{\mathbf{z}}$
$NiPS_3$	C2/m (12)	Monoclinic	$\begin{pmatrix}0 & \tau_{FL}^{xy} & 0\\ \tau_{FL}^{yx} & 0 & 0\\ 0 & \tau_{FL}^{yz} & 0\end{pmatrix}\mathbf{J}$	$\begin{pmatrix}M_x\,\tau_o^{x,xx}+M_z\,\tau_o^{z,xx} & M_y\,\tau_o^{y,yx} & 0\\ M_y\,\tau_o^{y,xy} & M_x\,\tau_o^{x,yy}+M_z\,\tau_o^{z,yy} & 0\\ M_z\,\tau_o^{z,xz} & 0 & 0\end{pmatrix}\mathbf{J}+\mathbf{M}\cdot\begin{pmatrix}\tau_o^{xx} & 0 & 0\\ 0 & \tau_o^{yy} & 0\\ 0 & 0 & 0\end{pmatrix}\mathbf{J}\,\hat{\mathbf{z}}$

“Spukhafte Fernwirkung!”

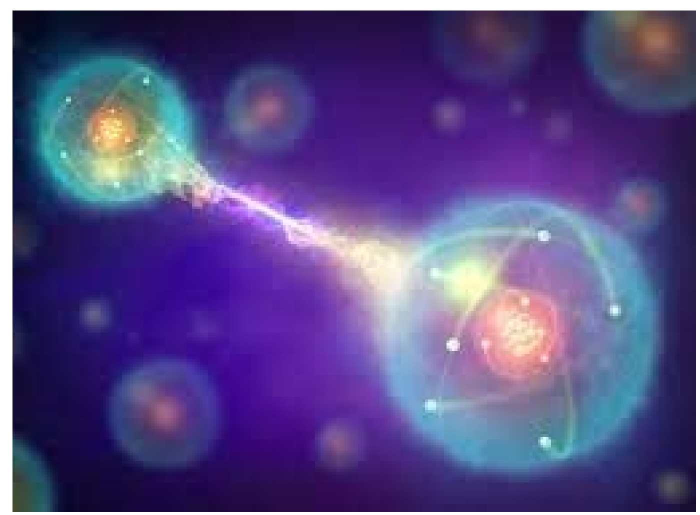


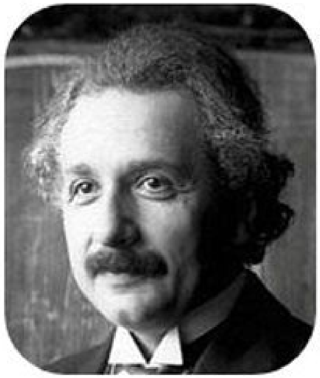
"Spukhafte Fernwirkung!"

Letter to Max Born(1947),
about the statistical approach to quantum mechanics

" *I cannot seriously believe in "it" because the theory cannot be reconciled with the idea that physics should represent a reality in space and time, free from spooky action at a distance*…"

(A. Einstein)




A. Einstein


B. Podolsky


N. Rosen

Einstein Podosly Rosen
« *thought experiment*»
Quantum Entanglement

MAY 15, 1935 PHYSICAL REVIEW VOLUME 47

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

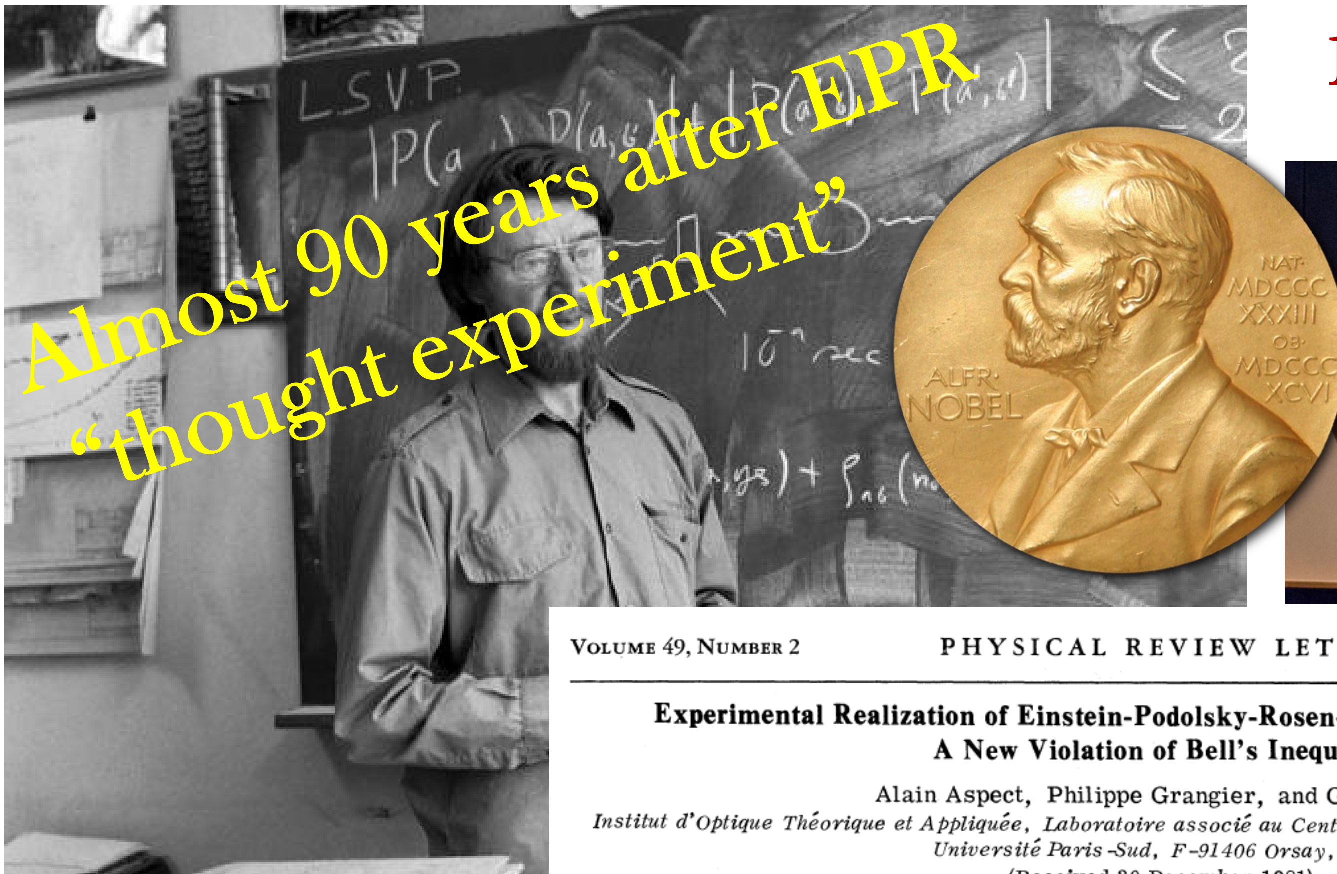
A. Einstein, B. Podolsky and N. Rosen, *Institute for Advanced Study, Princeton, New Jersey*
(Received March 25, 1935)

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-

30 years after (1964)…., John Bell proved that

no theory of nature that obeys locality and realism
can reproduce all the predictions of quantum theory



15 years after

VOLUME 49, NUMBER 2 PHYSICAL REVIEW LETTERS 12 JULY 1982

Experimental Realization of Einstein-Podolsky-Rosen-Bohm *Gedankenexperiment*: A New Violation of Bell's Inequalities

Alain Aspect, Philippe Grangier, and Gérard Roger
Institut d'Optique Théorique et Appliquée, Laboratoire associé au Centre National de la Recherche Scientifique, Université Paris-Sud, F-91406 Orsay, France

(Received 30 December 1981)

The linear-polarization correlation of pairs of photons emitted in a radiative cascade of calcium has been measured. The new experimental scheme, using two-channel polarizers (i.e., optical analogs of Stern-Gerlach filters), is a straightforward transposition of Einstein-Podolsky-Rosen-Bohm *gedankenexperiment*. The present results, in excellent agreement with the quantum mechanical predictions, lead to the greatest violation of generalized Bell's inequalities ever achieved.

