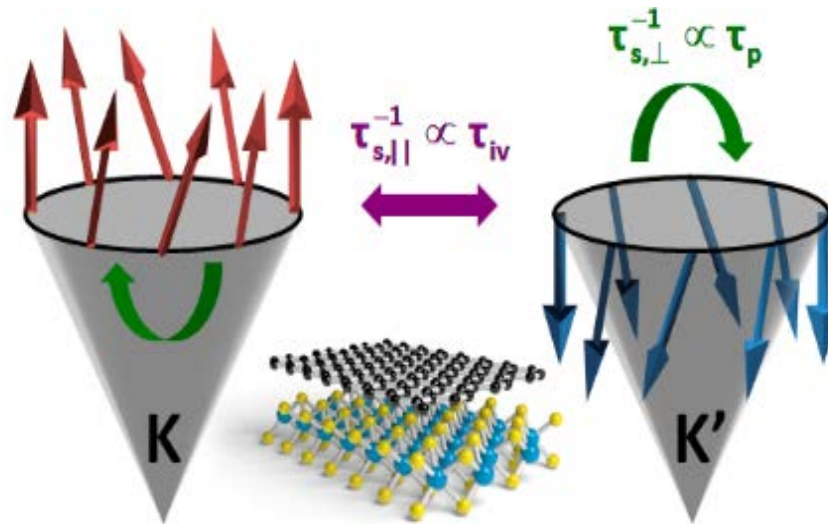


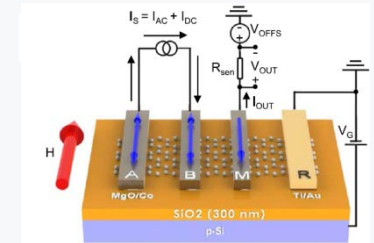
Recent Theoretical Advances in Graphene Spintronics

Stephan Roche

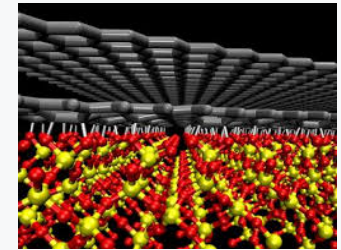


OUTLINE

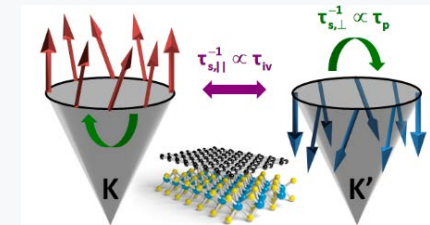
Why Spintronics using 2D Materials ?



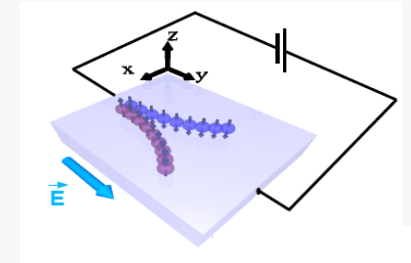
How the substrate controls spin dynamics?



*Giant spin transport anisotropy
in graphene induced by strong SOC
Proximity effect*



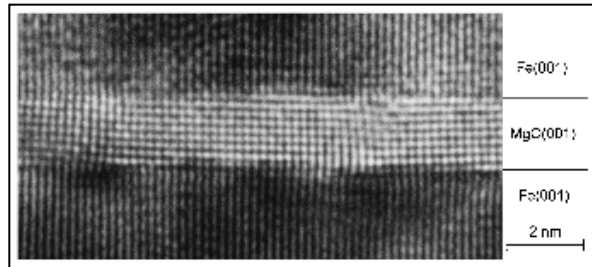
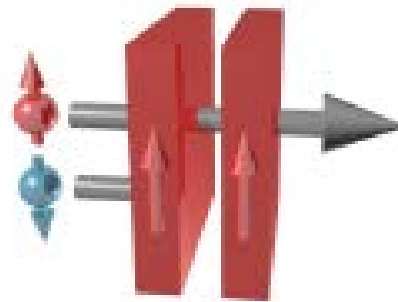
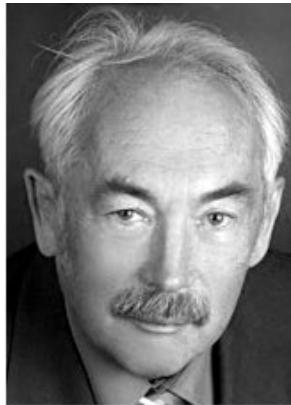
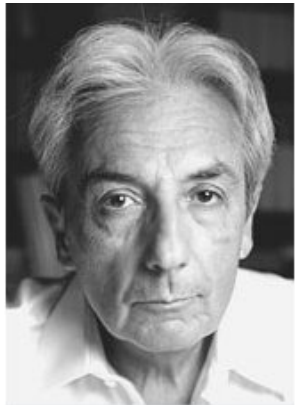
*Weak antilocalization & Spin Hall Effect
in Graphene/TMDC*



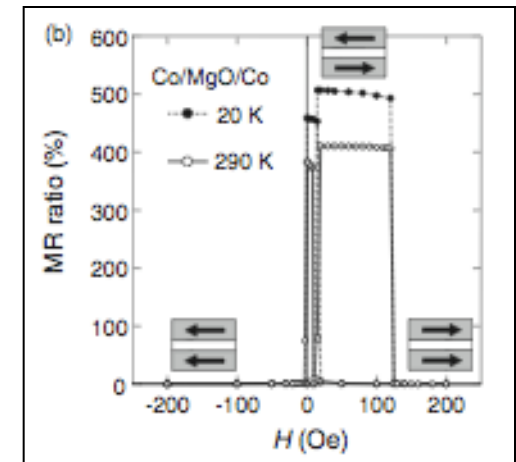
Spintronics and its industrial/Societal impact

Albert Fert

Peter Grünberg



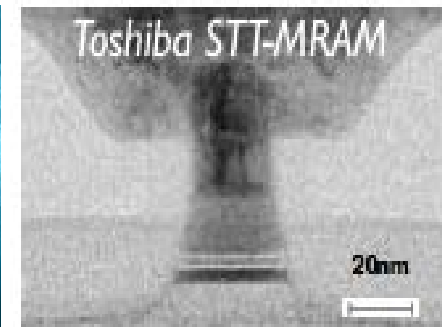
$$MR = \frac{R_{AP} - R_P}{R_P}$$



*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)

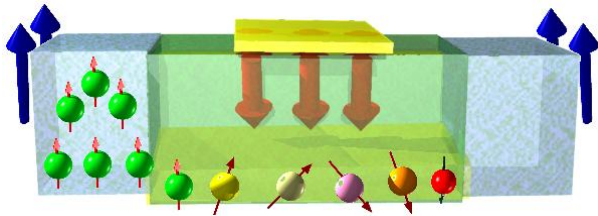
Spin transfer Torque MRAM



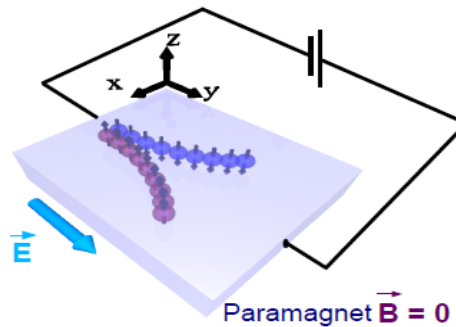
Spin-based information processing ?

Active devices based on **Spin manipulation** ?

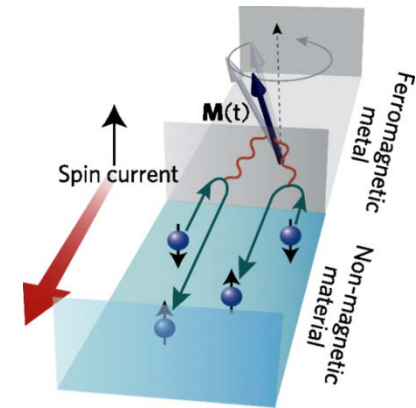
**Datta-Das
spin transistor**



Spin Hall Effect



Spin torques

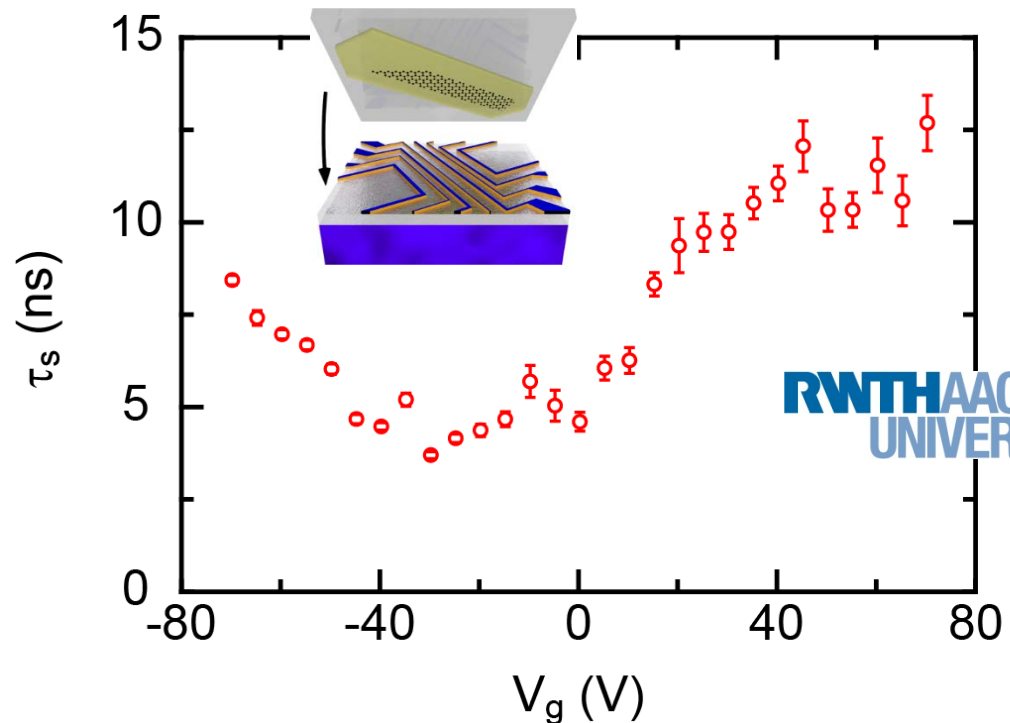
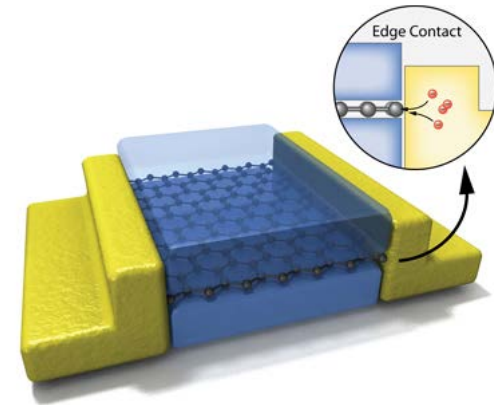
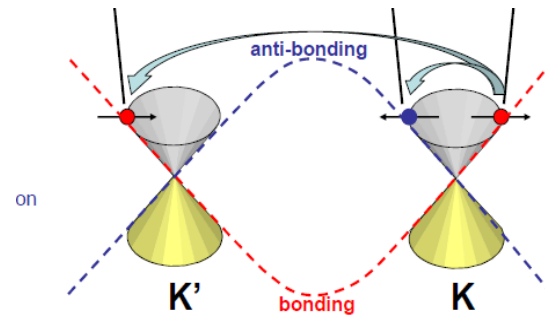


**Need for spin information transport on long distance (room T)
Spin injection and detection (ferromagnets/non magnetic materials)**

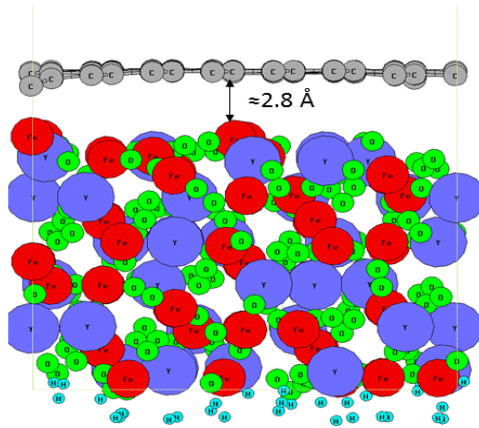
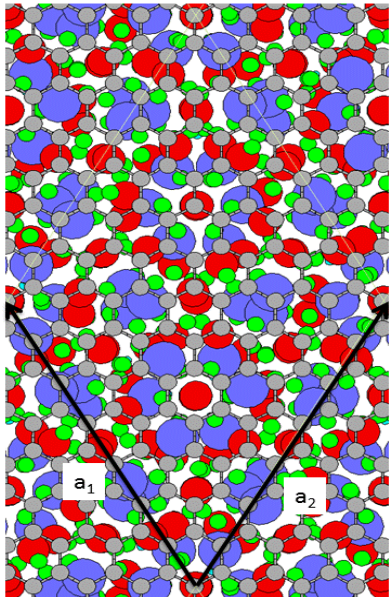
Metals/semiconductors... short spin diffusion length
(spin lifetime 0.1-1ns), 1% (or below) of MR signal

What makes graphene attractive

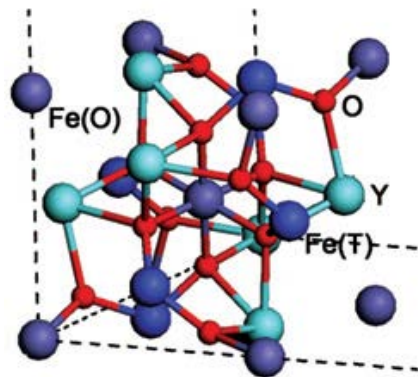
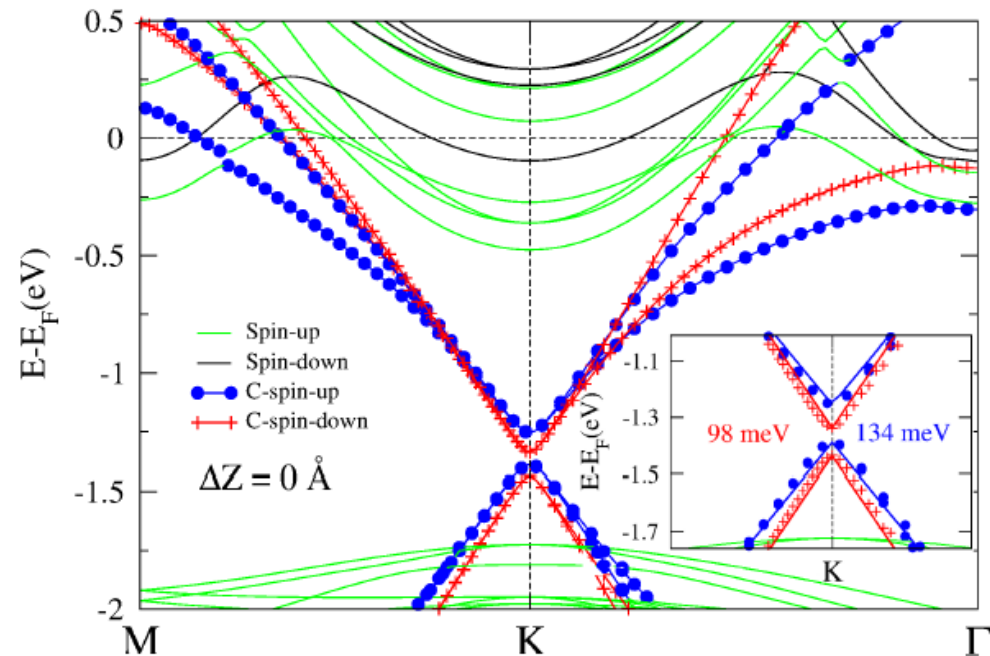
- Ambipolar/tuneable transport
- **Large mobilities**
($> 100\text{k cm}^2/\text{V.s}$ at RT, $1\text{M cm}^2/\text{V.s}$ at 4K)
- **Low spin-orbit interaction**
- Graphene properties can be tailored by proximity effects



Graphene/EuO and Graphene/Y₃Fe₅O



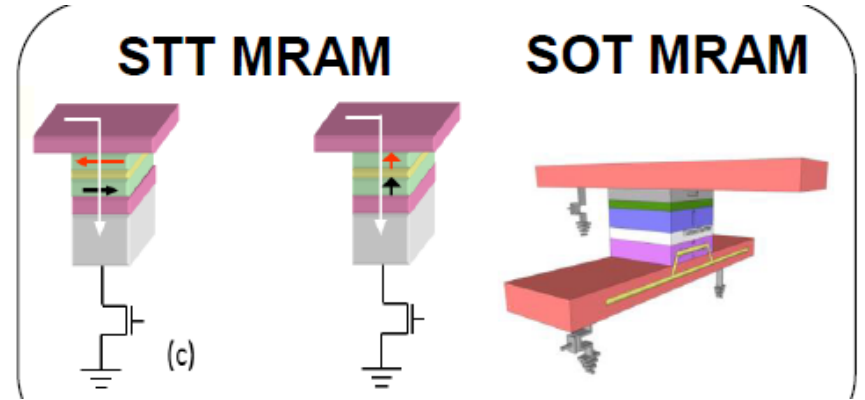
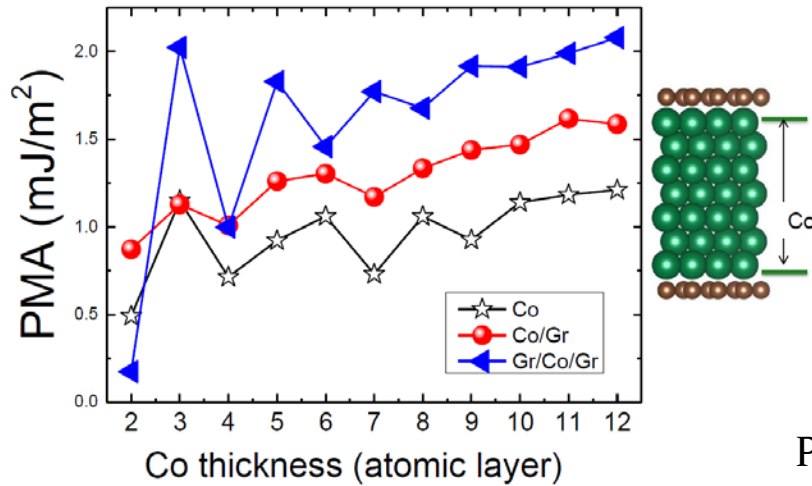
Spin Filtering and Exchange Splitting Gaps