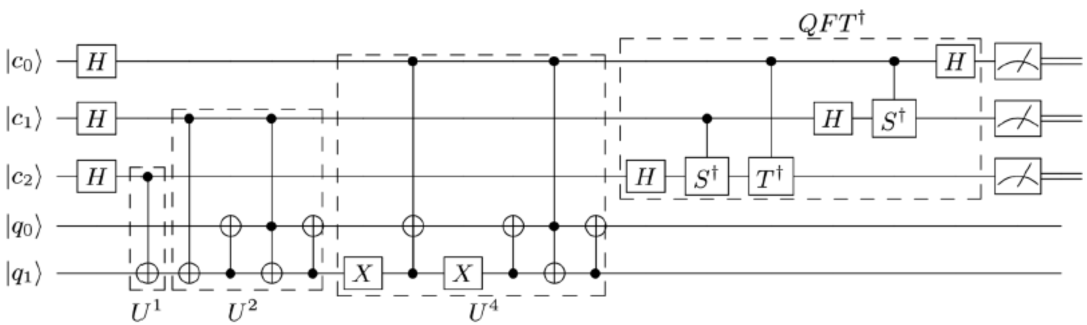
(practical?) **Quantum Computers**

- **IBM** – 400 Qubits plus quantum processor (2022)
- **D-Wave** 5000 Qubits quantum annealer
- **Microsoft** –Quantum Lab-Delft…. **"Chi l´ha visto?"**
- **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

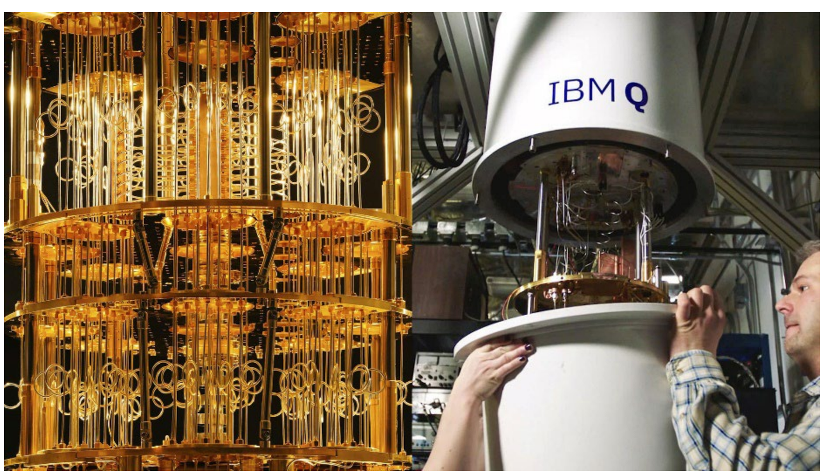
What available IBM quantum computer can do today?

Useful Quantum algortihm (Shor´s algorithm) factorizing very large number in prime numbers…(“quantum cryptography…”)



exponentially faster than the most efficient known classical factoring algorithm….

27-qubit quantum processor **ibmq_toronto**



scientific reports

Check for updates

OPEN

Demonstration of Shor’s factoring algorithm for N = 21 on IBM quantum processors

Unathi Skosana & Mark Tame

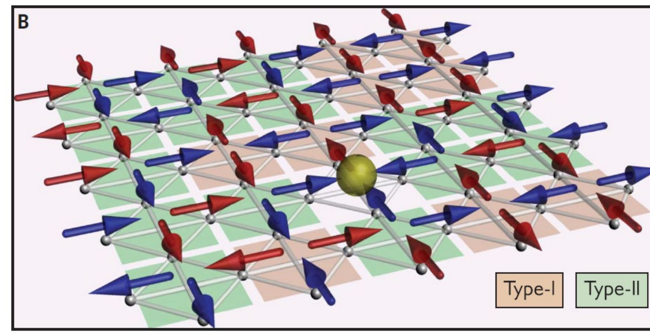
We report a proof-of-concept demonstration of a quantum order-finding algorithm for factoring the integer 21. Our demonstration involves the use of a compiled version of the quantum phase estimation routine, and builds upon a previous demonstration. We go beyond this work by using a configuration of approximate Toffoli gates with residual phase shifts, which preserves the functional correctness and allows us to achieve a complete factoring of $N = 21$. We implemented the algorithm on IBM quantum processors using only five qubits and successfully verified the presence of entanglement between the control and work register qubits, which is a necessary condition for the algorithm’s speedup in general. The techniques we employ may be useful in carrying out Shor’s algorithm for larger integers, or other algorithms in systems with a limited number of noisy qubits.

"Observation of topological phenomena in a programmable lattice of 1,800 qubits

A.D. King et al **Nature 560, 456 (2018)**

Topological quantum transition (Kosterlitz-Thouless)
Reproduced with Large scale simulation in a network of **1,800 in situ programmable superconducting niobium flux qubits**

A. D King et al., **Science 373, 576–580 (2021)**



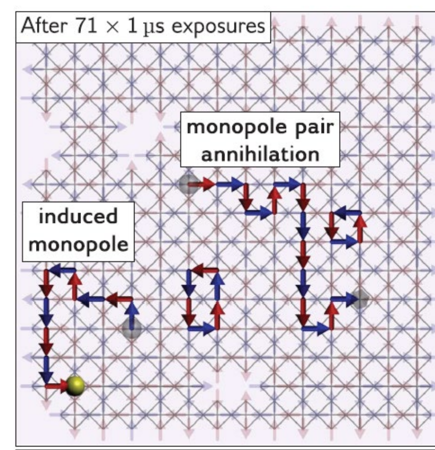
MAGNETISM

Qubit spin ice

$$\mathcal{H} = \mathcal{J}\left(\sum_{\langle ij\rangle} J_{ij}\hat{\sigma}_i^z\hat{\sigma}_j^z + \sum_i h_i\hat{\sigma}_i^z\right) - \Gamma\sum_i \hat{\sigma}_i^x$$

Andrew D. King[1*], Cristiano Nisoli[2*], Edward D. Dahl
Gabriel Poulin-Lamarre[1], Alejandro Lopez-Bezanilla[2]

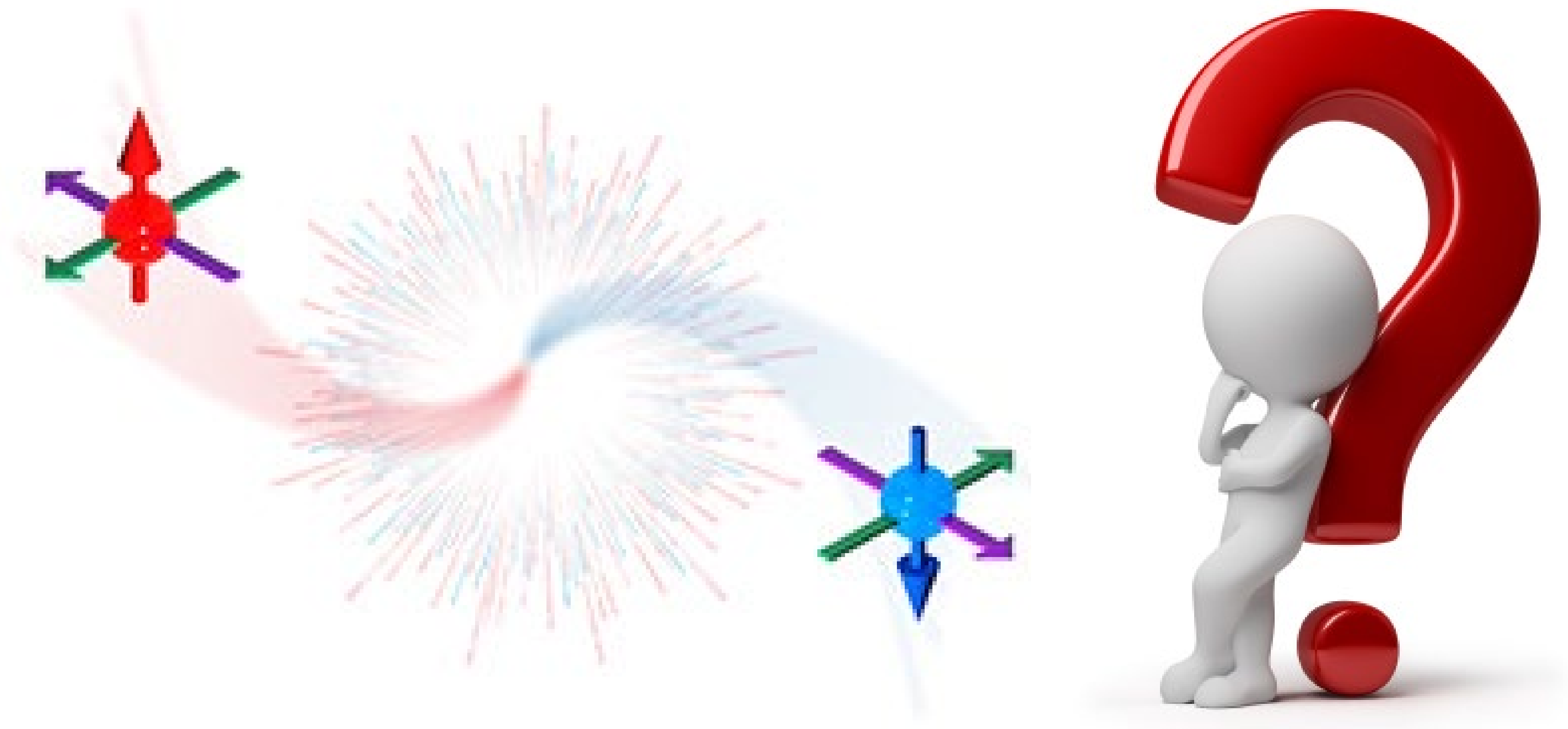
Artificial spin ices are frustrated spin systems that can be engineered, in which fine tuning of geometry and topology has allowed the design and characterization of exotic emergent phenomena at the constituent level. Here, we report a realization of spin ice in a lattice of superconducting qubits. Unlike conventional artificial spin ice, our system is disordered by both quantum and thermal fluctuations. The ground state is classically described by the ice rule, and we achieved control over a fragile degeneracy point, leading to a Coulomb phase. The ability to pin individual spins allows us to demonstrate Gauss's law for emergent effective monopoles in two dimensions. The demonstrated qubit control lays the groundwork for potential future study of topologically protected artificial quantum spin liquids.

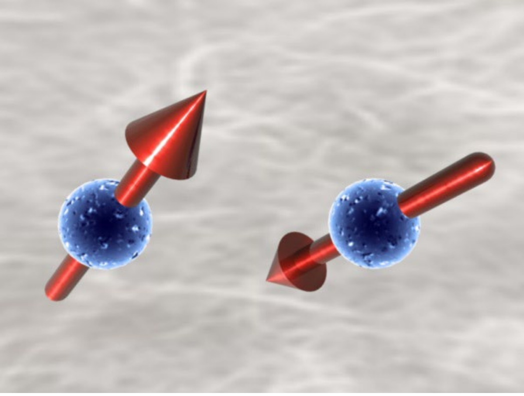


Entanglement in Quantum Matter

as a ressource for

Quantum information





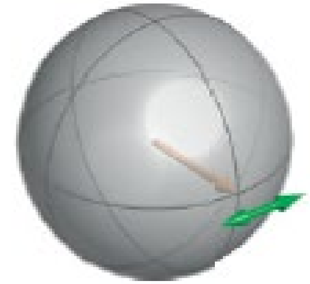
Particles in Graphene

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..

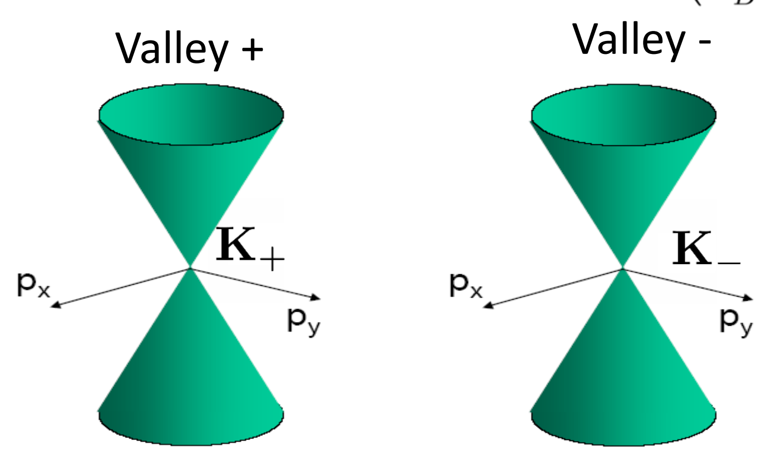
No disorder, No spin-orbit interaction

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

DIRAC Fermions

GAPLESS ***Linear energy dispersion***

and velocity 10^6m/s

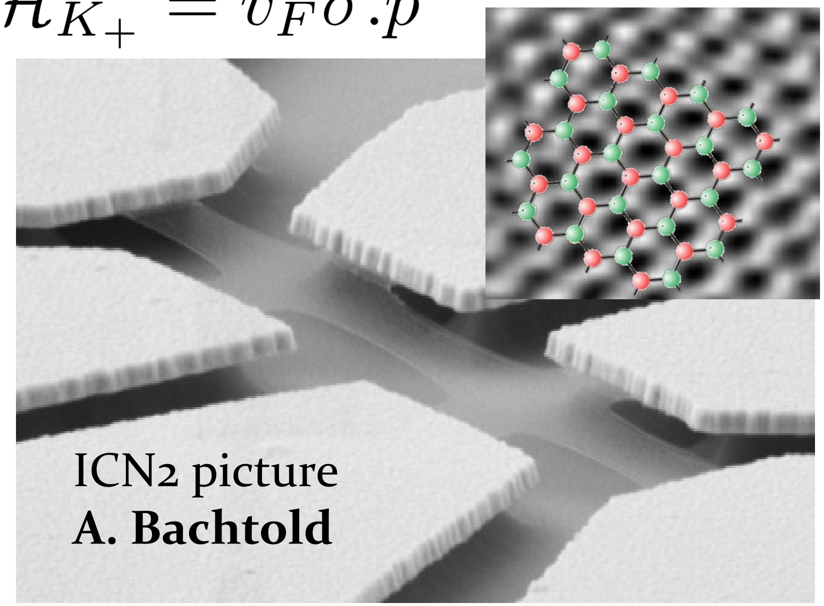


"Unique properties of Clean graphene"

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

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

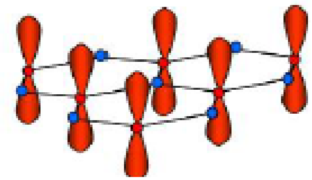
$$\mathcal{H}_{K_+} = v_F\vec{\sigma}.\vec{p}$$