Exchange splitting (G/YIG) = 40 meV

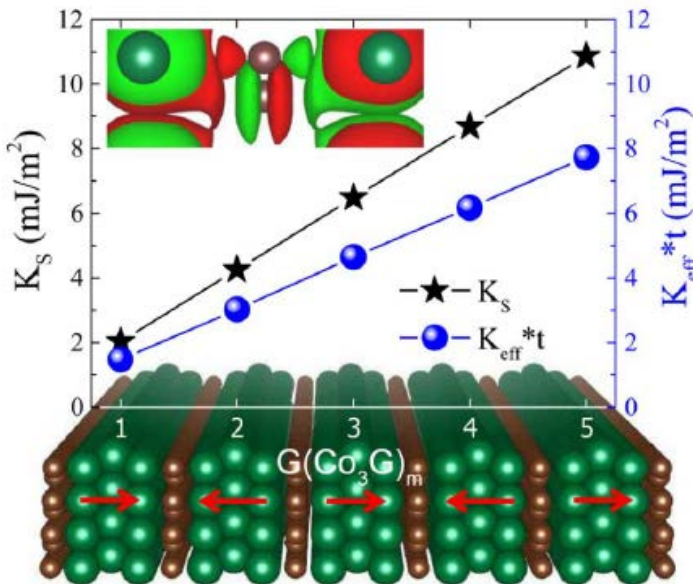
Yang, Hallal, Waintal, Roche, Chshiev, *PRL* **110**, 046603 (2013)
Hallal et al. *2D materials* **4**, 025074 (2017)

Potential of 2d Materials for STT-MRAM technologies



Perpendicular Magnetic Anisotropy in FM/Ox and FM/Graphene interfaces :
Strongly enhanced PMA of Co realized by graphene coating

Layer and orbital resolved contributions unveil the PMA mechanisms
Superlattice structures to obtain Giant PMA



$$K_{eff} = \frac{K_s}{t_{Co}} - E_{demag}$$

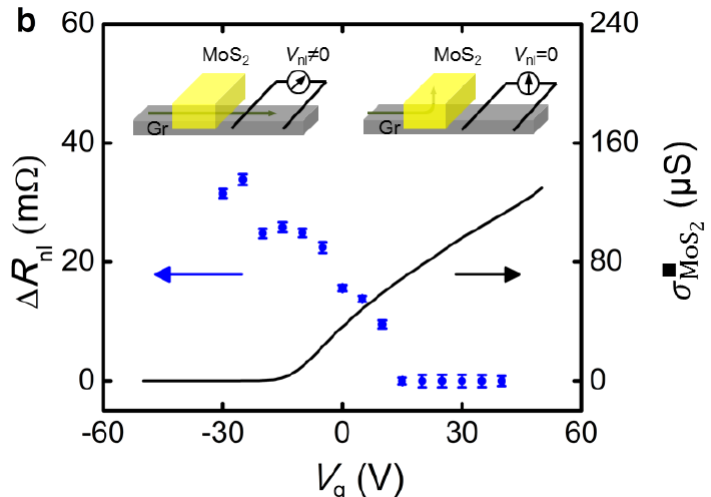
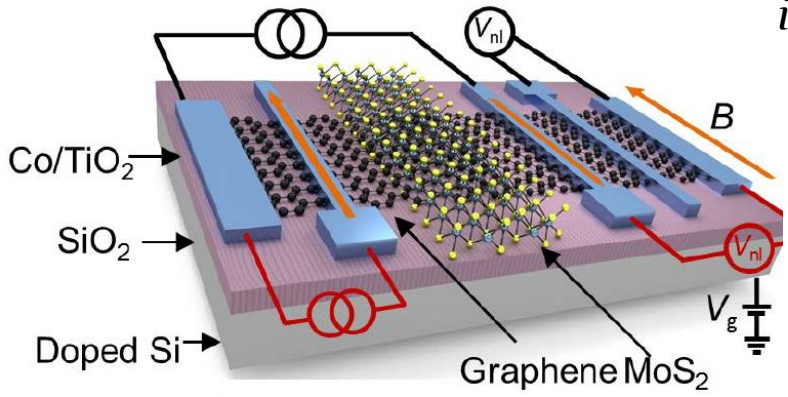
Yang, Chshiev et al, **Nano Letters** 16, 145 (2015)

Graphene-based Spintronic logic demonstrators

W. Yan et al.

Nature Comm. 7, 13372 (2016)

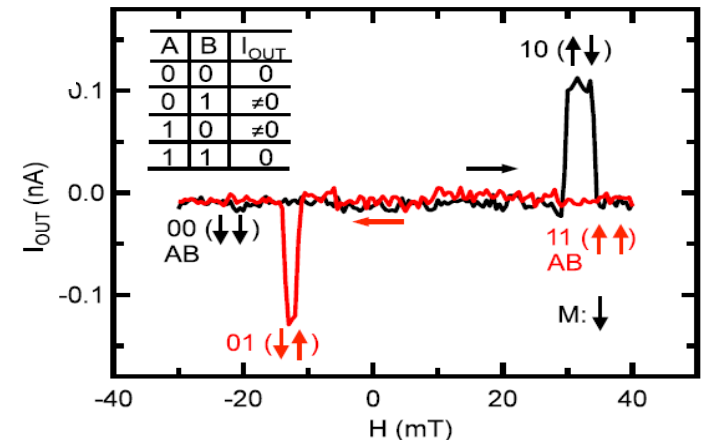
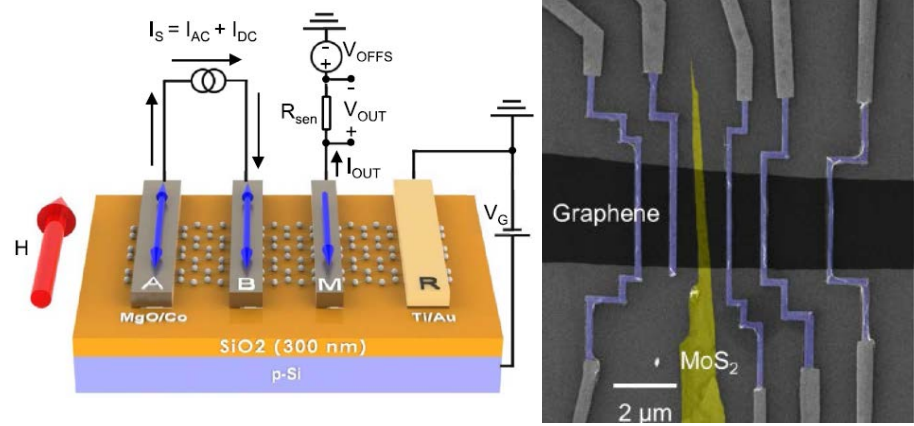
SPIN-FET



Hua Wen et al.

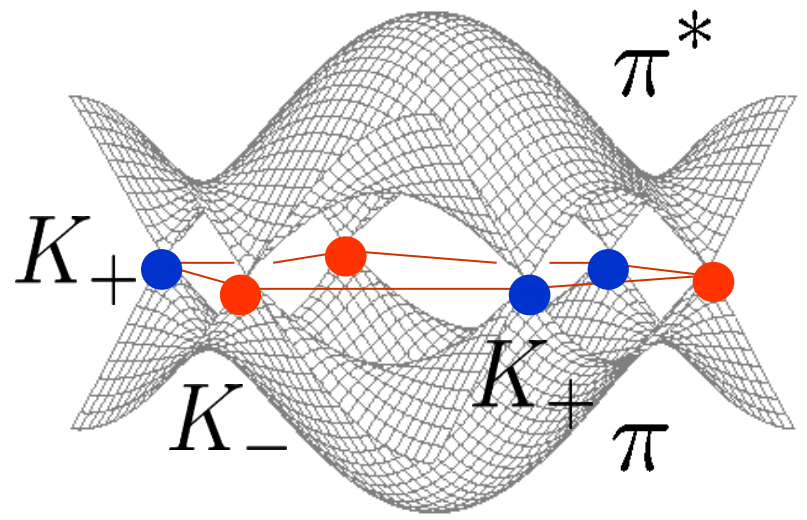
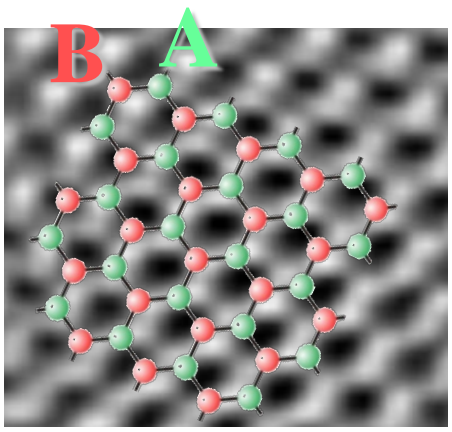
Phys. Rev. Applied 5, 044003 (2016)

Experimental demonstration of XOR operation in graphene Magnetologic Gates at room temperature



Massless Dirac Fermions in 2D graphene

Sublattice Pseudospin (and valley isospin) & spin quantum degrees of freedom

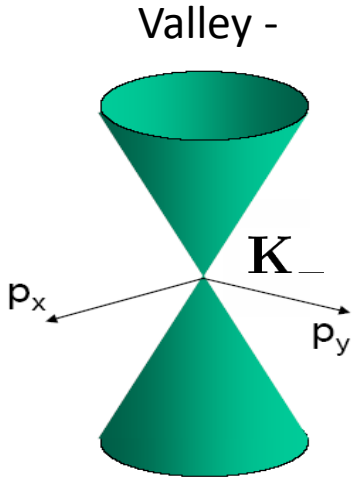
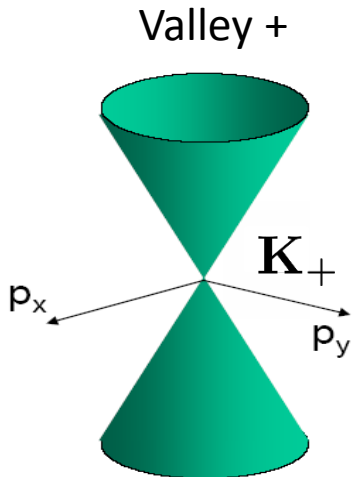


Two valleys -Sublattices A and B - Spin 1/2

*Full effective Hamiltonian for low-energy properties
(8-components wavefunction)*

$$\left(\begin{array}{cccccccc}
 0 & p_x - ip_y & 0 & 0 & 0 & 0 & 0 & 0 \\
 p_x - ip_y & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & -p_x + ip_y & 0 & 0 & 0 & 0 \\
 0 & 0 & -p_x + ip_y & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & 0 & p_x - ip_y & 0 & 0 \\
 0 & 0 & 0 & 0 & p_x - ip_y & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & 0 & 0 & 0 & -p_x + ip_y \\
 0 & 0 & 0 & 0 & 0 & 0 & -p_x + ip_y & 0
 \end{array} \right) \begin{pmatrix} \Psi_{A,+}^{\uparrow} \\ \Psi_{B,+}^{\uparrow} \\ \Psi_{A,-}^{\uparrow} \\ \Psi_{B,-}^{\uparrow} \\ \Psi_{A,+}^{\downarrow} \\ \Psi_{B,+}^{\downarrow} \\ \Psi_{A,-}^{\downarrow} \\ \Psi_{B,-}^{\downarrow} \end{pmatrix}$$

Massless Dirac Fermions in 2D graphene



$$\vec{Q} = K_+ + \vec{p}/\hbar$$

linearization close to Fermi level

Two valleys -> Dirac cones

$$E(\vec{p}) = v_F |\vec{p}|$$

$$\mathcal{H}_{K_+} = v_F \vec{\sigma} \cdot \vec{p} = v_F (p_x \sigma_x + p_y \sigma_y)$$

Pseudo-spinors are eigenstate of the **helicity operator**

$$\hat{h} = \frac{1}{2} \vec{\sigma} \cdot \frac{\vec{p}}{|\vec{p}|}$$

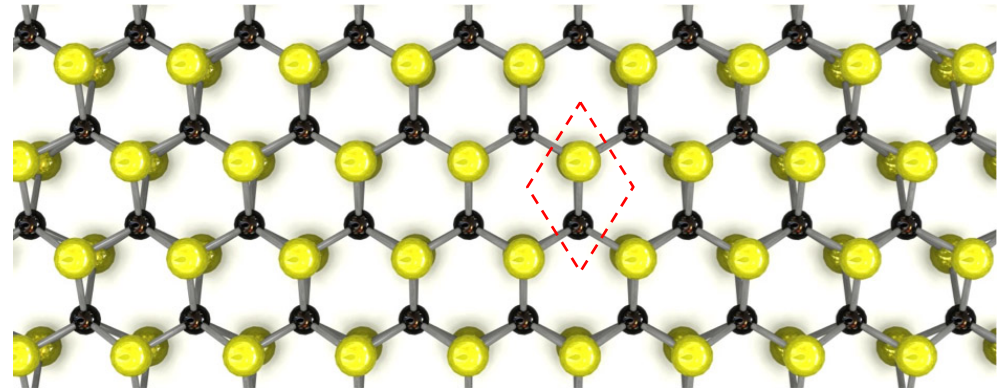
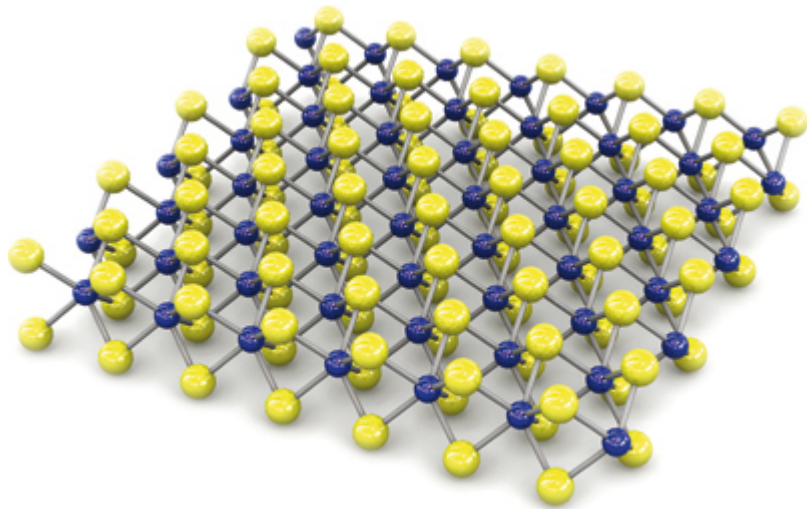
$$\Psi_{\vec{p}} = \frac{1}{\sqrt{2}} \left(\Psi_{\vec{p}}(A) \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \Psi_{\vec{p}}(B) \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right) = \frac{1}{\sqrt{2}} \begin{pmatrix} s e^{i\theta_p/2} \\ e^{-i\theta_p/2} \end{pmatrix}$$

“pseudospin” = sublattice index : **up (on A) / down (on B)**

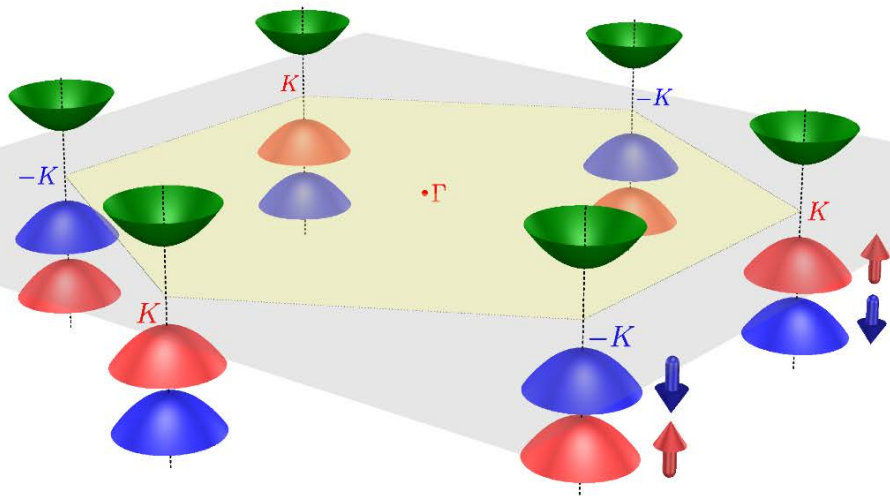
$$\tan \theta_p = \frac{p_y}{p_x}$$

Transition Metal dichalcogenides (monolayer)

Hexagonal lattice structure



Massive Dirac Fermions
partially filled d-orbitals(metal)



Gap ~ 2 eV

Spin-Split vbands $\sim 150 - 400$ meV


Valley pseudospin $\pm K$ ($\tau = \pm 1$)

Spin-valley locking

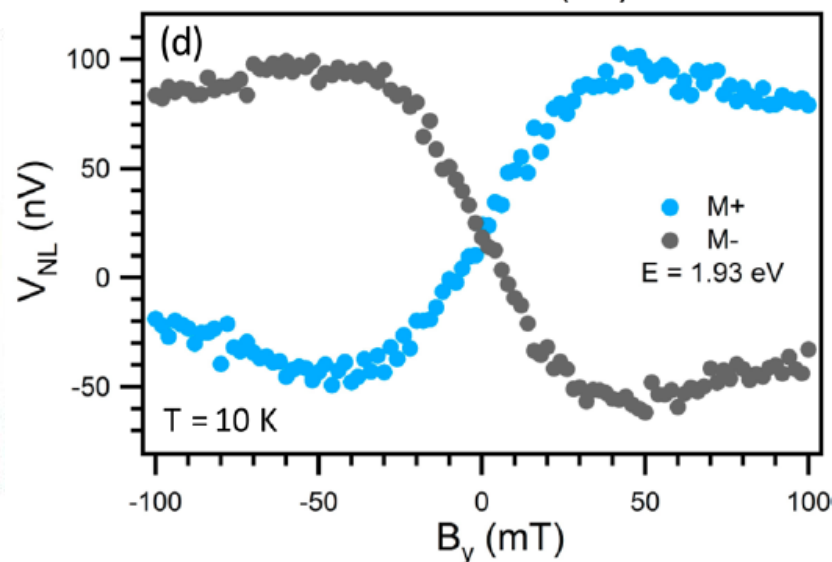
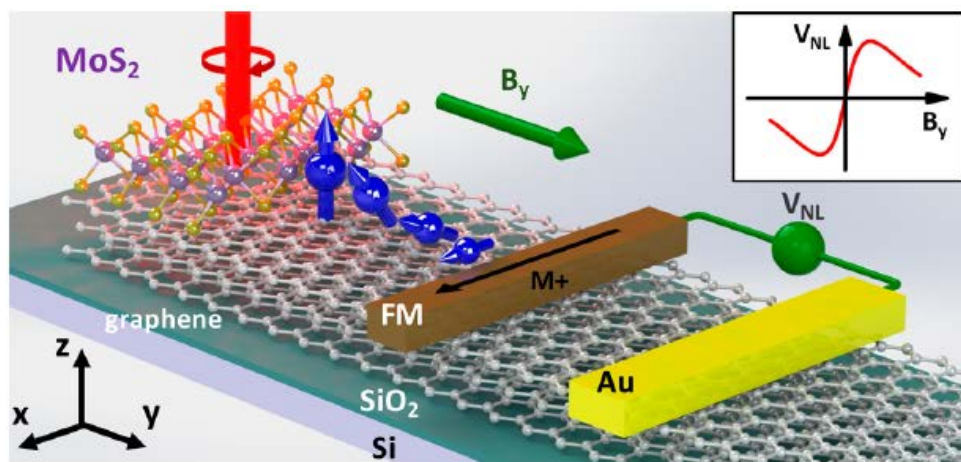
$$\mathcal{H} = at(\tau_z k_x \hat{\sigma}_x + k_y \hat{\sigma}_y) + \frac{\Delta}{2} \sigma_z + \lambda_{SO} \tau_z \hat{s}_z$$

D. Xiao et al **Phys. Rev. Lett** 108, 196802 (2016)

Opto-Valleytronic Spin Injection in Monolayer MoS₂/Few-Layer Graphene Hybrid Spin Valves

Yunqiu Kelly Luo,[†] Jinsong Xu,[†] Tiancong Zhu,[†] Guanzhong Wu,[†] Elizabeth J. McCormick,[†] Wenbo Zhan,[†] Mahesh R. Neupane,[‡] and Roland K. Kawakami^{*,†} 

Nano Lett. 17 (6), 3877 (2017)



Multifunctional 2D spintronic/valleytronic devices and applications !