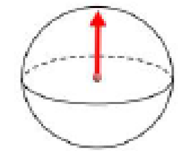
pseudospin

A sublattice : p_z

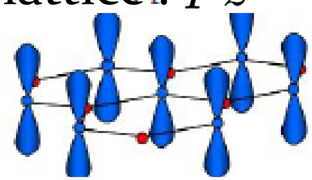
Spinor Representation



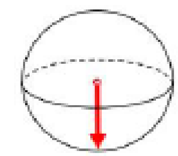
$|\Psi_A\rangle$



B sublattice : p_z



$|\Psi_B\rangle$

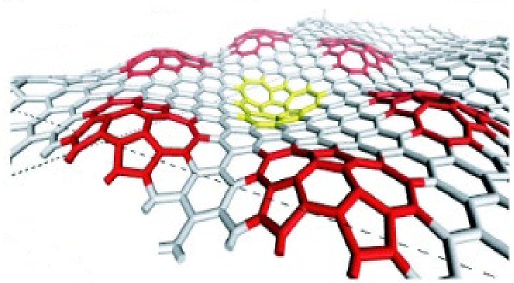


And related Berry's phase

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 ?**

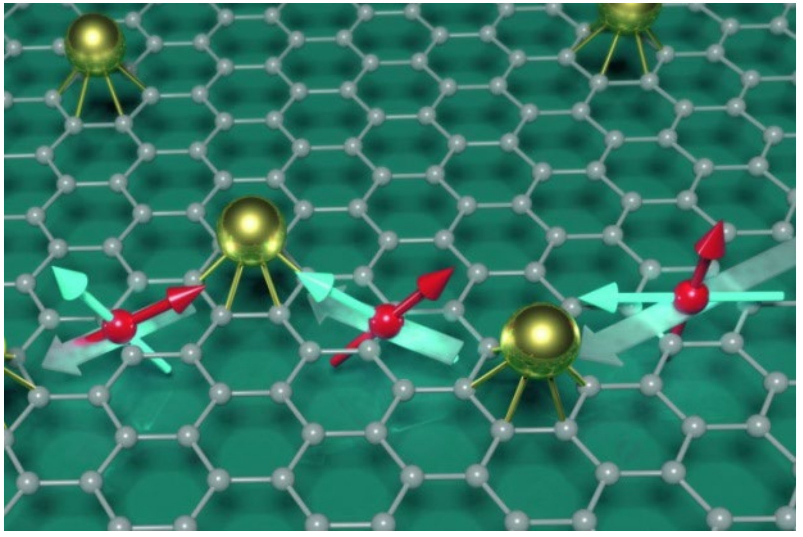
nature physics

ARTICLES

PUBLISHED ONLINE: 14 SEPTEMBER 2014 | DOI: 10.1038/NPHYS3083

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]*

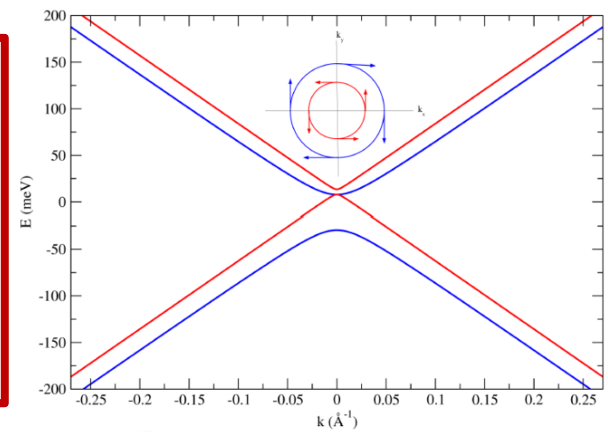


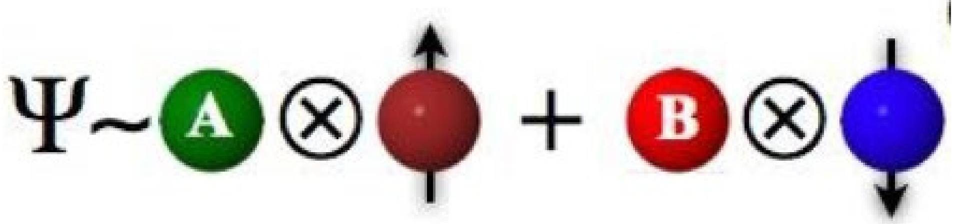
$$\vec{P}(E,t) = \frac{\langle\psi_\uparrow(t)|\,[1_\sigma\otimes\vec{s}]\,\delta(E-\mathcal{H}^{\text{eff}}) + \delta(E-\mathcal{H}^{\text{eff}})\,[1_\sigma\otimes\vec{s}]\;|\psi_\uparrow(t)\rangle}{2\langle\psi_\uparrow(t)|\delta(E-\mathcal{H}^{\text{eff}})\;|\psi_\uparrow(t)\rangle}$$

Spin-Pseudospin entanglement

$$
\begin{aligned}
h_0(\vec{k}) &= \hbar v_F(\eta\sigma_x k_x + \sigma_y k_y) \otimes 1_s \\
h_R(\vec{k}) &= \bar{\lambda}_R\left(\eta\left[\sigma_x \otimes s_y\right] - \left[\sigma_y \otimes s_x\right]\right) \\
h_I(\vec{k}) &= \bar{\lambda}_I\eta\left[\sigma_z \otimes s_z\right]
\end{aligned}
$$

$$
\begin{aligned}
\Psi^{I}_{\vec{k},\pm} &= \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes |\uparrow\rangle \pm \begin{pmatrix} i \\ 0 \end{pmatrix} \otimes |\downarrow\rangle \\
\Psi^{II}_{\vec{k},\pm} &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes |\uparrow\rangle \pm \begin{pmatrix} 0 \\ i \end{pmatrix} \otimes |\downarrow\rangle
\end{aligned}
$$

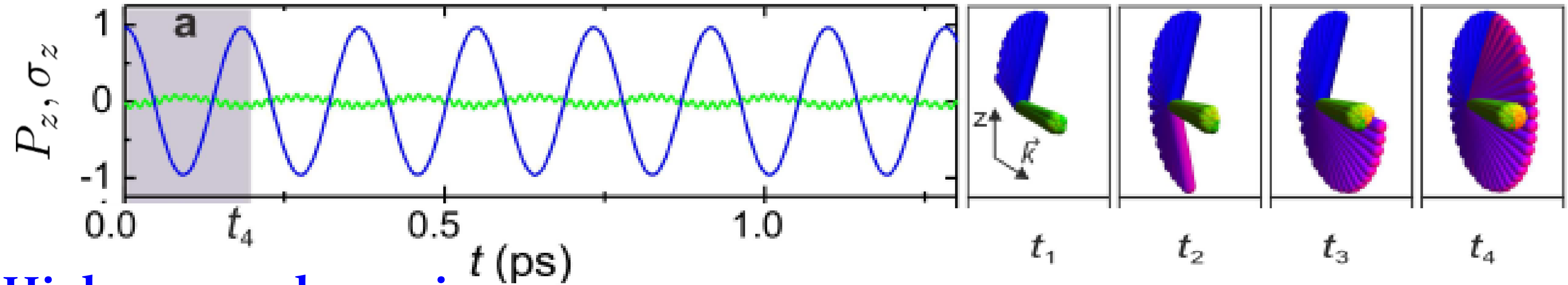




a change in sublattice (pseudospin) index entails a change in spin index

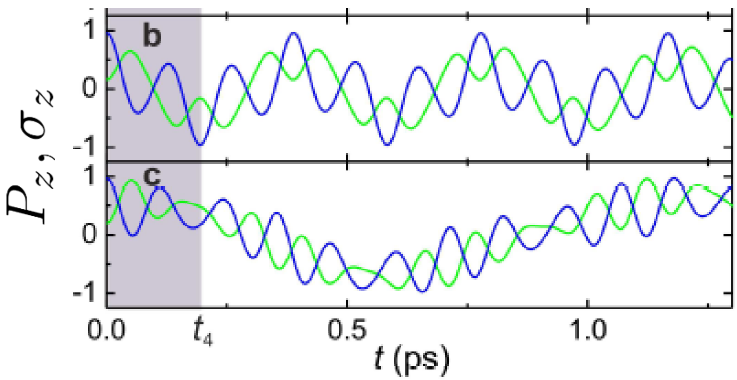
Low energy spin and pseudospin are completely locked

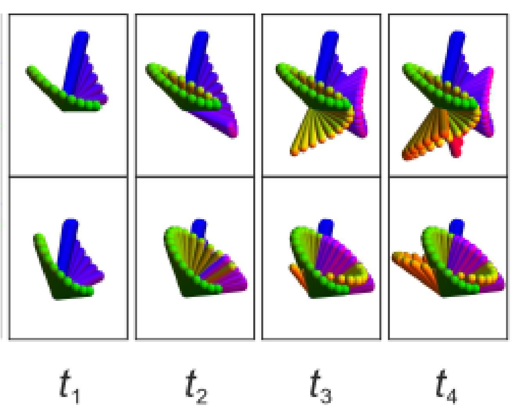
Spin-Pseudospin dynamics

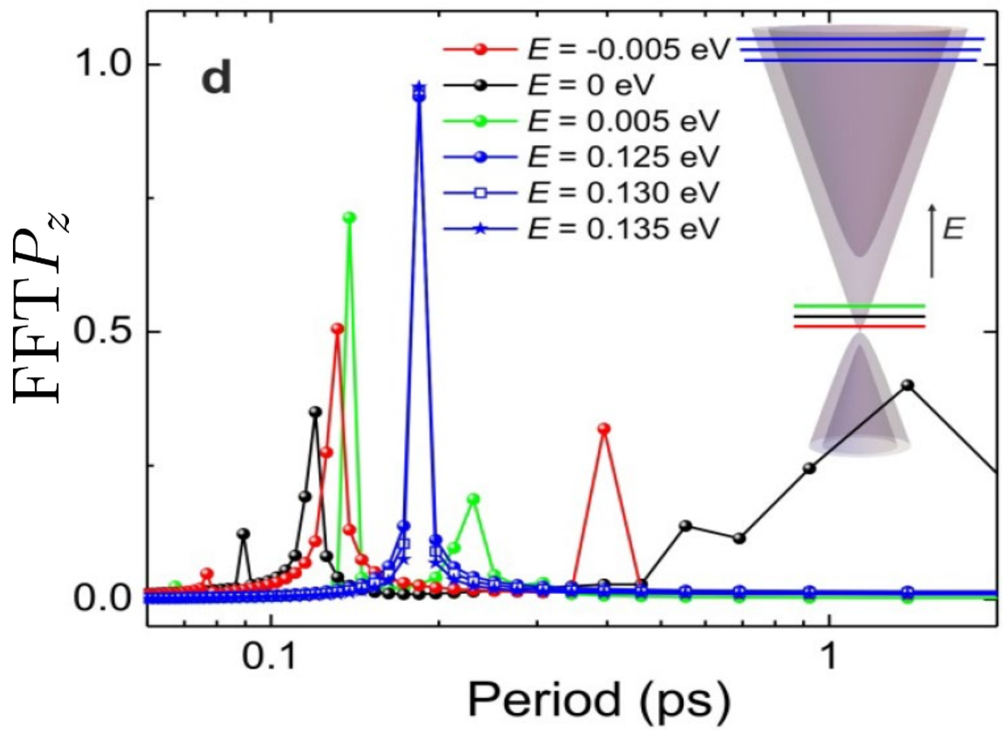


High energy dynamics

Low-energy dynamics

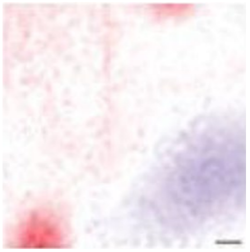






Stronger dephasing at Dirac point

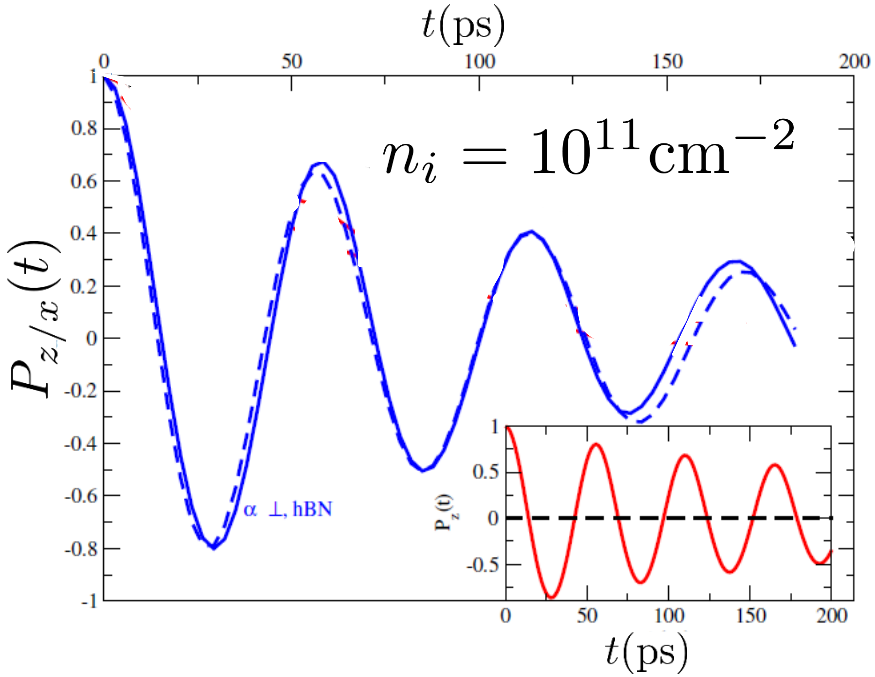
Dephasing results combination of non-uniform spin precession freq and broadening



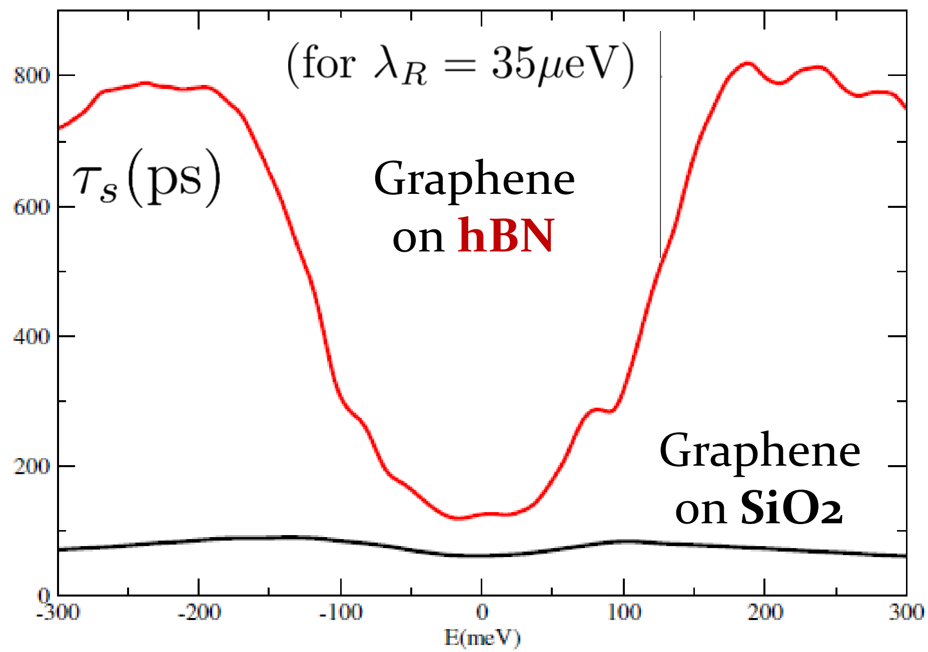
Graphene on hBN

electron-hole puddles drive the relaxation

$$\tau_p^{\mathrm{hBN}}/T_\Omega \geq 1$$



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



Dephasing driven by an
entangled dynamics between spin and pseudospin

$$\tau_s(E) \approx 4T_\Omega \approx 4\frac{\pi\hbar}{\lambda_R}$$

$$\tau_s \simeq 1 - 10 \text{ ns}$$

(for $\lambda_R \to 5\mu\mathrm{eV}$)