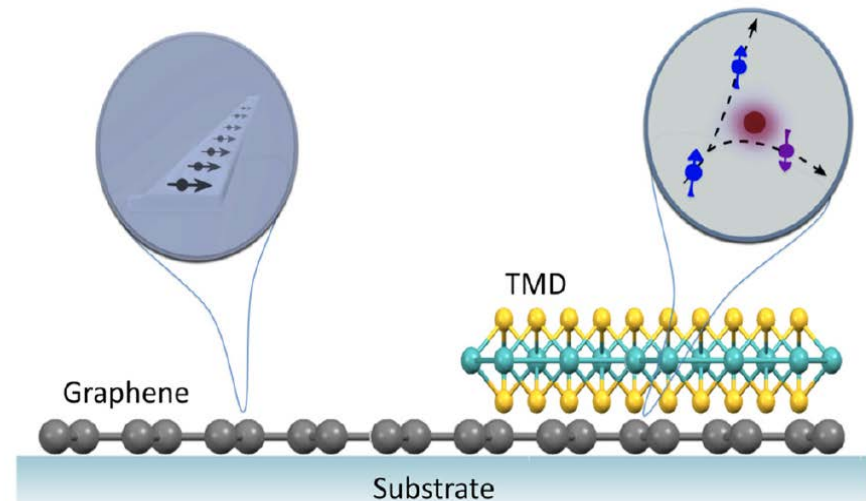
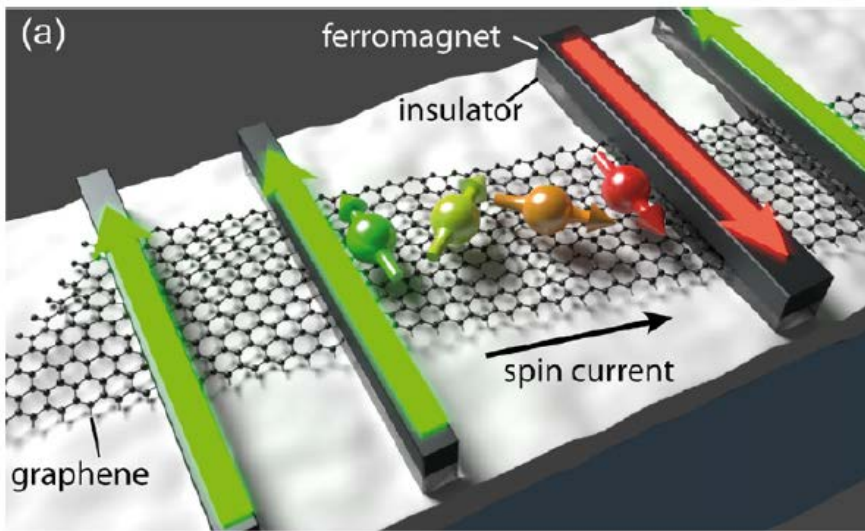
2D Materials

EDITORIAL

Graphene spintronics: the European Flagship perspective

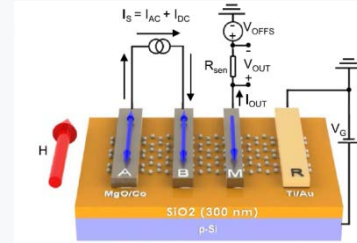
Stephan Roche^{1,2}, Johan Åkerman^{3,4,5}, Bernd Beschoten⁶, Jean-Christophe Charlier⁷, Mairbek Chshiev^{8,9}, Saroj Prasad Dash¹⁰, Bruno Dlubak¹², Jaroslav Fabian¹¹, Albert Fert¹², Marcos Guimarães^{13,19}, Francisco Guinea^{14,15}, Irina Grigorieva¹⁴, Christian Schönberger¹⁶, Pierre Seneor¹², Christoph Stampfer¹⁷, Sergio O Valenzuela^{1,2}, Xavier Waintal^{9,18} and Bart van Wees¹⁹

2D Mater. 2 (2015) 030202

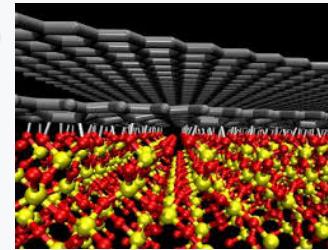


OUTLINE

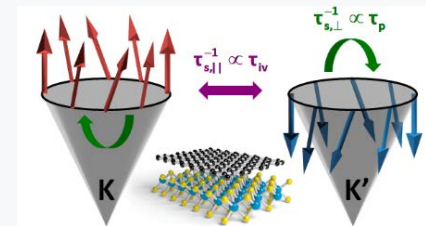
Why Spintronics using 2D Materials ?



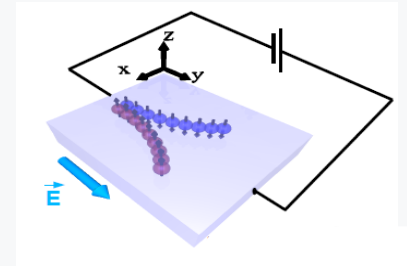
How the substrate controls spin dynamics?



*Giant spin transport anisotropy
in graphene induced by strong SOC
Proximity effect*



*Spin Hall Effect & Weak antilocalization
in Graphene/TMDC*



“Unprecedented spin lifetimes in ultraclean graphene”??

Homogeneous Rashba + disorder (density of impurities)

Numerical calculation of the spin relaxation time by performing Monte Carlo simulations

*Along any given classical trajectory $[\mathbf{r}(t), \mathbf{k}(t)]$
the spin dynamics is described by Bloch spin equation*

$$\frac{d\mathbf{S}}{dt} = \Omega_R[\mathbf{r}(t)](\mathbf{n}[\mathbf{k}(t)] \wedge \mathbf{S})$$

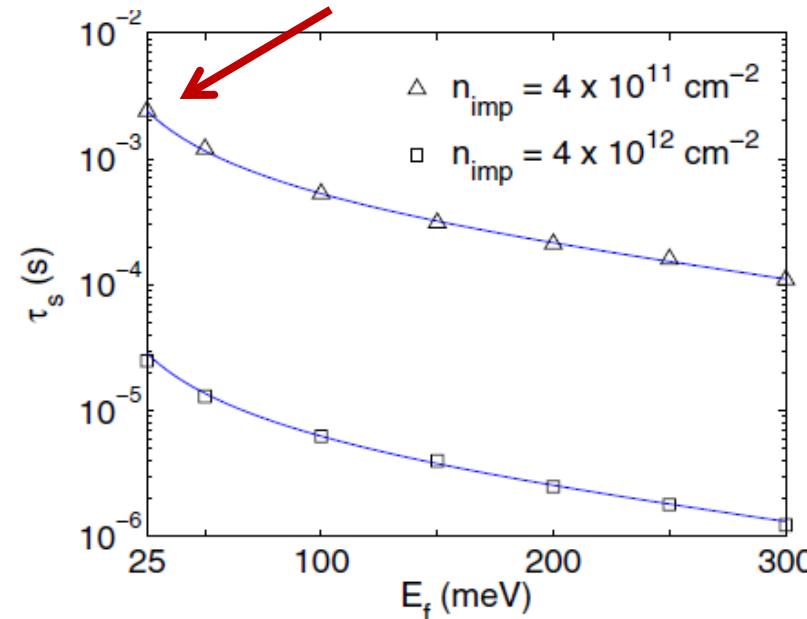
Spin lifetime is calculated by averaging over random trajectories with different initial momenta, assuming

$$t \gg \tau_{tr}$$

$$S_\alpha(t) \sim e^{-t/\tau_\alpha}$$

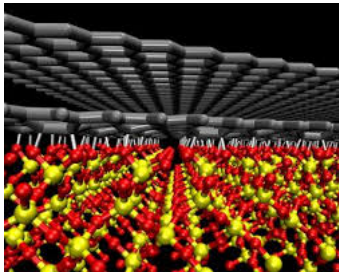
$$\tau_\alpha \rightarrow \mu\text{s} - \text{ms}!!!$$

**Maximum at Dirac point
Elliot Yaffet**

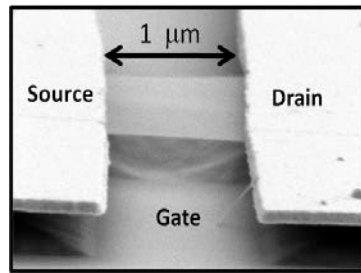


Experimental spin lifetime features

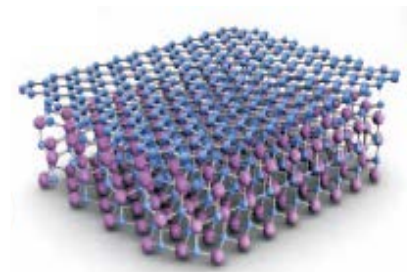
*Graphene
on SiO₂*



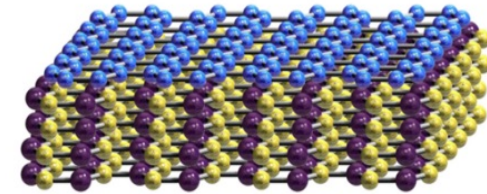
*Suspended
Graphene*



*Epitaxial graphene
on SiC*



*Graphene
on BN*

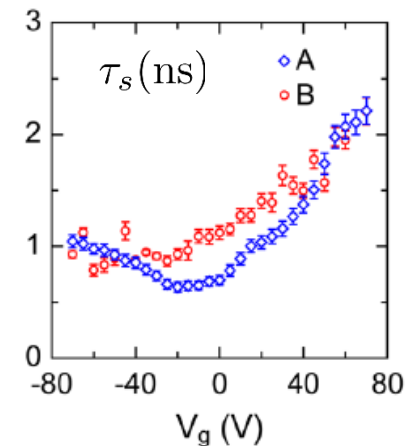
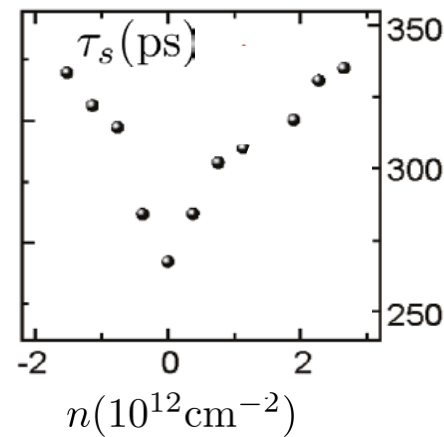


charge mobility $\mu \sim 100 - 100.000 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$

Room temperature

$$\tau_s \sim 0.1 - 10 \text{ ns}$$

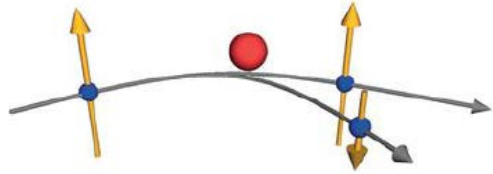
- Avsar et al, *Nano Lett.* **11**, 2363 (2011)
Drögeler et al. *Nano Lett.* **14**, 6050 (2014)
Guimarães et al *Phys Rev Lett* **113**, 086602 (2014)



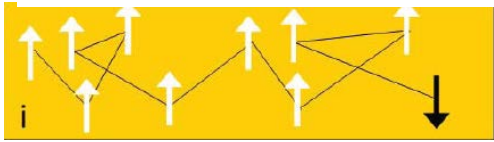
Which relaxation mechanism at play ?

Metals

Elliott-Yafet mechanism



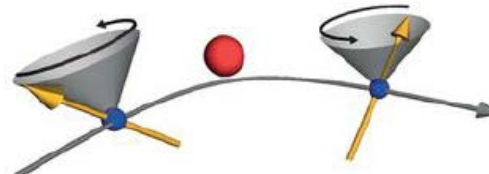
$$\tau_s \sim 10^4 - 10^6 \tau_p$$



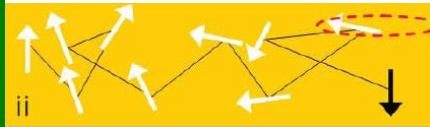
$$\tau_s^{EY} \sim \epsilon_F^2 \tau_p / \lambda_R^2$$

Small gap semiconductor

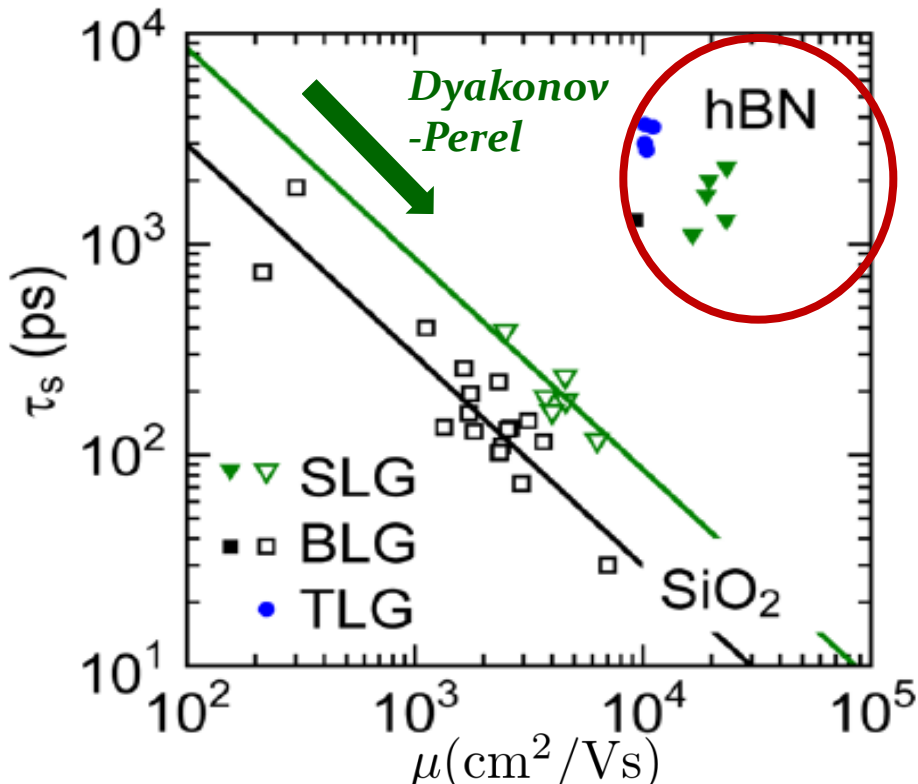
Dyakonov-Perel mechanism



$$\tau_s \sim \frac{1}{\tau_p}$$



$$\tau_s^{DP} \sim \hbar^2 / (\lambda_R^2 \tau_p)$$



Drögeler et al. *Nano Lett.* 14, 6050 (2014)

Guimarães et al *PRL* 113, 086602 (2014)

Cleaner samples for SiO₂ substrates lead to lower spin lifetime

“opposite trend” for hBN Substrates?

Origin of spin dephasing

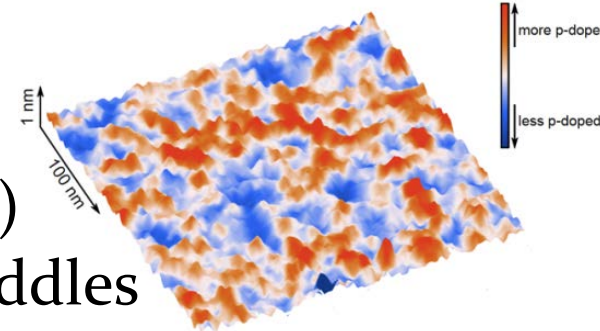
Spin-orbit coupling in graphene

“clean limit”

Intrinsic
spin-orbit coupling



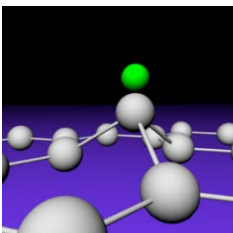
Substrate effects
(Rashba electric field)
and electron-hole puddles



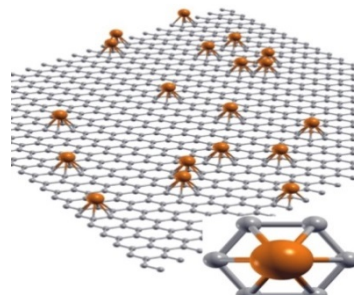
“dirty limit”

*Etching transfer processes : contamination with ionic impurities
(from metal etchants) or **metallic residues (from incomplete etching)**,
+ PMMA residues (transfer)*

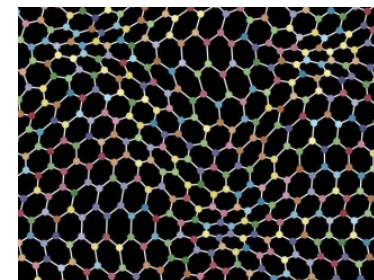
sp³ defects
(σ - π hybridization)
Hydrogen ad-atoms-



Transition- metal adatoms
(Cu, Ni, Au,...)



Deformation fields
(Strain, ripples, bubbles...)

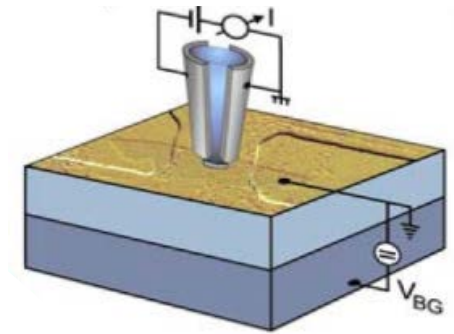
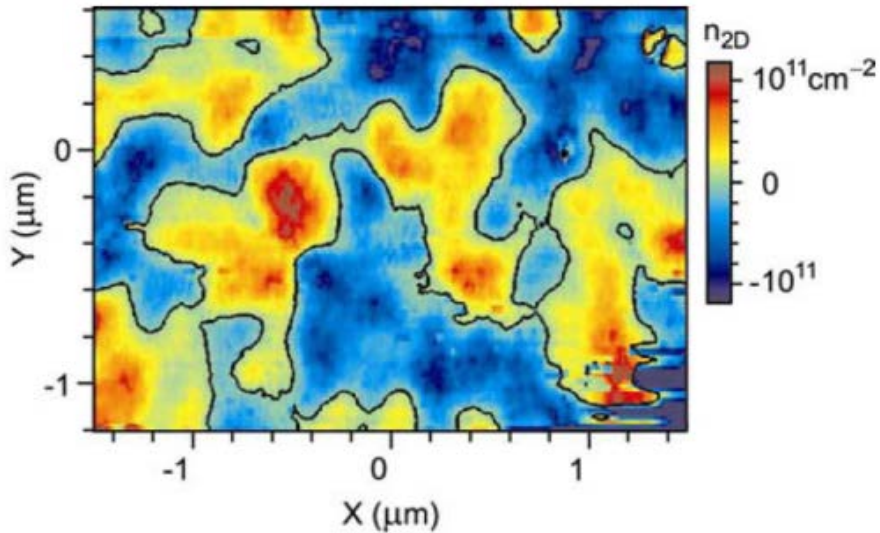


Spin relaxation in supported clean graphene

-beyond semiclassical approximations-

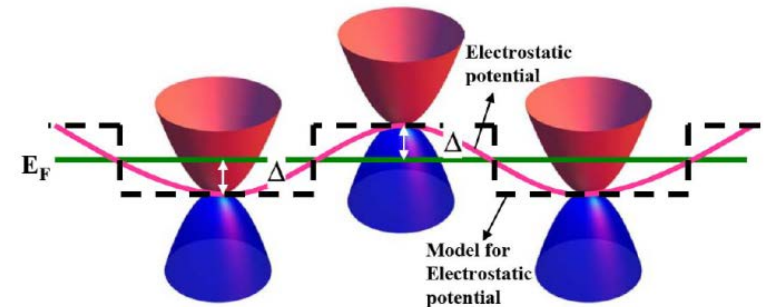
Disorder: Electron-holes puddles

Spatial (long range) charge density fluctuations



Electrons locally screen charged impurities trapped in the substrate

J. Martin et al, **Nat. Phys. 4, 144 (2008)**



Spin-orbit interaction :

Uniform Rashba SOC-field $10 \mu\text{eV}$

(substrate effect/mirror symmetry breaking)

$\tau_s \sim \mu\text{s} - \text{ms} ???$

Tight-binding Modelling

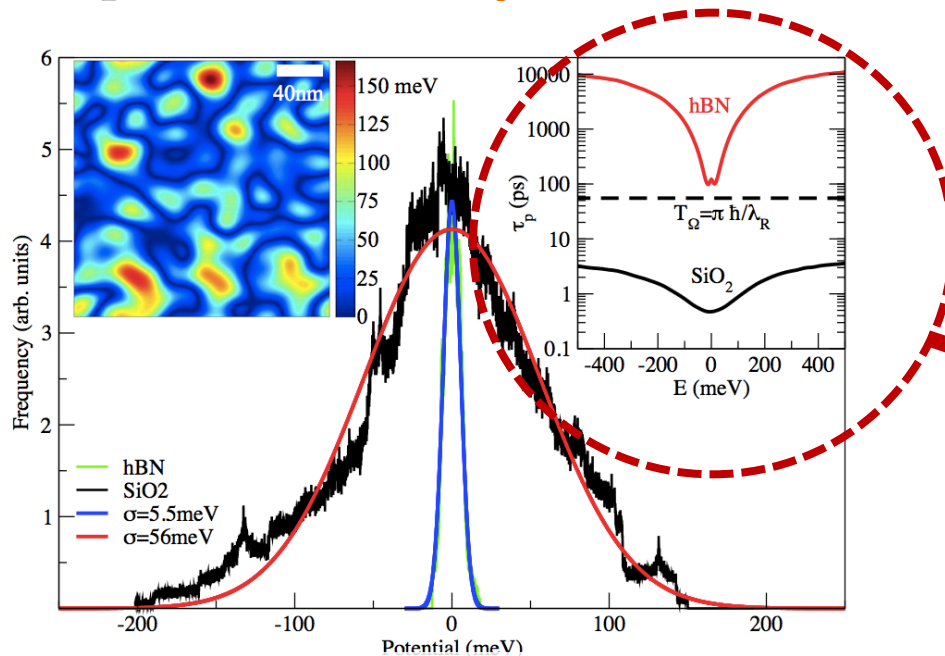
$$\mathcal{H} = -\gamma_0 \sum_{\langle ij \rangle} c_i^\dagger c_j + \sum_{\langle i \rangle} V_i c_i^\dagger c_i + iV_R \sum_{\langle ij \rangle} c_i^\dagger \vec{z} \cdot (\vec{s} \times \vec{d}_{ij}) c_j$$

Screened Coulomb potential

Long range (Gaussian) potential

$$V_i = \sum_{\alpha=1}^{N_\alpha} \varepsilon_\alpha \exp(-|\mathbf{r}_\alpha - \mathbf{r}_i|^2 / (2\xi^2))$$

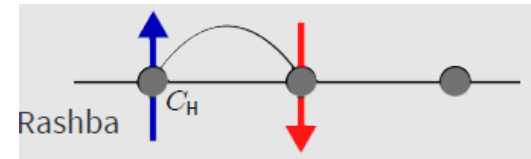
Shaffique Adam et al **Phys. Rev. B** 84, 235421 (2011)



Onsite energy distribution of the π -orbitals with standard deviation for hBN (5meV) & SiO₂ (56meV)

Rashba SOC

$$V_R \sim 20\mu\text{eV}$$

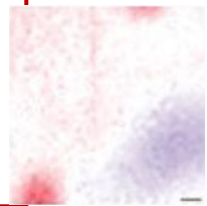
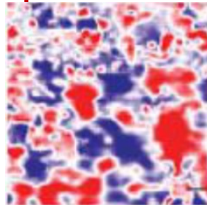


Graphene on SiO₂


$$\tau_p^{\text{SiO}_2} / T_\Omega \ll 1$$

Graphene on hBN

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



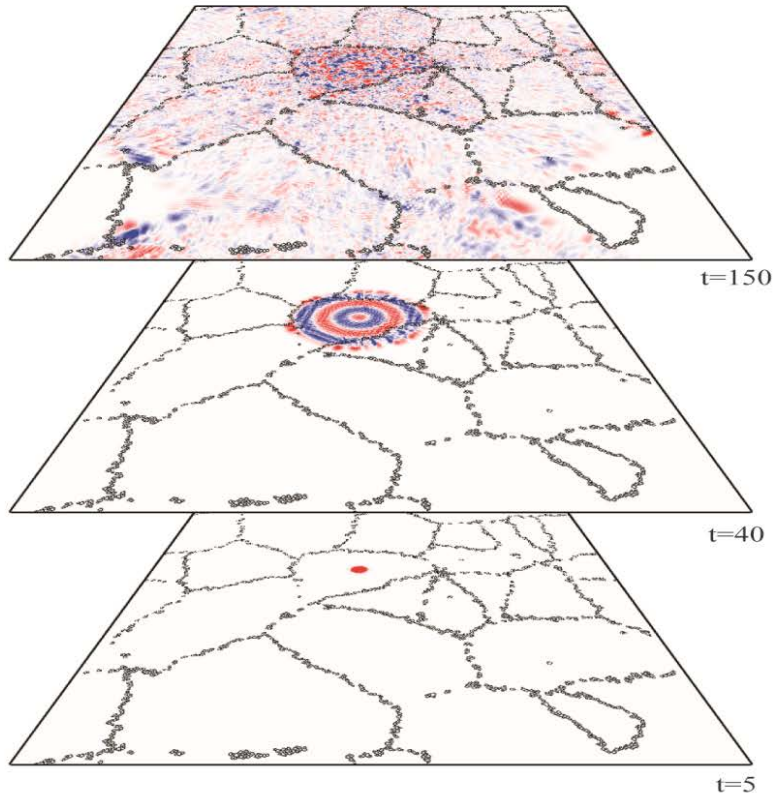
Spin dynamics of propagating wavepacket



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

Local spin density in real space

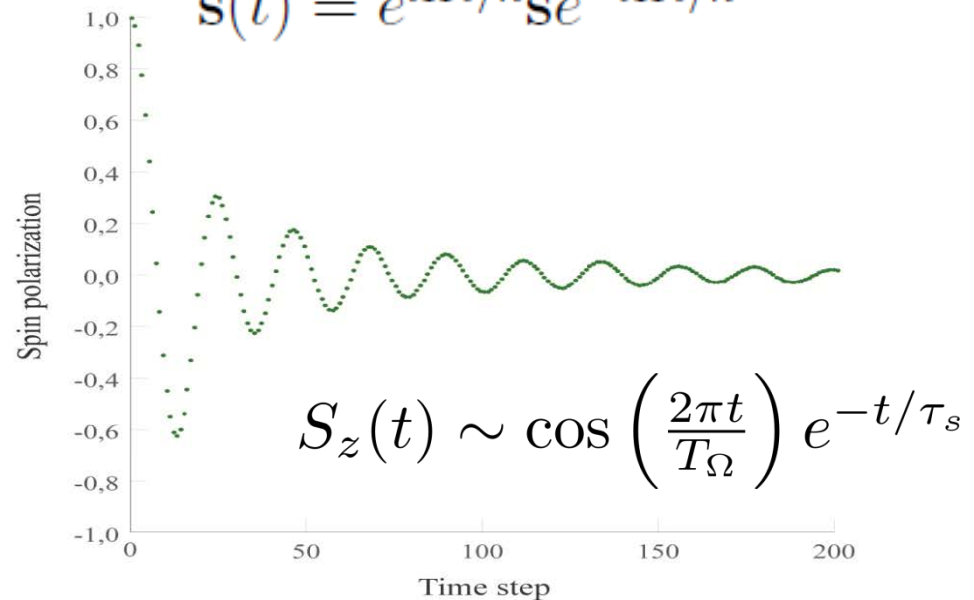
$$s_i(t) = |\Psi_i^{\uparrow}(t)|^2 - |\Psi_i^{\downarrow}(t)|^2$$

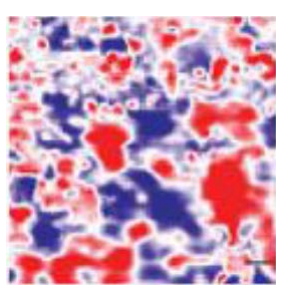


Time evolution of the wavepacket
spin polarization

$$\vec{S}(E, t) = \frac{\text{Tr}[\delta(E - H)\hat{\mathbf{s}}(t)]}{\text{Tr}[\delta(E - H)]}$$

$$\hat{\mathbf{s}}(t) = e^{iHt/\hbar}\hat{\mathbf{s}}e^{-iHt/\hbar}$$

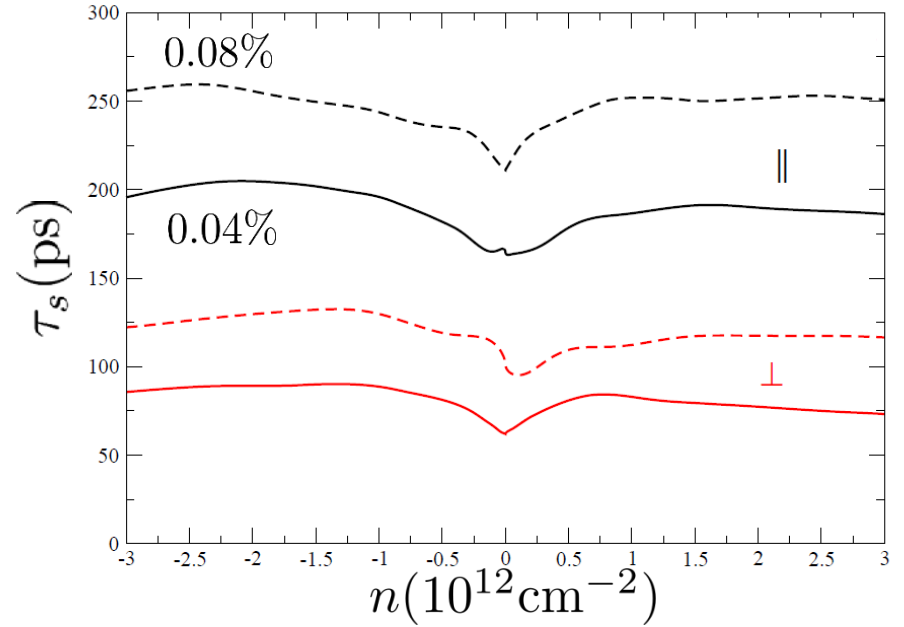
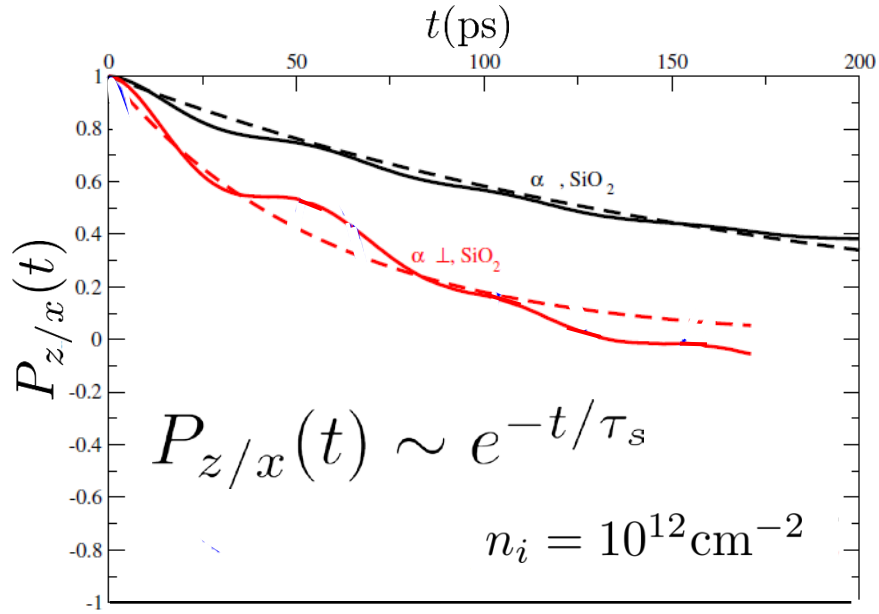




Graphene on SiO₂

electron-hole puddles drive the relaxation

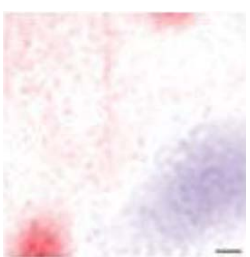
$$\tau_p^{\text{SiO}_2} / T_\Omega \ll 1$$



$$\tau_s \sim \frac{1}{n_i} \quad \text{increases with defect density}$$

$$\tau_s^\perp / \tau_s^\parallel \rightarrow 0.5$$

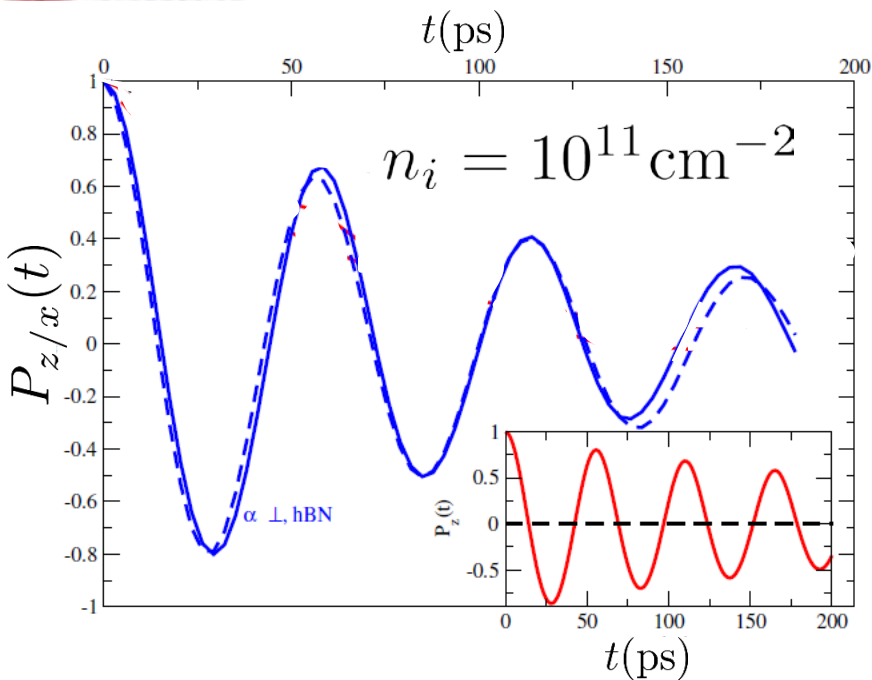
Dyakonov-Perel
relaxation mechanism



Graphene on hBN

electron-hole puddles drive the relaxation

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

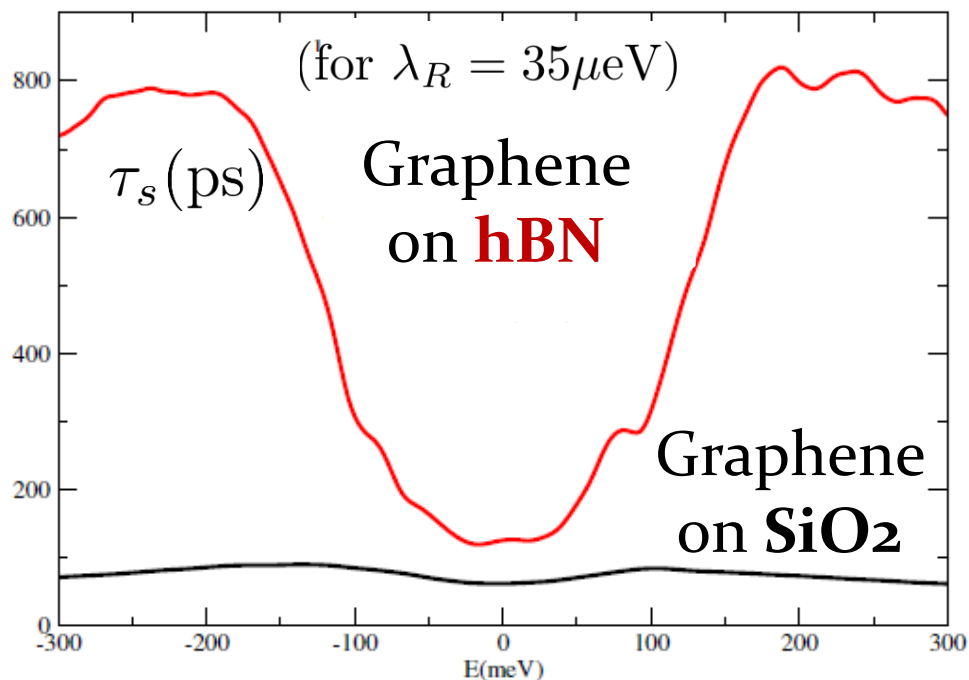


$$P_{z/x}(t) \sim \cos\left(\frac{2\pi t}{T_\Omega}\right) e^{-t/\tau_s}$$

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

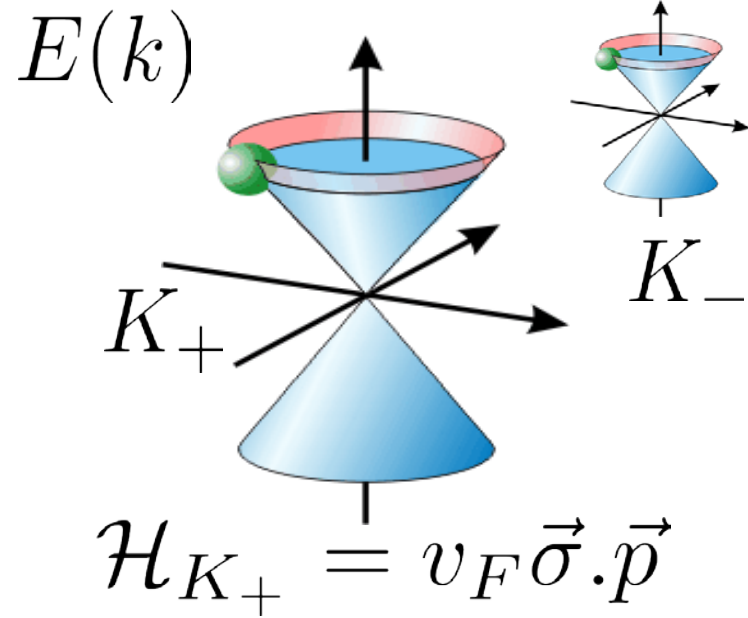
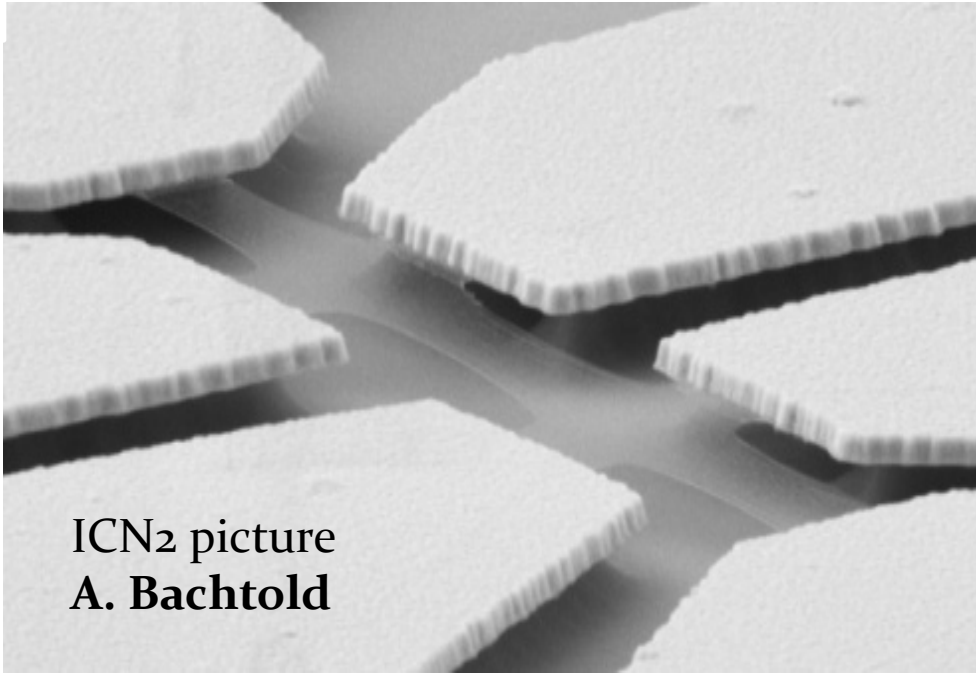
$$\tau_s \simeq 1 - 10 \text{ ns}$$

(for $\lambda_R \rightarrow 5 \mu\text{eV}$)



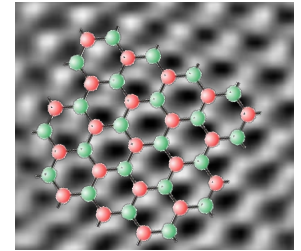
What is the origin of dephasing/relaxation mechanism?