D. Van Tuan et al, **Nature Physics 10, 857 (2014)**
,, **Sci. Reports 6, 21046 (2016)**
A.W. Cummings and SR, **PRL 116, 086602 (2016)**

PHYSICAL REVIEW B **102**, 041403(R) (2020)

Rapid Communications

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

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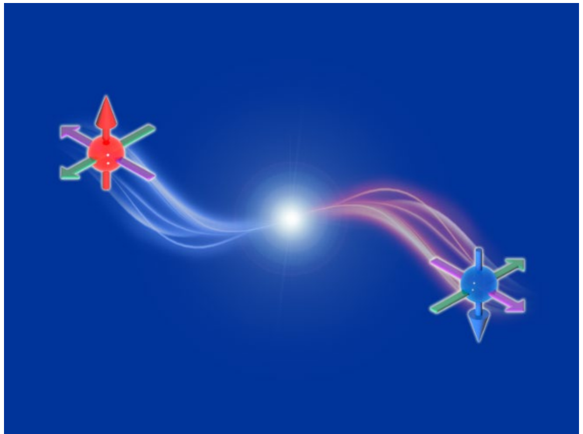
We demonstrate the emergence and dynamics of intraparticle entanglement in massless Dirac fermions. This entanglement, generated by spin-orbit coupling, arises between the spin and sublattice pseudospin of electrons in graphene. The entanglement is a complex dynamic quantity but is generally large, independent 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)

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

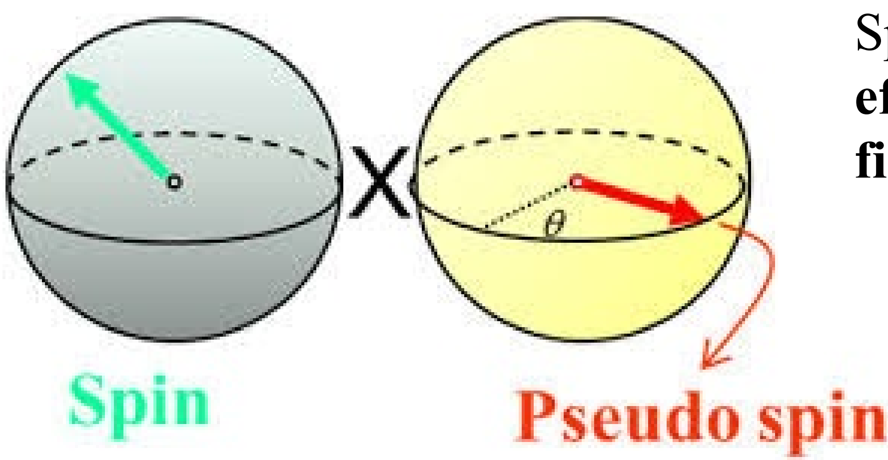
diagonalising an operator R which is built from the general ***two-qubit*** *density matrix*

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

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)

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



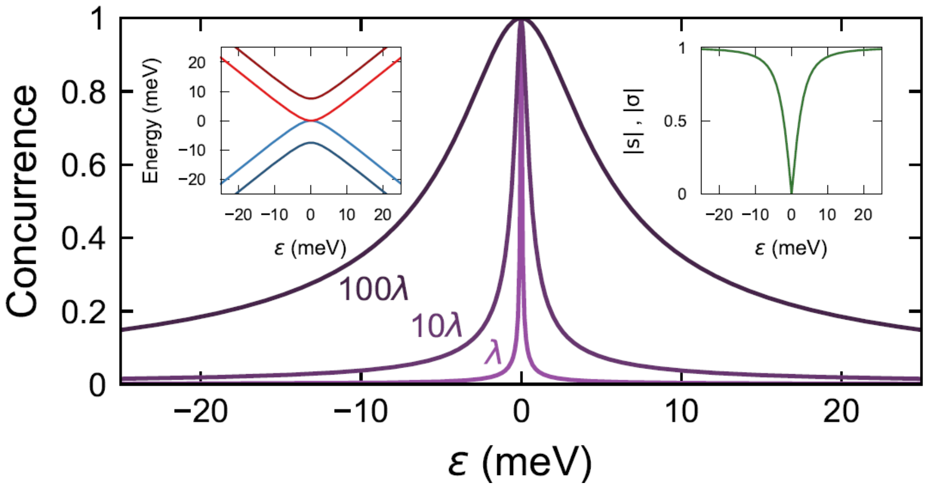
Spin and pseudospin will precess around **effective magnetic and pseudomagnetic fields** (oscillation freq. $\omega_{\mathrm{R}} = 2\lambda_{\mathrm{R}}/\hbar$)

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

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

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

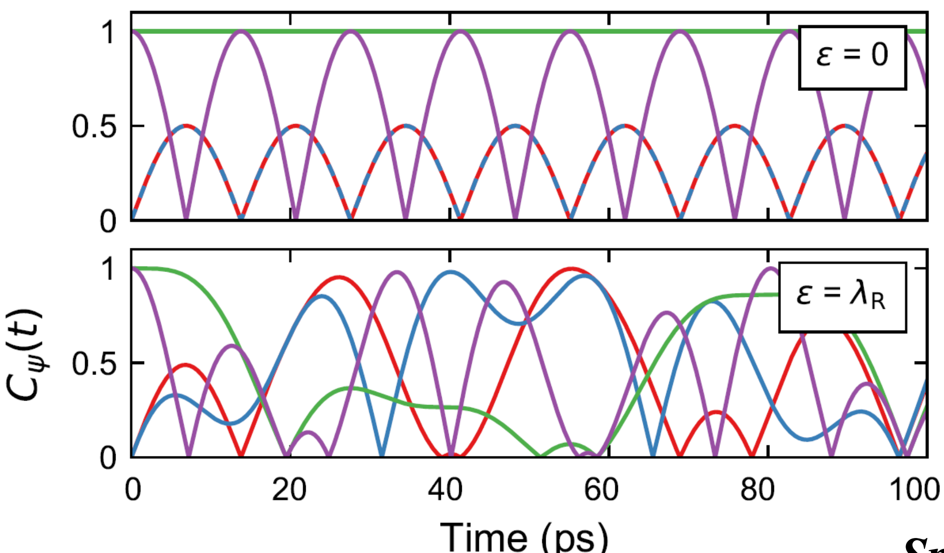
$$\hat{\mathcal{H}} = \hbar v_{\mathrm{F}} \left(\tau \hat{\sigma}_x k_x + \hat{\sigma}_y k_y \right) \otimes \hat{s}_0 + \lambda_{\mathrm{R}} \left(\tau \hat{\sigma}_x \otimes \hat{s}_y - \hat{\sigma}_y \otimes \hat{s}_x \right)$$



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

In the eigenstates basis of H

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



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

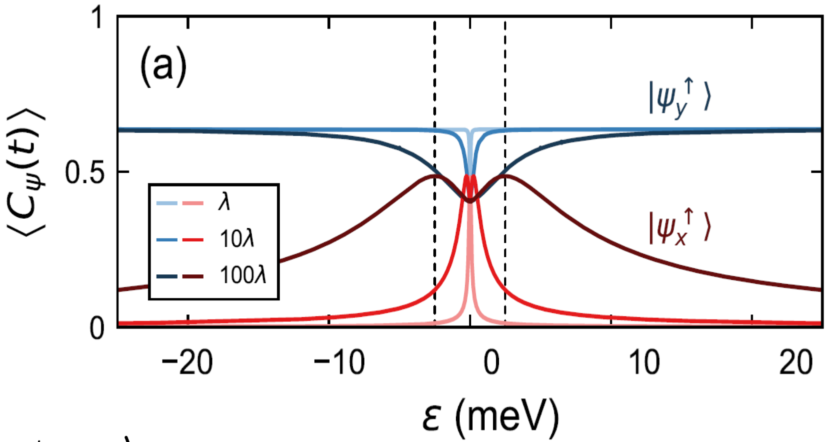
Time-evolution of concurrence
for different initial states