“Unique properties of Clean graphene”



pseudospin

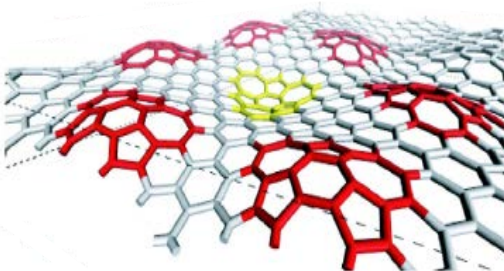
$$|\Downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$



Long range potential

Intravalley scattering

(short momentum transfer)

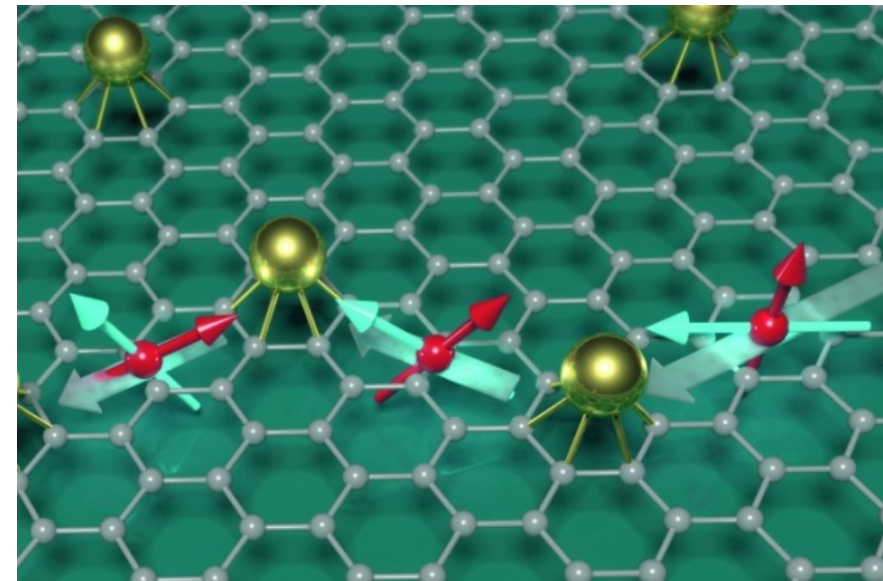
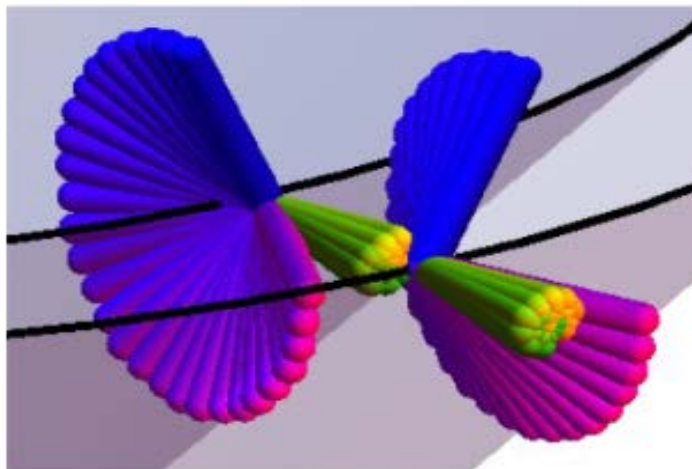
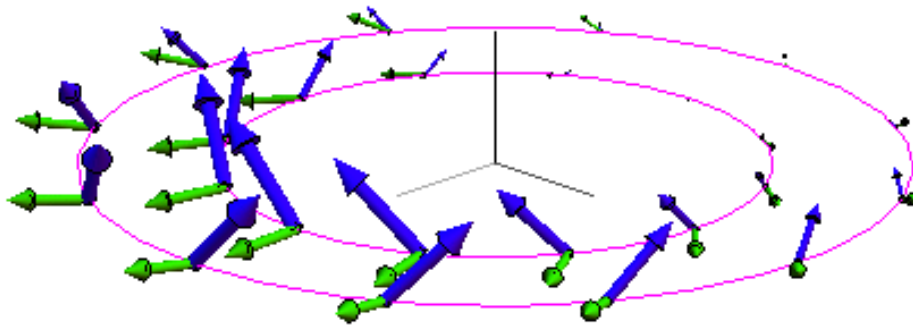


Anomalous quantum transport

- 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 ?**

Pseudospin-driven spin relaxation mechanism in graphene

Dinh Van Tuan^{1,2}, Frank Ortmann^{1,3,4}, David Soriano¹, Sergio O. Valenzuela^{1,5} and Stephan Roche^{1,5*}



$$\Psi \sim \text{A} \otimes \uparrow + \text{B} \otimes \downarrow$$

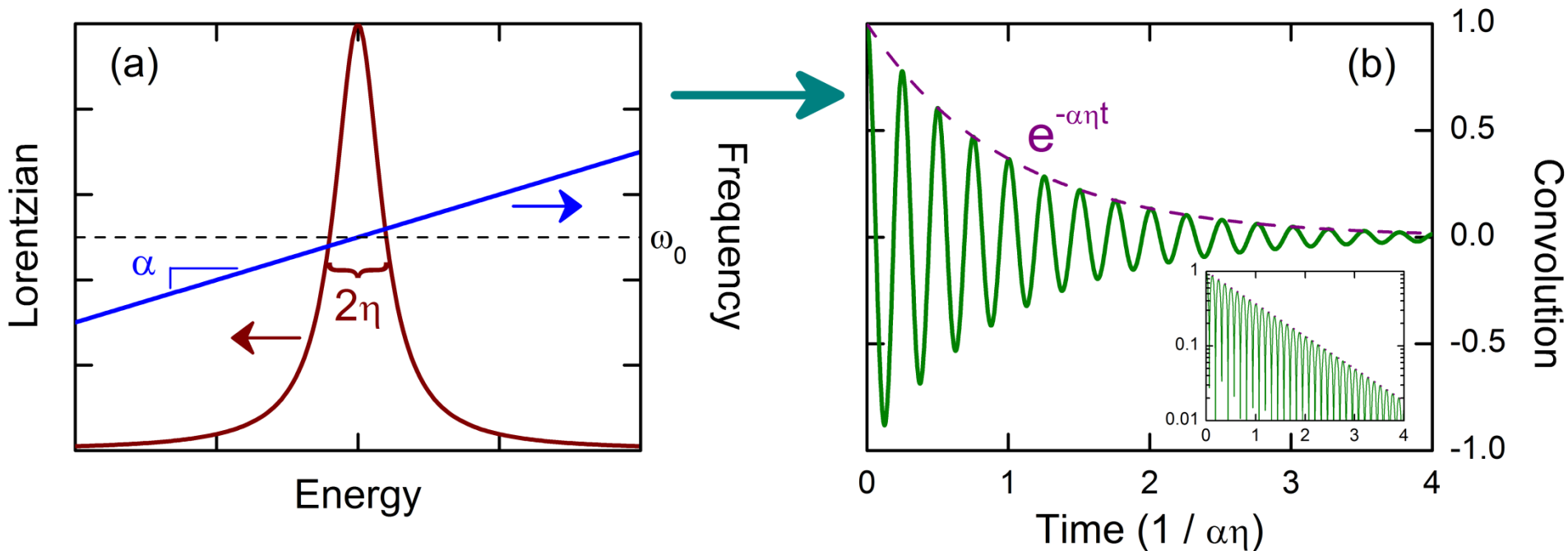
Relaxation in the ultraclean limit...

spin precession frequency varies linearly with energy

$$\omega(E) = \omega_0 + \alpha E$$

charge carriers occupy a Lorentzian distribution in energy

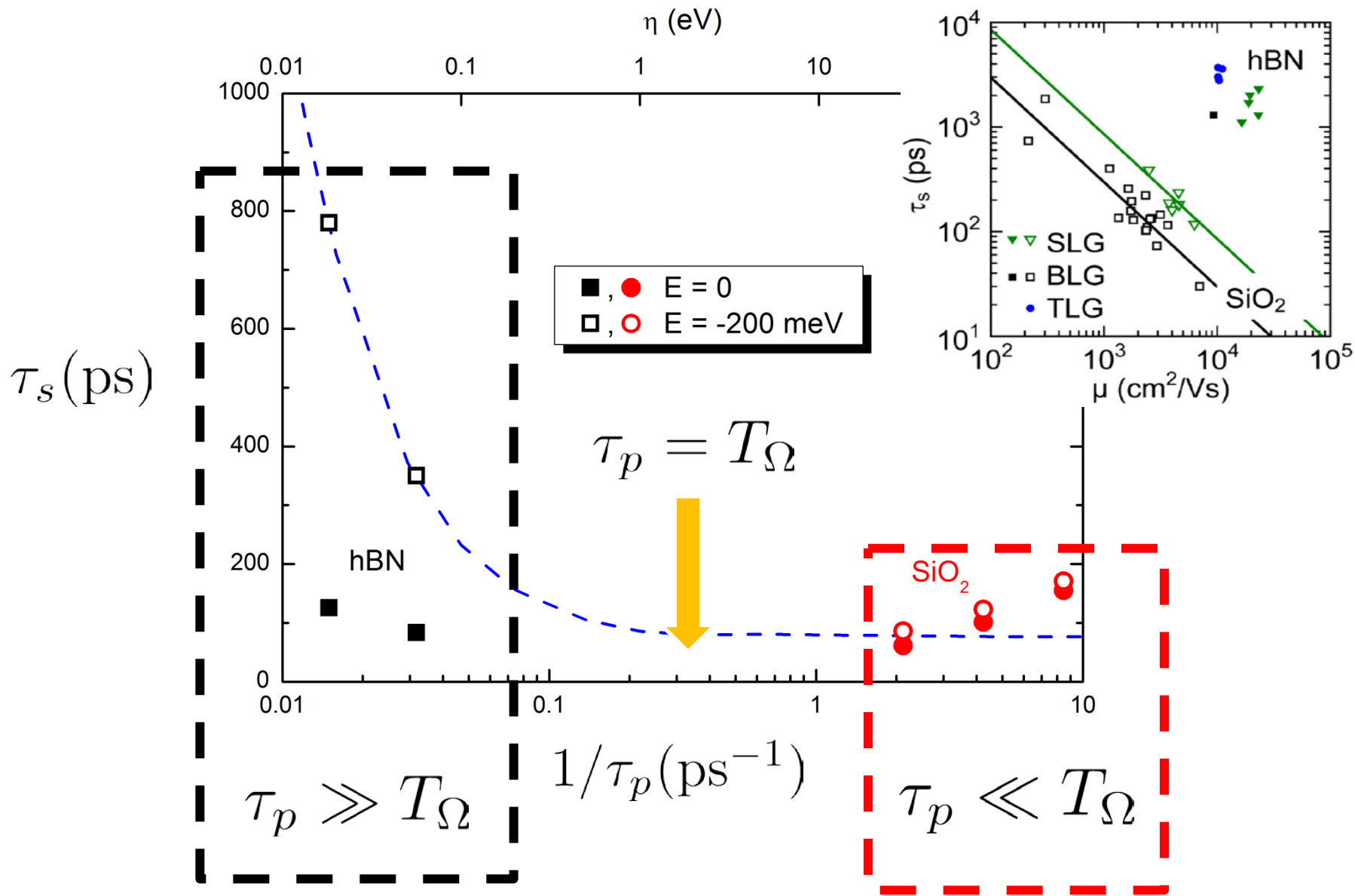
$$\mathcal{L}(E) = \eta / [\pi \cdot (E^2 + \eta^2)]$$



Exponentially-decaying cosine, with frequency ω_0 and decay time $1/\alpha\eta$

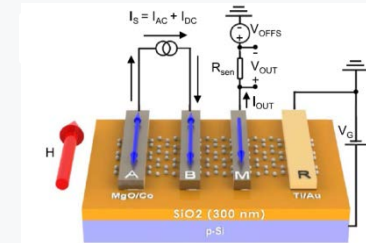
$$s(t) = \mathcal{L}(E) \circ \cos(\omega(E)t) = e^{-\alpha\eta t} \cdot \cos(\omega_0 t)$$

Crossover between “pure dephasing” and scattering-induced Dyakonov-Perel

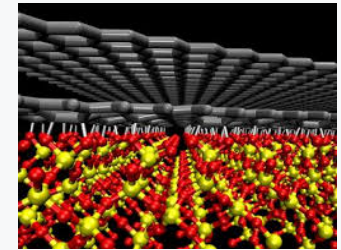


OUTLINE

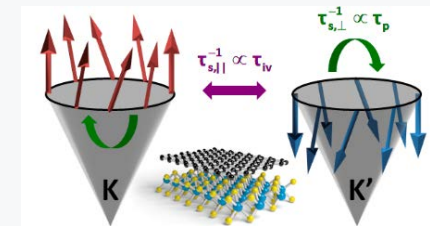
Why Spintronics using 2D Materials ?



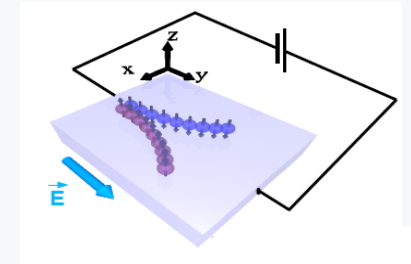
How the substrate controls spin dynamics?



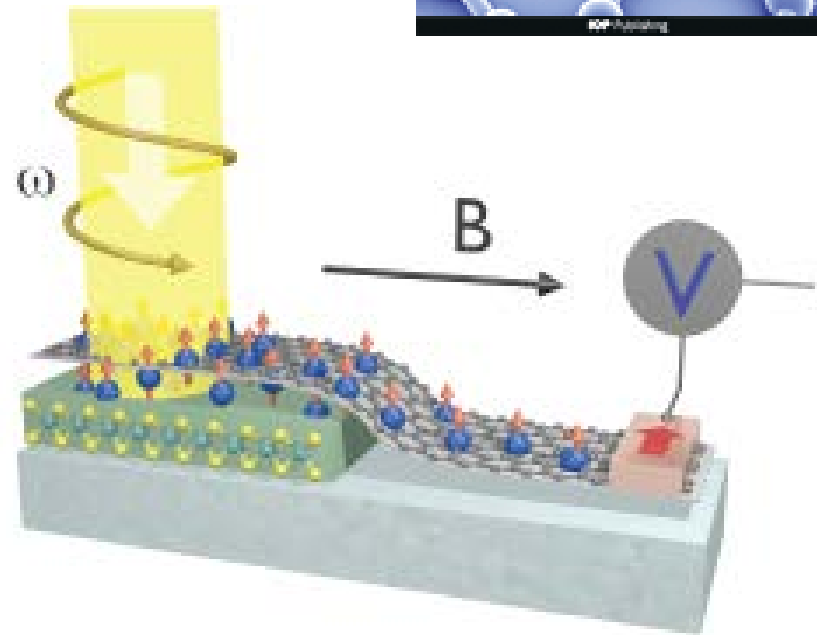
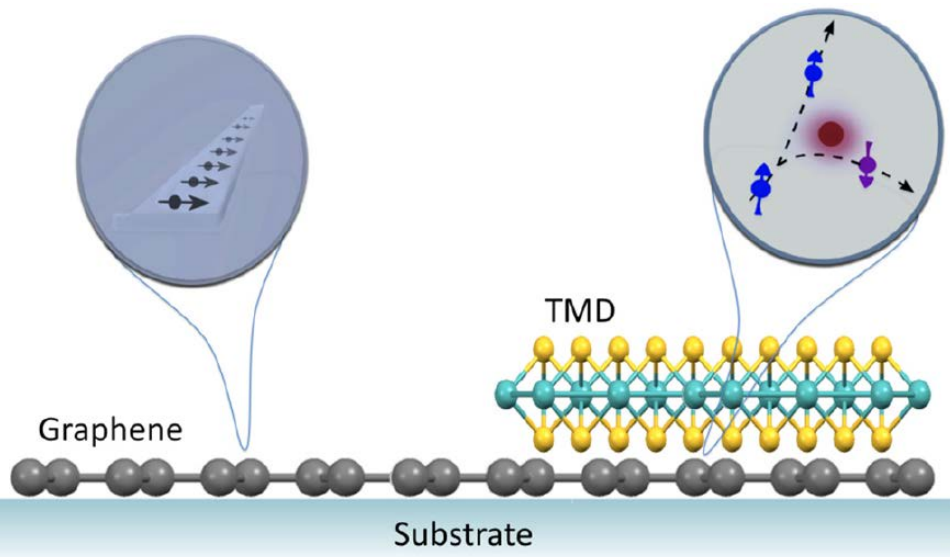
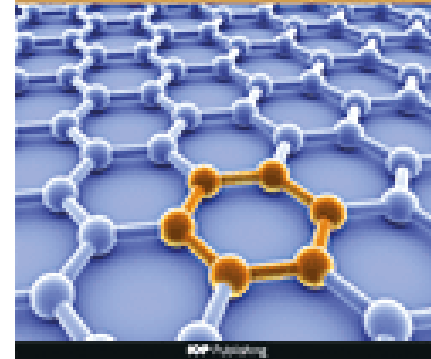
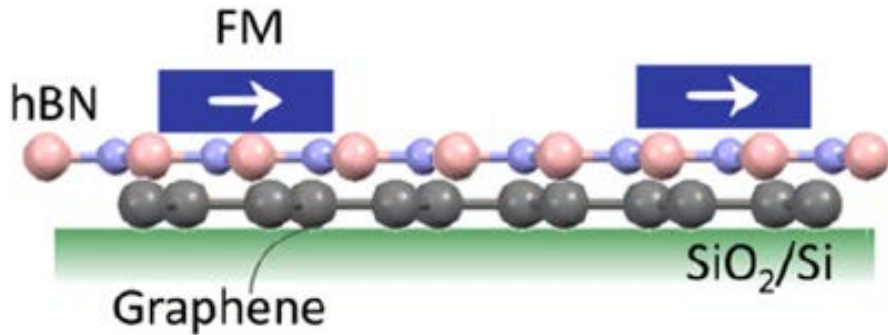
***Giant spin transport anisotropy
in graphene induced by strong SOC
Proximity effect***



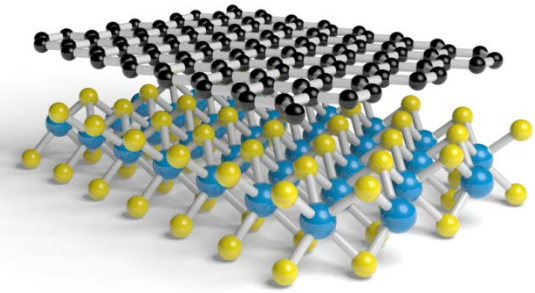
***Weak antilocalization & Spin Hall Effect
in Graphene/TMDC***



Hybrid devices of graphene and other 2D materials



Realistic Model of Graphene/TMDC with interface disorder



DFT-TB model from

M. Gmitra, D. Kochan, P. Högl, & J. Fabian

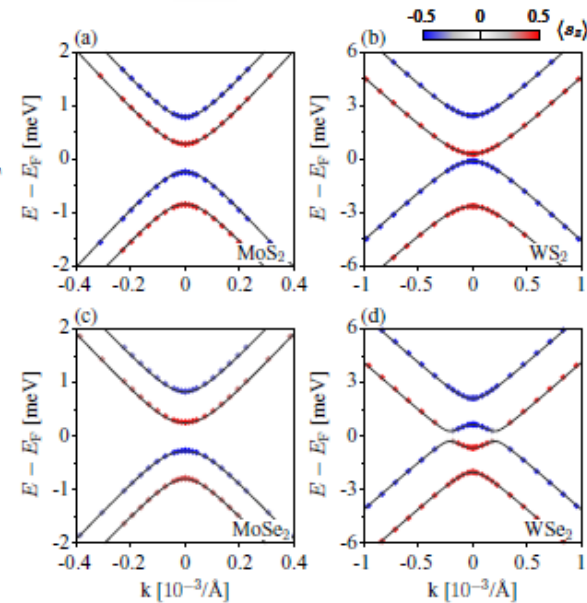
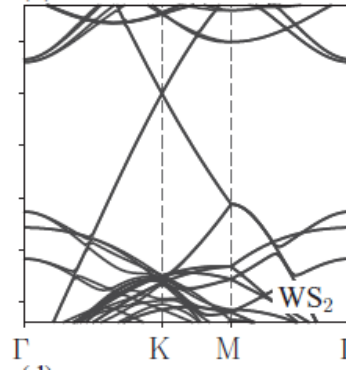
PRB 93, 155104 (2016)

$$H_0 = -t \sum_{\langle i,j \rangle} (a_i^\dagger b_j + b_i^\dagger a_i) + \frac{\Delta}{2} \sum_i (a_i^\dagger a_i - b_i^\dagger b_i)$$

$$H_{\text{so}} = \frac{2i}{3} \sum_{\langle i,j \rangle, \sigma} (\hat{\mathbf{s}} \times \mathbf{d}_{i,j})_{z, \sigma, \bar{\sigma}} \lambda_R a_{i, \sigma}^\dagger b_{j, \bar{\sigma}} + h.c$$

$$+ \frac{2i}{3} \sum_{\langle\langle i,j \rangle\rangle, \sigma} (\hat{\mathbf{s}} \times \mathbf{D}_{i,j})_{z, \sigma, \bar{\sigma}} \left(\lambda_{\text{PIA}}^{(A)} a_{i, \sigma}^\dagger a_{j, \bar{\sigma}} + \lambda_{\text{PIA}}^{(B)} b_{i, \sigma}^\dagger b_{j, \bar{\sigma}} \right)$$

$$+ \frac{i}{3\sqrt{3}} \sum_{\langle\langle i,j \rangle\rangle, \sigma} \nu_{i,j} (\hat{s}_z)_{\sigma, \sigma} (\lambda_I^{(A)} a_{i, \sigma}^\dagger a_{j, \sigma} - \lambda_I^{(B)} b_{i, \sigma}^\dagger b_{j, \sigma}),$$

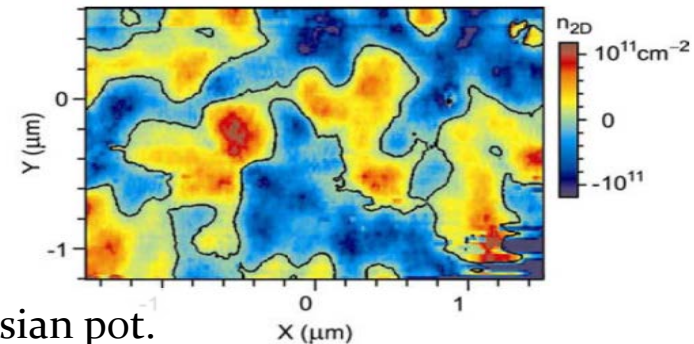


Random distribution of n_p electron-hole puddles

S. Adam et al. PRB 84, 235421 (2011)

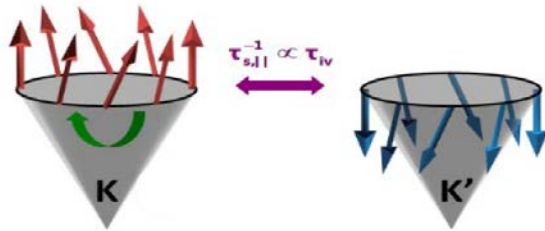
$$U_n(\mathbf{r}) = u_n \exp\left(-\frac{(\mathbf{r} - \mathbf{R}_n)^2}{2\xi_p^2}\right) \quad \xi_p = \sqrt{3}a \quad \text{Puddle range}$$

$u_n \in [-U_p, U_p]$ \mathbf{R}_n is the position of the center of the Gaussian pot.

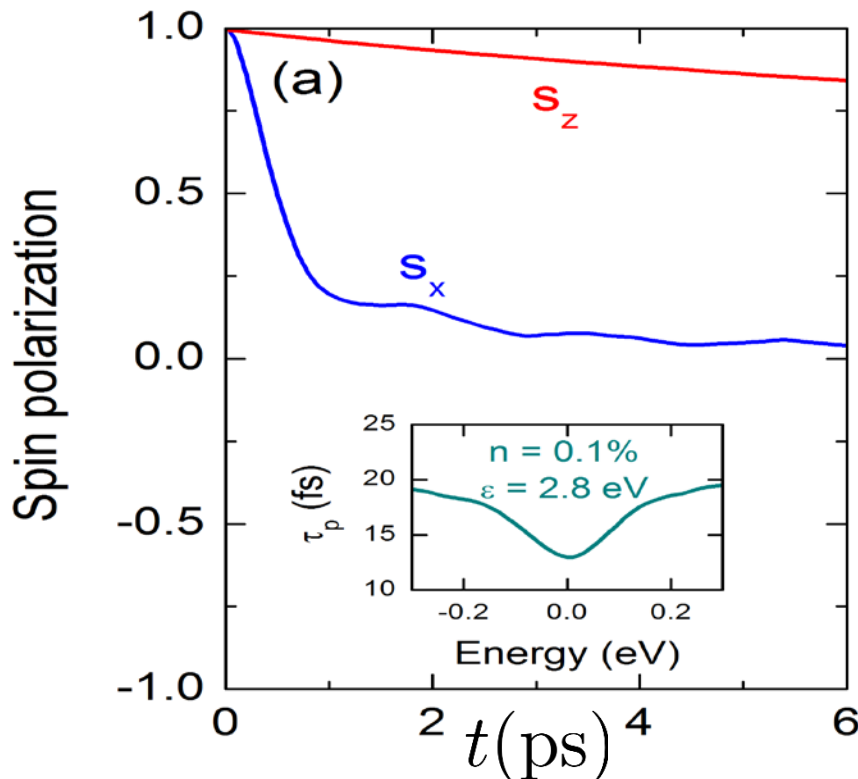


Spin dynamics for graphene/TMDC+ el-h puddles

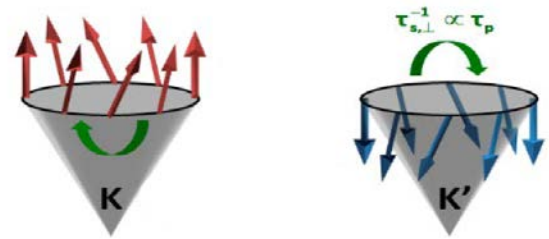
A. W. Cummings, J.H. García, J. Fabian, S. Roche, [arXiv:1705.10972](https://arxiv.org/abs/1705.10972)



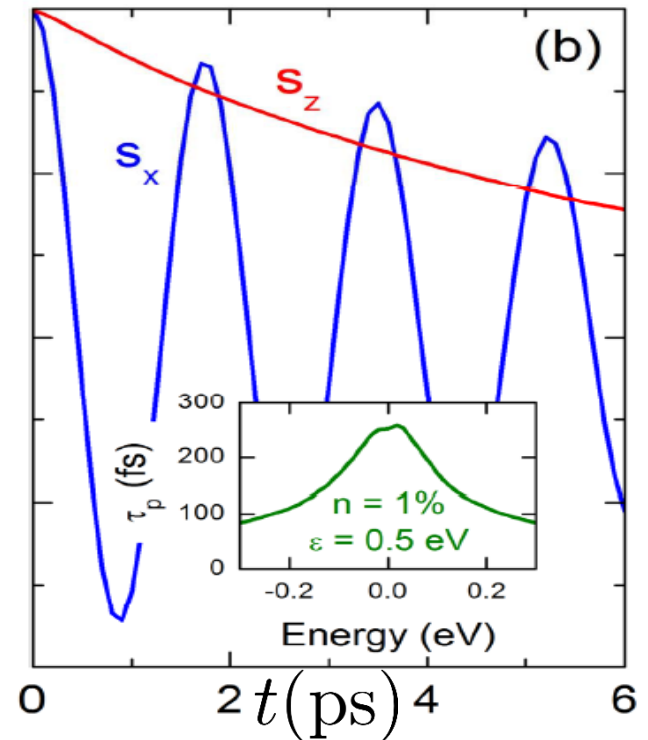
Strong valley mixing



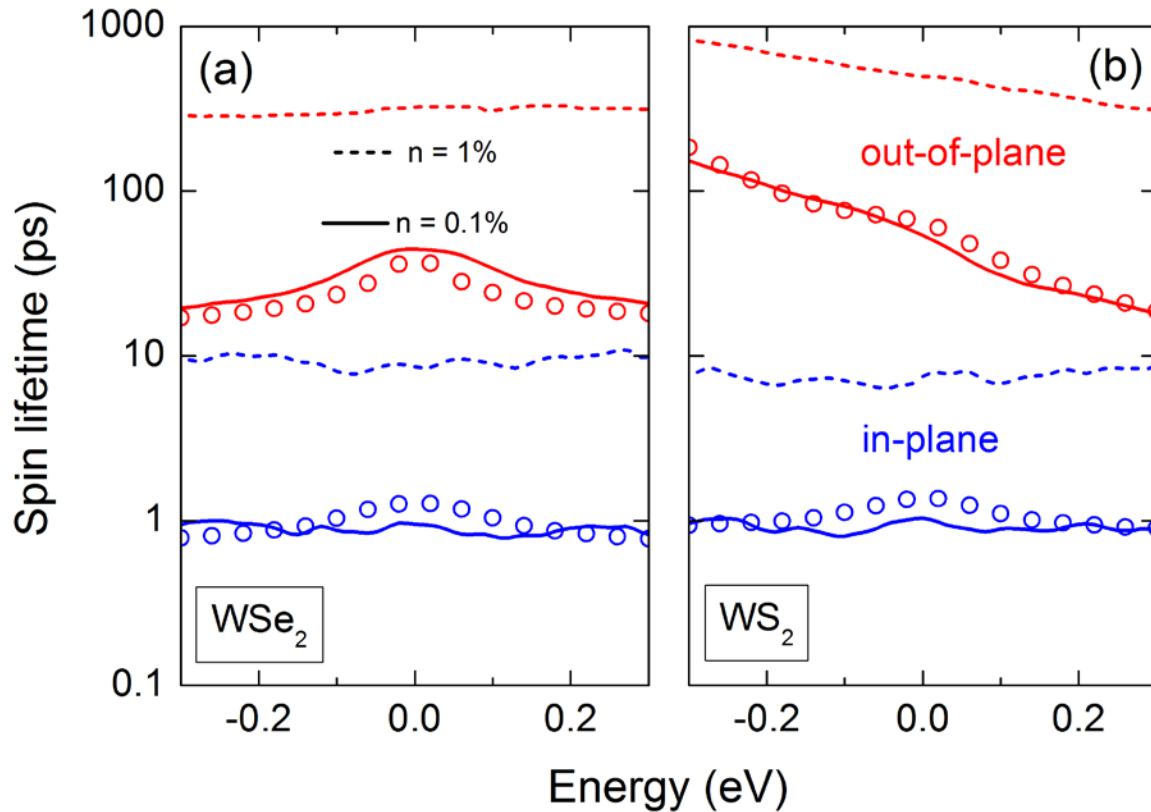
$$S_\alpha \simeq \exp(-t/\tau_{s,\alpha}) \cos(\omega_z t)$$



Intravalley scattering



Spin lifetimes in Graphene/TMDC (strong valley mixing)



Lifetime values

$$\tau_{s,\perp} \in [10, 1000] \text{ps}$$

$$\tau_{s,\parallel} \in [1, 10] \text{ps}$$

Dyakonov-Perel mechanism

$$\tau_{s,\perp} \& \tau_{s,\parallel} \sim 1/n_p$$

Giant anisotropy

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

Symbols:

Effective spin-orbit fields
arising from the SOC terms
+ equation of motion of
density matrix

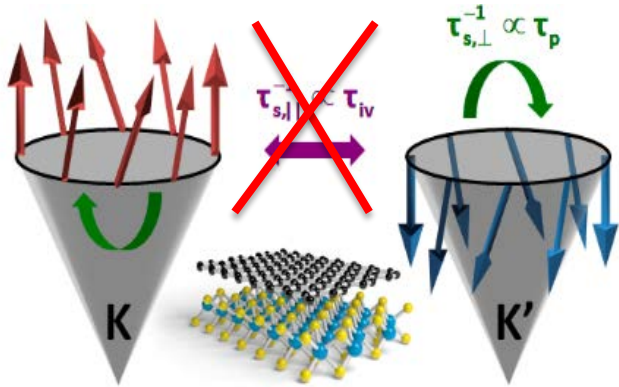
$$H = H_0 + \frac{1}{2} \hbar \vec{\omega}(t) \cdot \vec{s}$$

$$\overline{\omega_\alpha(t) \omega_\beta(t')} = \delta_{\alpha\beta} \overline{\omega_\alpha^2} e^{-|t-t'|/\tau_{c,\alpha}},$$

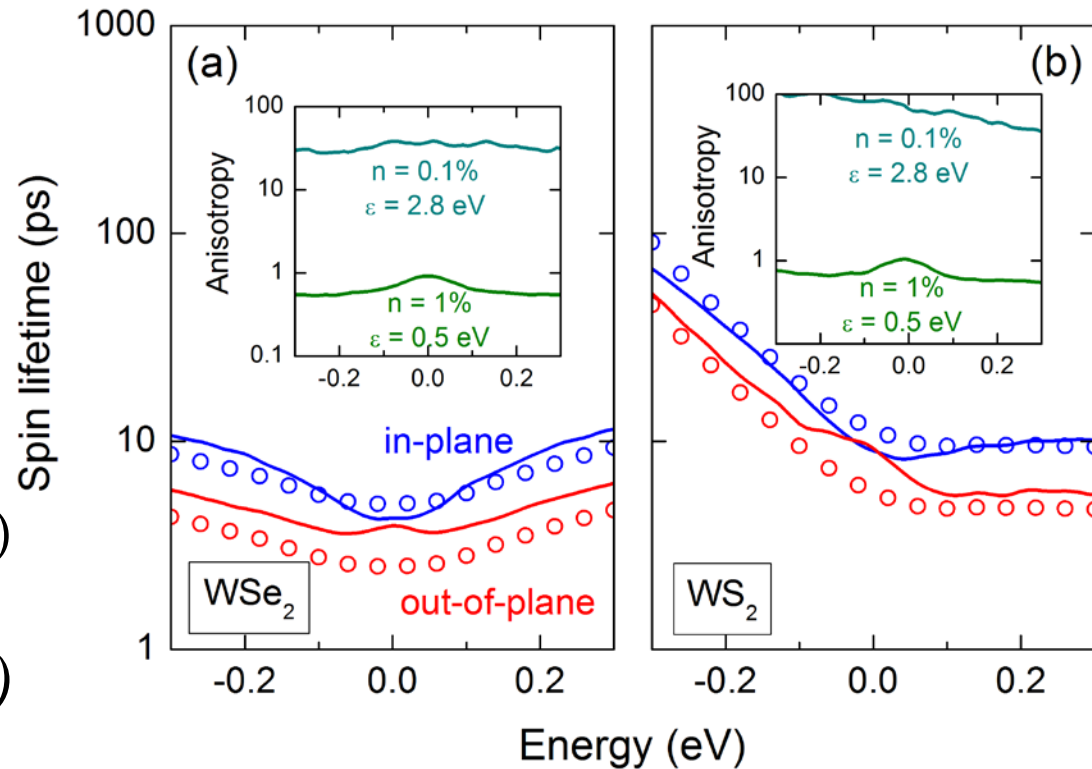
$$\frac{d\overline{\rho_I(t)}}{dt} = \left(\frac{1}{i\hbar}\right)^2 \int_0^{t \gg \tau_c} \overline{[V_I(t), [V_I(t'), \rho_I(t)]]} dt',$$

$$V_I(t) = \frac{1}{2} \hbar \vec{\omega}(t) \cdot \vec{s}_I(t) \text{ and } \vec{s}_I(t) = e^{iH_0 t/\hbar} \vec{s} e^{-iH_0 t/\hbar}$$