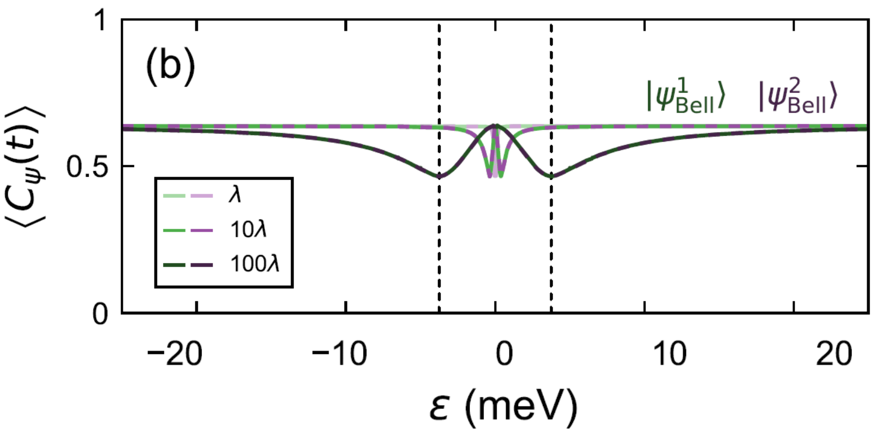
$$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 & 0 & 0 \end{bmatrix}^{\mathrm{T}} = \frac{1}{\sqrt{2}} \left(|A\rangle + |B\rangle \right) \otimes |\uparrow\rangle = |\psi_x^{\uparrow}\rangle$$

pseudospin along x, spin along z

States initially unentangled acquired
Spin-pseudospin entanglement during propagation

Emergence, persistent & robust spin-pseudospin entanglement



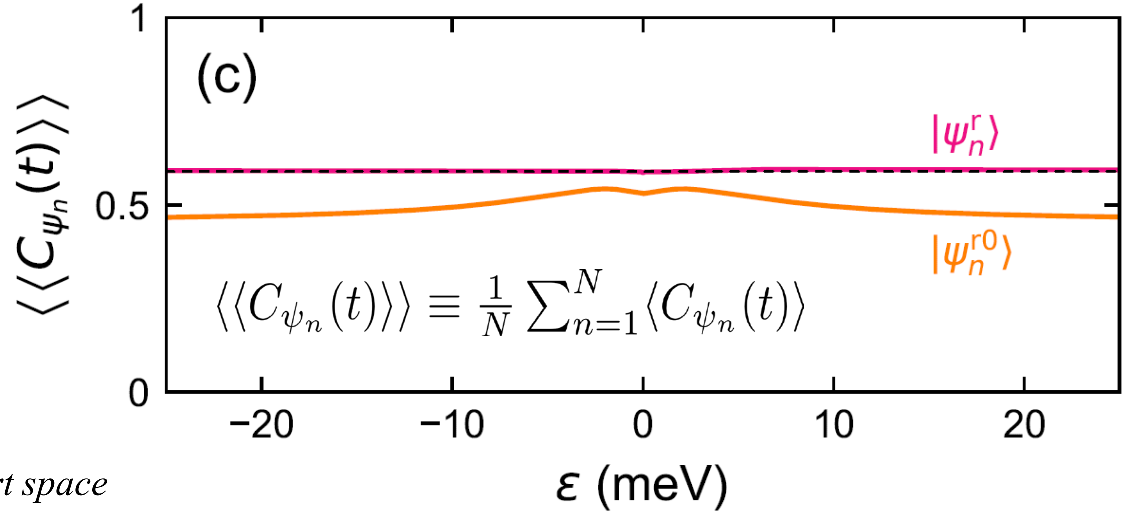


$$|\psi_n^{r_0}\rangle$$

*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



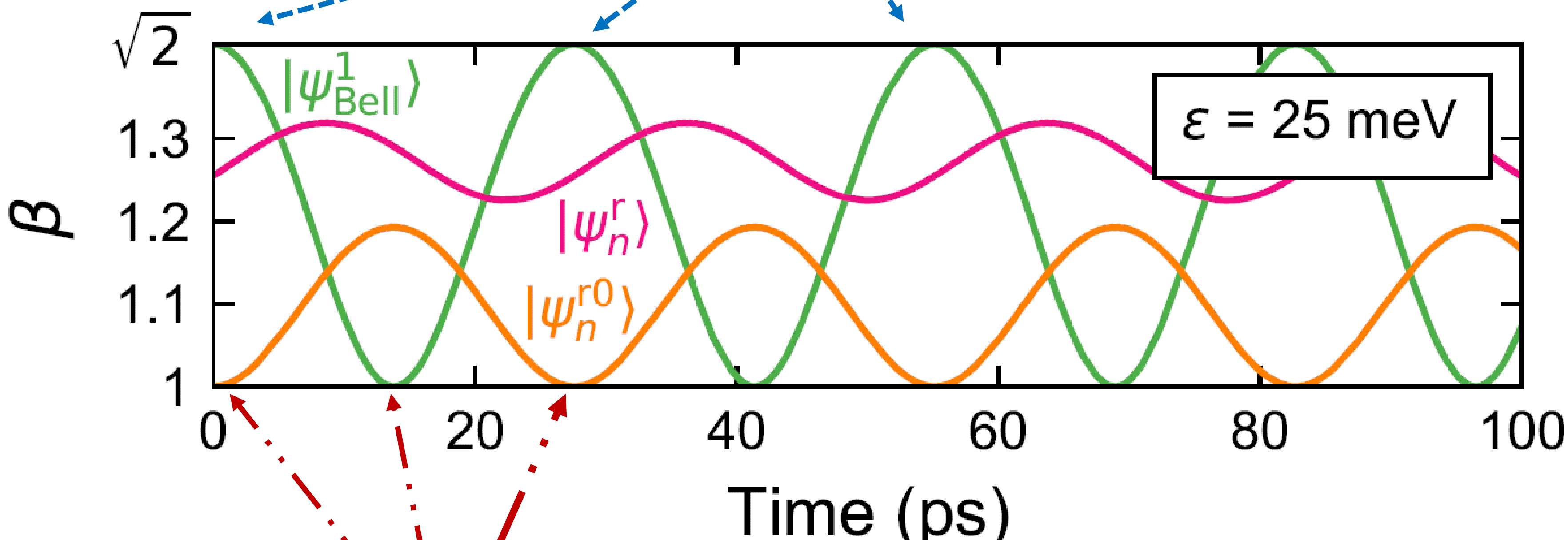
Even arbitrarily initial state develops a final entanglement

(entanglement resilient to scattering)

Time-dependent violation of the Bell inequality
(CHSH variant)

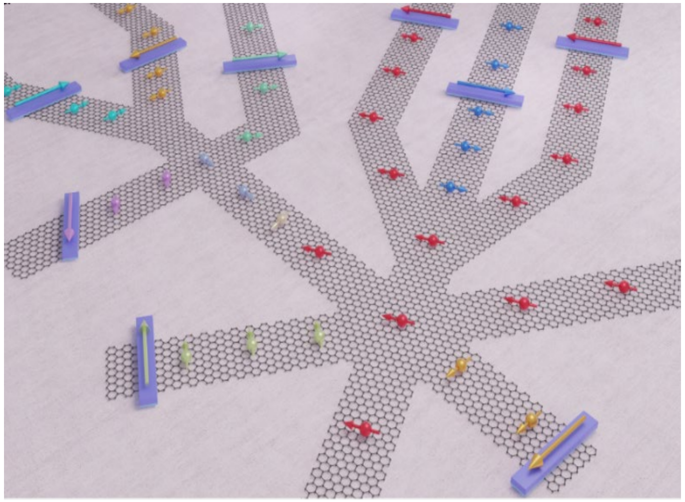
$$\beta = \sqrt{1 + C_\psi^2}$$

Maximally entangled states



Unentangled states

Whatever the initial state
There is always an emerging intraparticle entangelement ressource generated during the dynamics