Spin transport anisotropy in Graphene/TMDC (intravalley scattering only)



higher quality interfaces
Spin lifetimes (out-of-plane)
much smaller
(even smaller than in-plane)



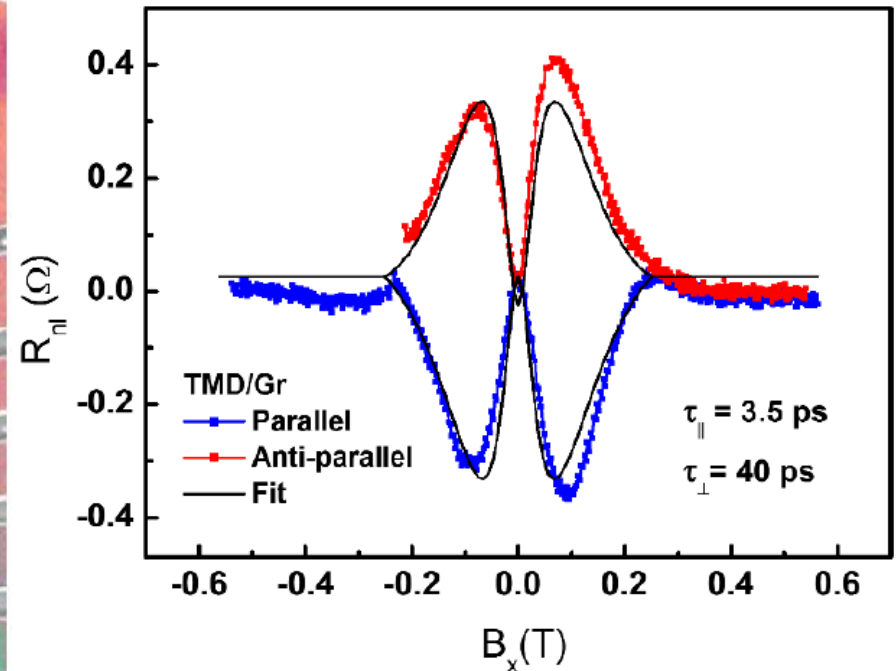
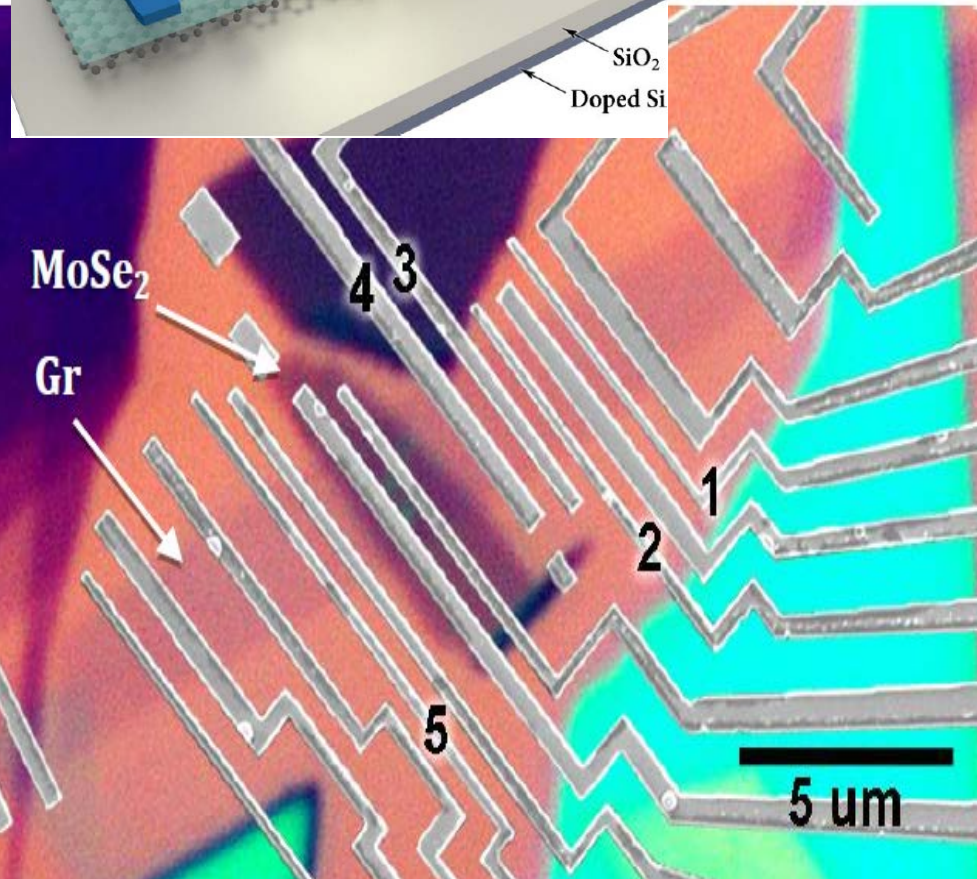
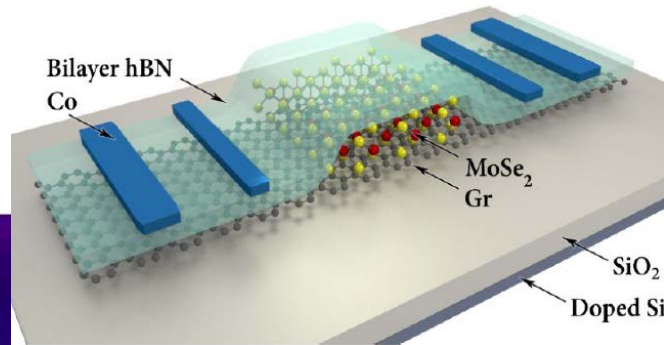
Anisotropy around 1/2

(as in conventional Rashba disordered systems)

Experimental confirmation

Group of Bart van Wees

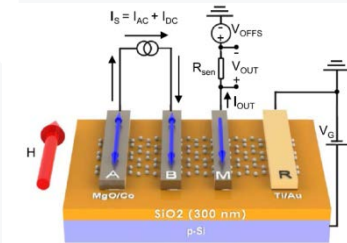
T.S. Ghiasi et al, [arXiv:1708.04067](https://arxiv.org/abs/1708.04067)



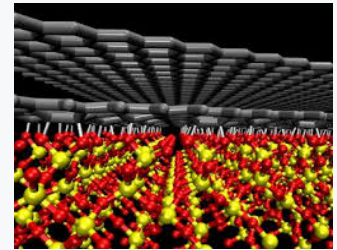
$$\tau_{\perp} / \tau_{\parallel} \simeq 10-40$$

OUTLINE

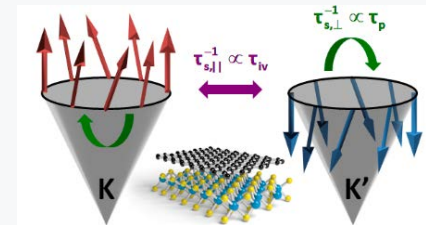
Why Spintronics using 2D Materials ?



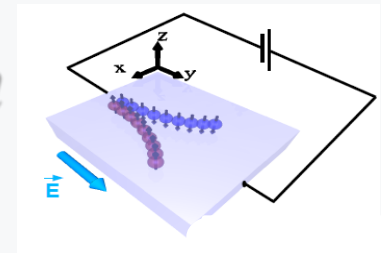
How the substrate controls spin dynamics?



*Giant spin transport anisotropy
in graphene induced by strong SOC
Proximity effect*



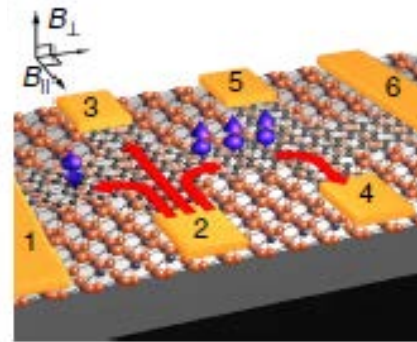
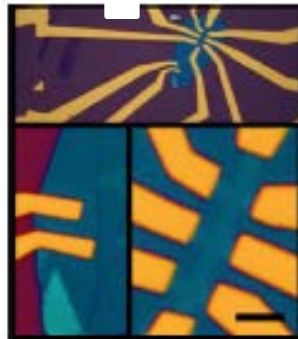
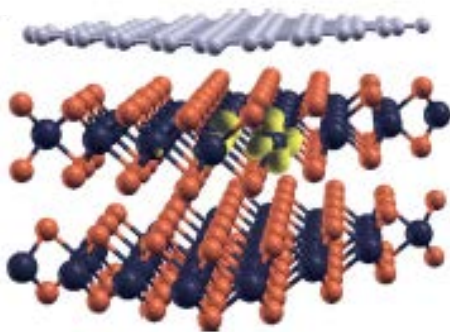
*Spin Hall Effect & Weak antilocalization
in Graphene/TMDC*





Spin-orbit proximity effect in graphene

A. Avsar^{1,2}, J.Y. Tan^{1,2}, T. Taychatanapat^{1,2}, J. Balakrishnan^{1,2}, G.K.W. Koon^{1,2,3}, Y. Yeo^{1,2}, J. Lahiri^{1,2}, A. Carvalho⁴, A.S. Rodin⁴, E.C.T. O'Farrell^{1,2}, G. Eda^{1,2}, A.H. Castro Neto^{1,2} & B. Özyilmaz^{1,2,3}

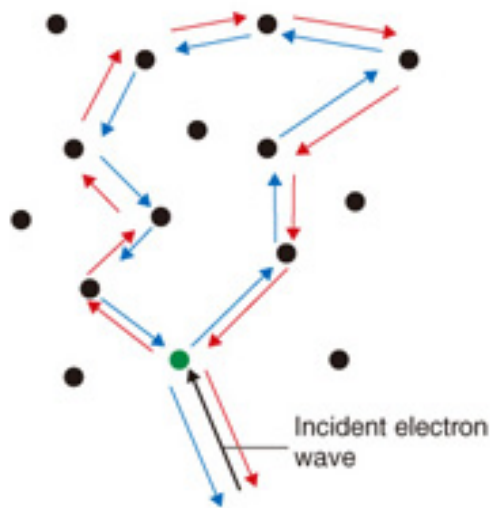


$$\tau_s \simeq 5 - 10 \text{ ps}$$

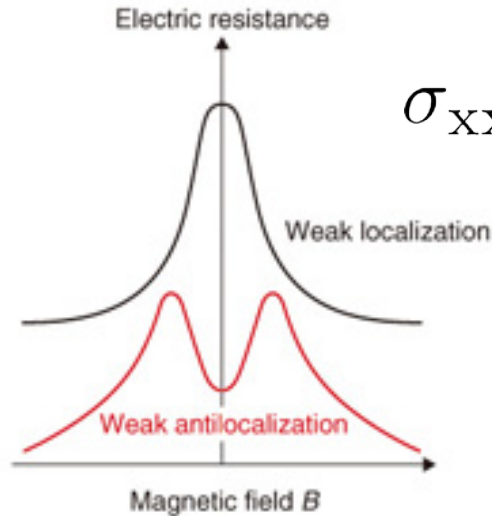
*“Graphene acquires spin-orbit coupling up to **17 meV**, three orders of magnitude higher than its intrinsic value, without modifying the structure of the graphene.*

The proximity SOC leads to the spin Hall effect even at room temperature, and opens the door to spin field effect transistors”

Weak (anti)-localization by proximity effect



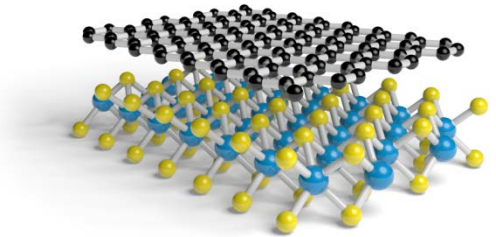
(a) Generation mechanism



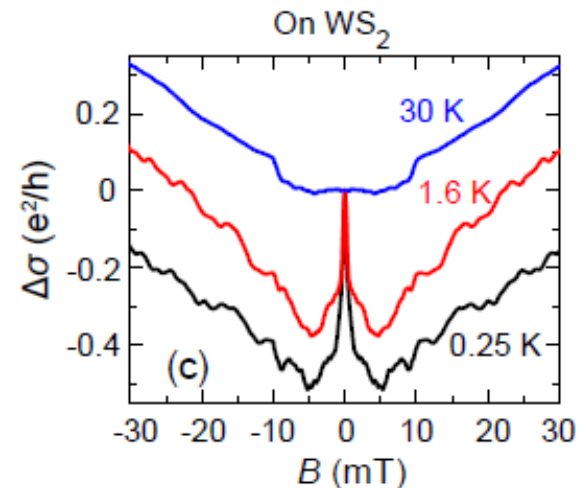
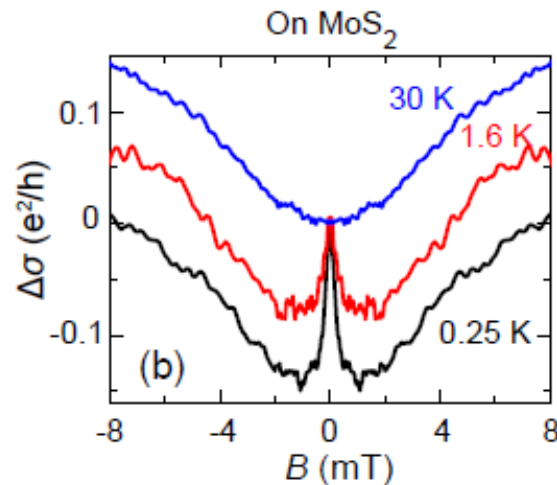
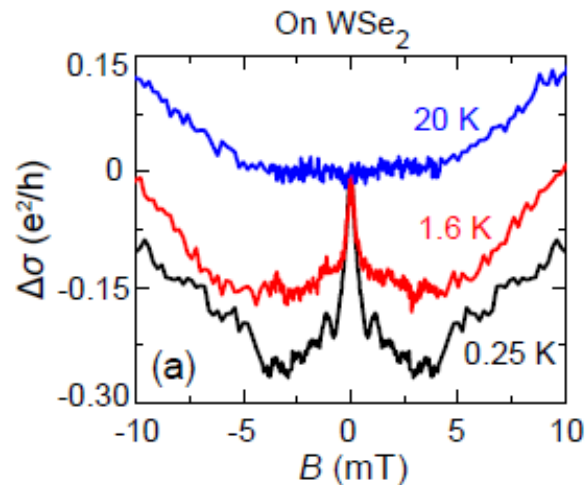
(b) Magneto-resistance effect

$$\sigma_{xx}(\varepsilon_F) = \sigma_{sc}(\varepsilon_F) + \delta\sigma(\varepsilon_F)$$

Sign of the **quantum correction**
Changes in presence of spin-orbit
coupling



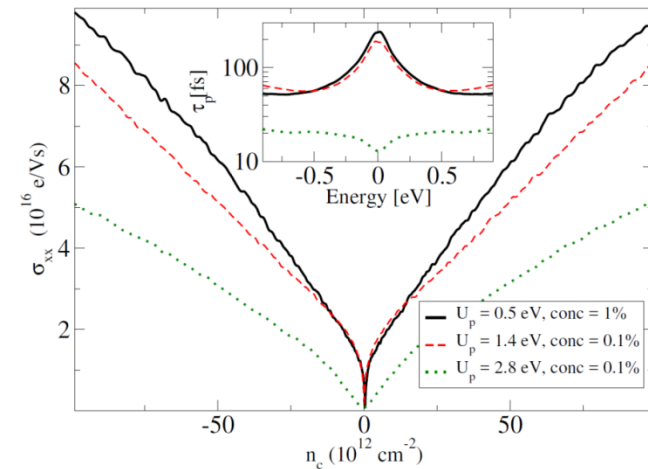
Wang et al, **PHYSICAL REVIEW X 6, 041020 (2016)**



Localization effects for graphene/WS₂ + el-h puddles

Scaling theory of localization

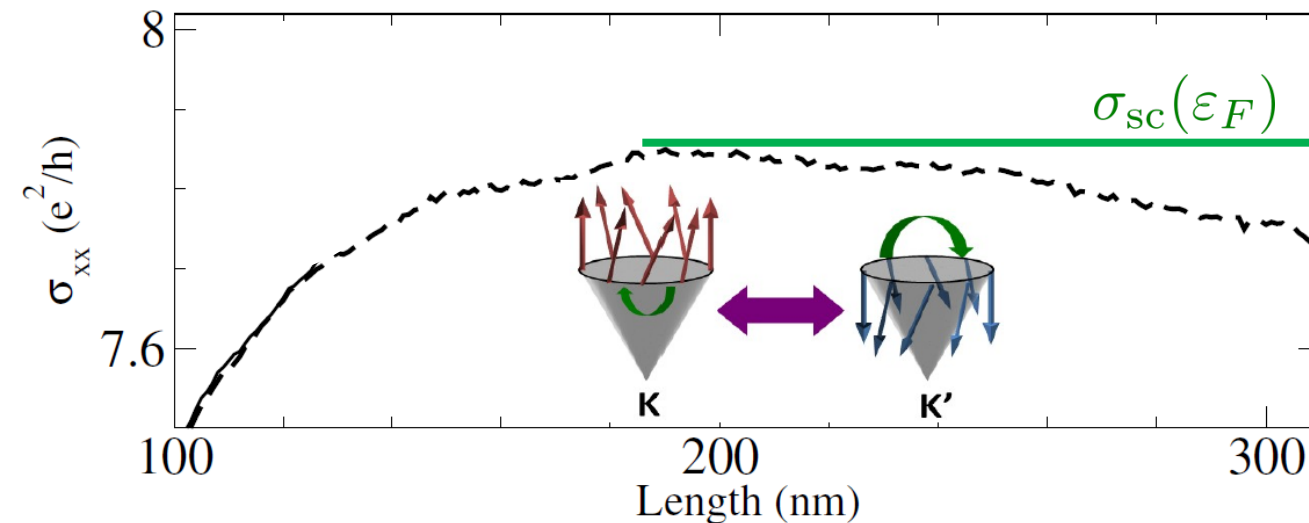
$$\sigma_{XX}(\varepsilon_F) = \sigma_{SC}(\varepsilon_F) + \delta\sigma(\varepsilon_F)$$



$$\tau_p = \frac{\sigma_{SC}(\varepsilon_F)}{v_F^2 \rho(\varepsilon_F)}$$

Case of strong scatterers (puddles) and large intervalley scattering

SOC switch OFF



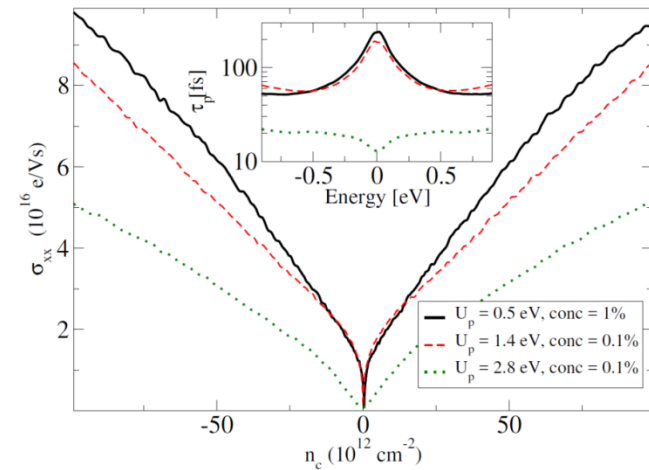
$$\delta\sigma = -\frac{2e^2}{\pi h} \log(L/\ell_e)$$