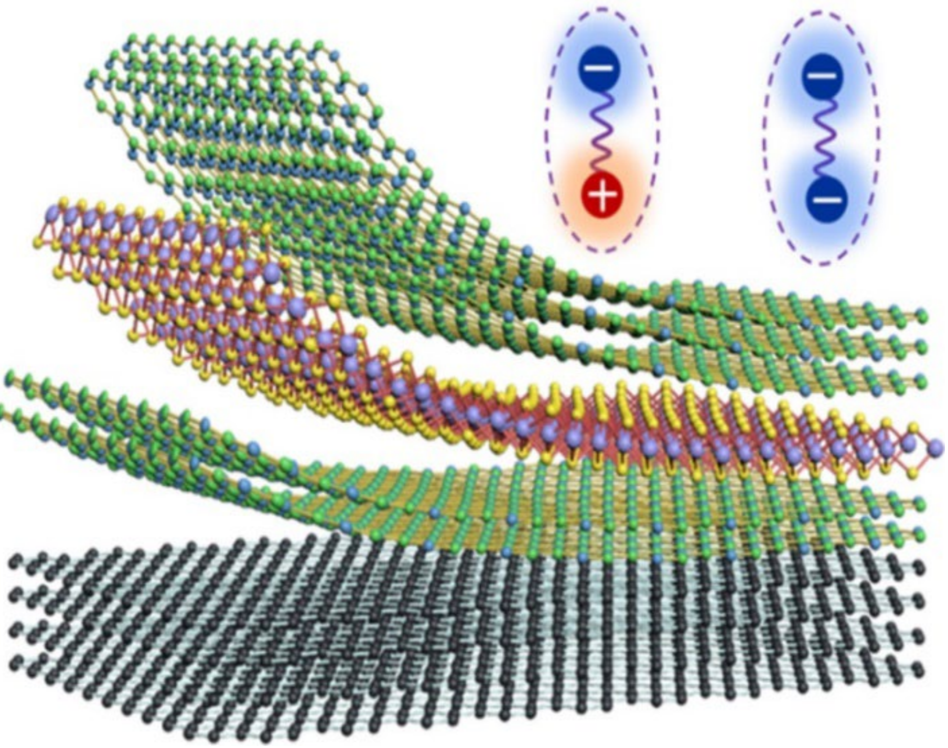


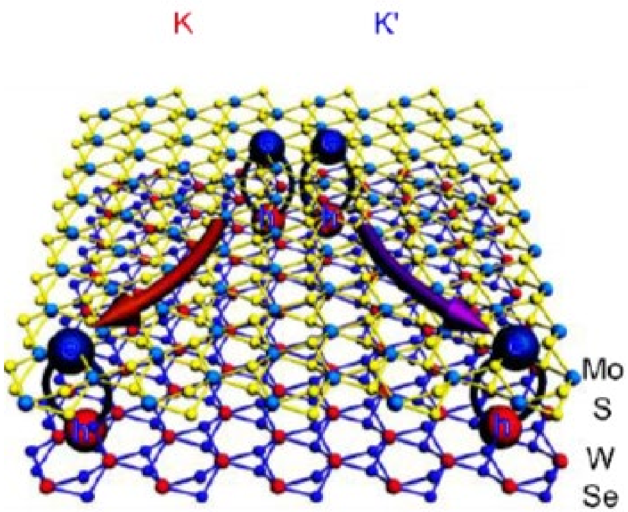
Van der Waals heterostructures
Dirac-Topological Matter

*opportunities to **manipulate DoFs by external fields***
(electromagnetic, deformation fields, proximity effects…)

Two (more)-particle entanglement

generation, manipulation & detection
using intraparticle vs interparticle DoFs





Time-evolution of non-local correlations

Conference and Advanced School on Low-Dimensional Quantum Systems

ICTP

Slides available upon request

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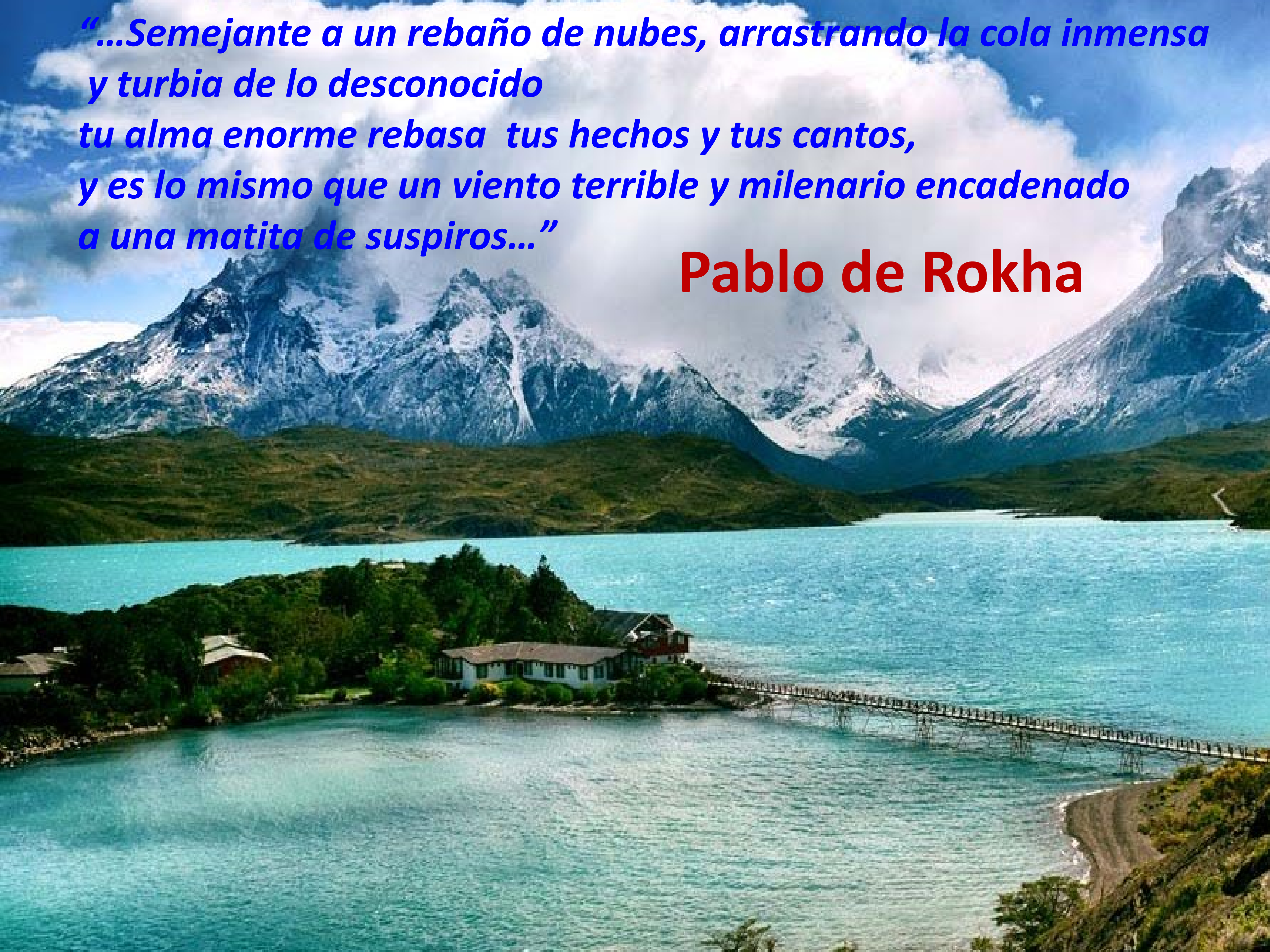
"…Semejante a un rebaño de nubes, arrastrando la cola inmensa
y turbia de lo desconocido
tu alma enorme rebasa tus hechos y tus cantos,
y es lo mismo que un viento terrible y milenario encadenado
a una matita de suspiros…"
Pablo de Rokha