Weak localization

Localization effects for graphene/WS₂ + el-h puddles

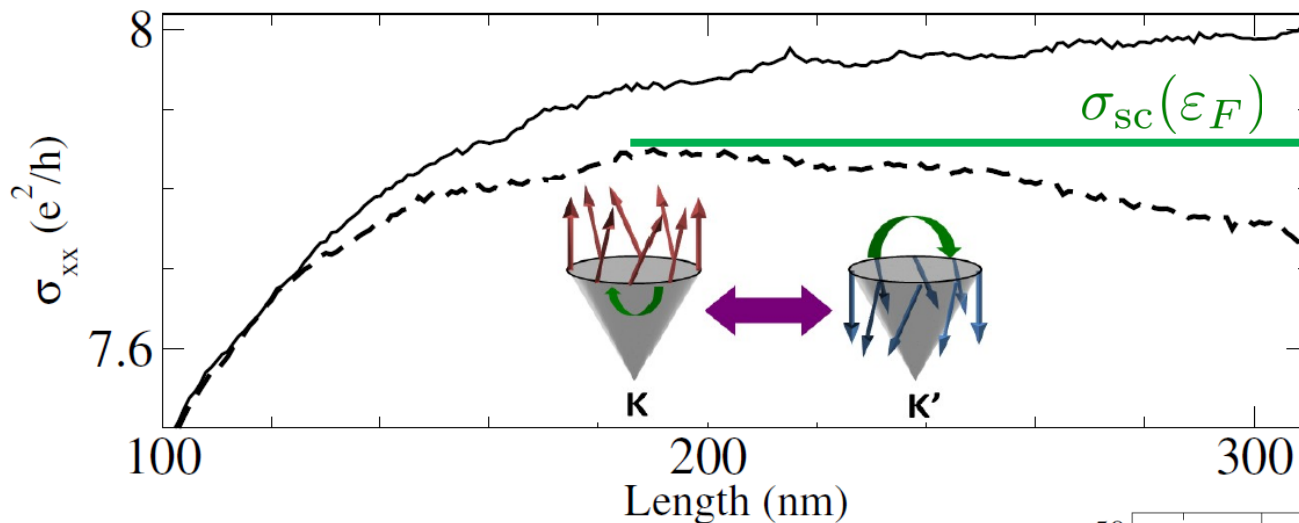
Scaling theory of localization

$$\sigma_{XX}(\varepsilon_F) = \sigma_{SC}(\varepsilon_F) + \delta\sigma(\varepsilon_F)$$



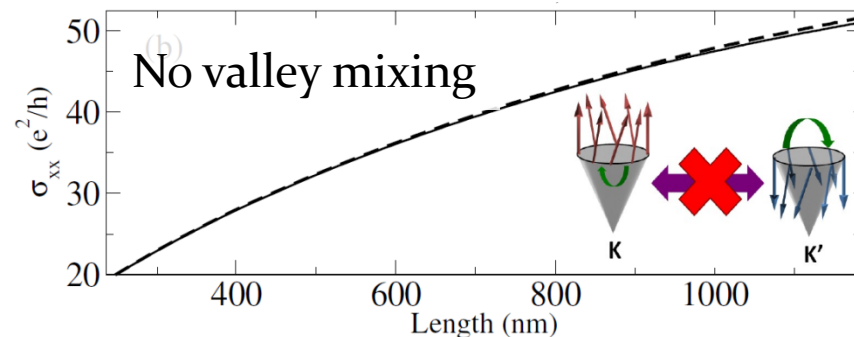
Case of strong scatterers (puddles) and large intervalley scattering

SOC switch ON



$$\delta\sigma = + \frac{2e^2}{\pi h} \log(L/\ell_e)$$

Weak Antilocalization



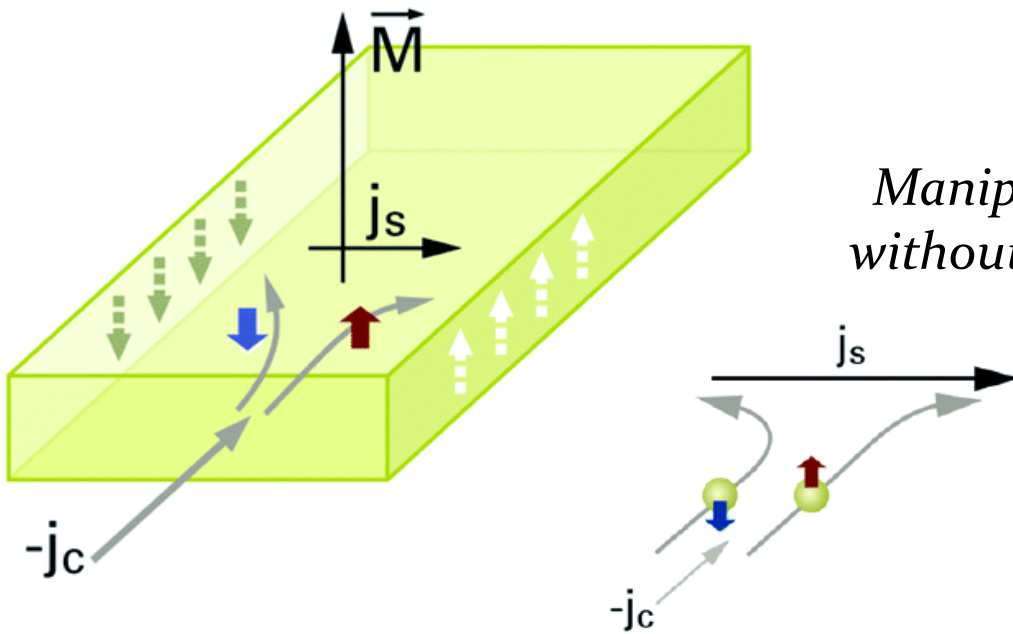
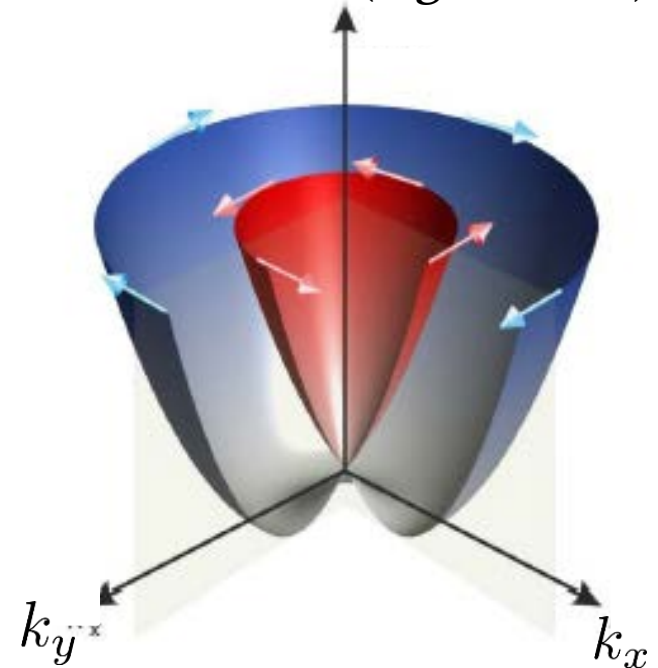
Spin Hall Effect

Manipulation of spin by electrical means without the use of ferromagnetic materials or magnetic fields

Intrinsic mechanism

Sinova (2005),...

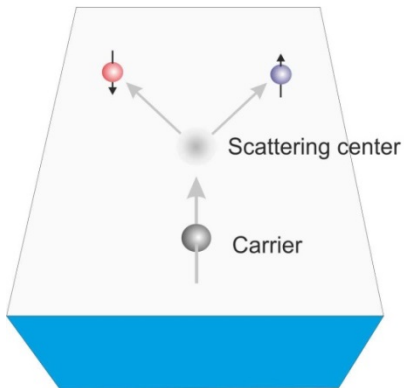
Band Structure (e.g. Rashba)



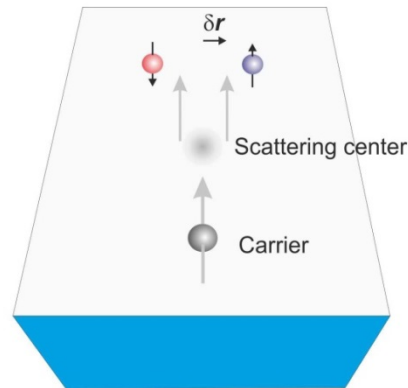
Extrinsic mechanisms

Dyakonov-Perel (1971); Hirsh (1999)

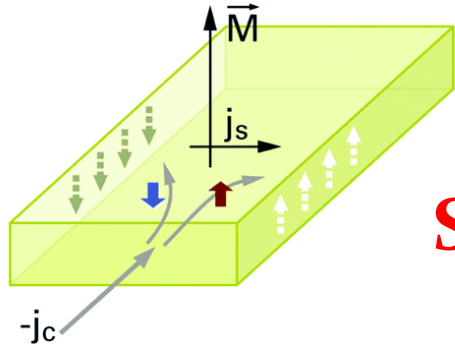
Skew Scattering



Side-Jump Scattering



Computing SHE figure of merit in clean/disordered graphene/TMDC interfaces

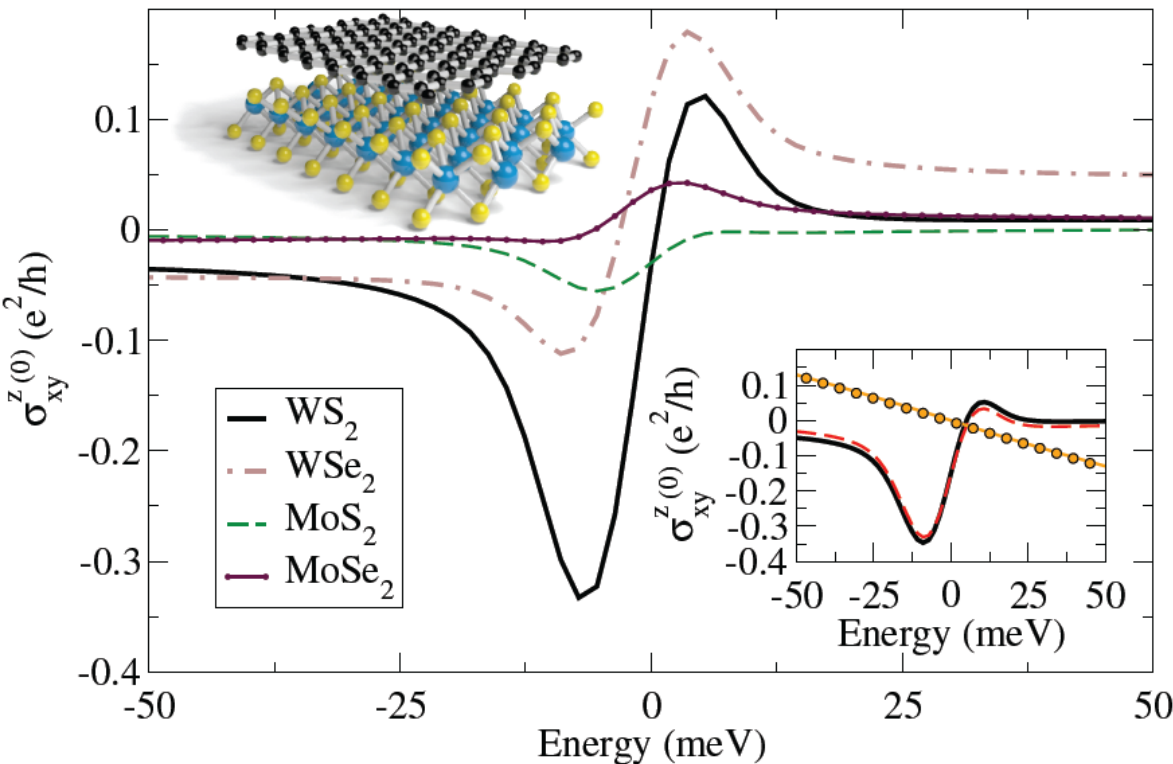


$$\theta_{sH}$$

Spin Hall angle

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

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



Dissipative SHE

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

“Clean case” :

“intrinsic SHE”

WS₂ leads to larger Spin Hall conductivity (larger SHA)

Spin Hall Kubo conductivity

in large scale disordered graphene models

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

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

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

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

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

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

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**

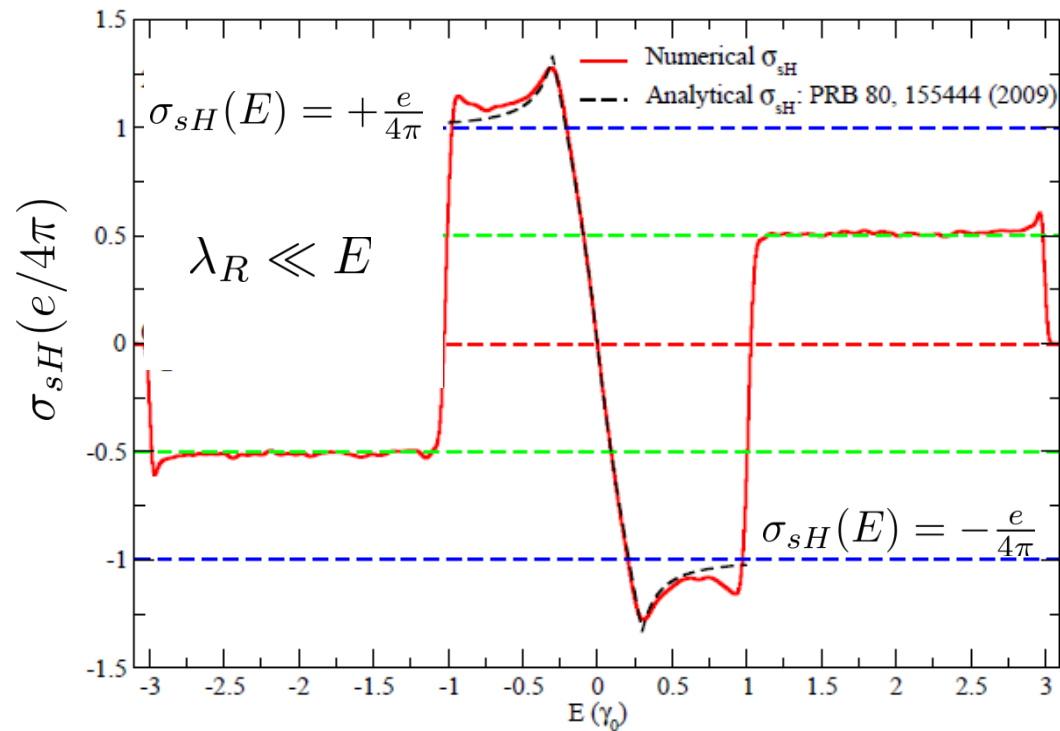
Validation: homogeneous SOCs

Homogeneous Rashba SOC λ_R (no intrinsic SOC)

Analytical result for the spin Hall conductivity

A. Dyrdal, V. K. Dugaev, and J. Barnas, **Phys. Rev. B. 80, 155444 (2009)**

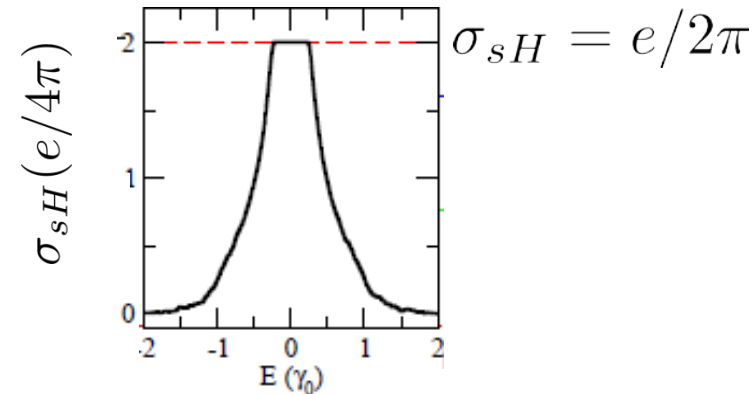
$$\sigma_{sH}(E) = \begin{cases} -\frac{e}{4\pi} \frac{\text{sign}(E)E^2}{(E^2 - \lambda_R^2)} & \text{for } |E| \geq 2\lambda_R \\ -\frac{e}{4\pi} \frac{E(E + 2\text{sign}(E)\lambda_R)}{2\lambda_R(E + \text{sign}(E)\lambda_R)} & \text{for } |E| < 2\lambda_R \end{cases}$$



Homogeneous intrinsic SOC
(QSHE)

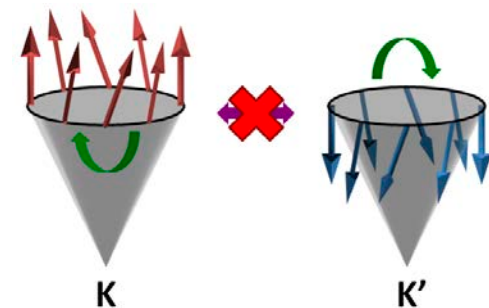
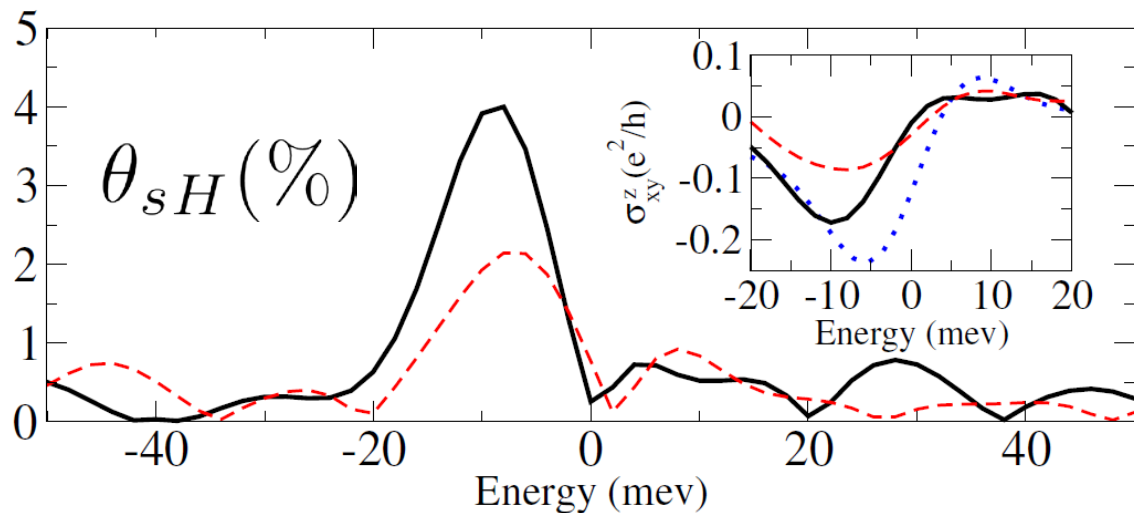
Plateau in the bulk bandgap

Sheng, Sheng, Ting, Haldane,
Phys. Rev. Lett. 95, 136602 (2005)

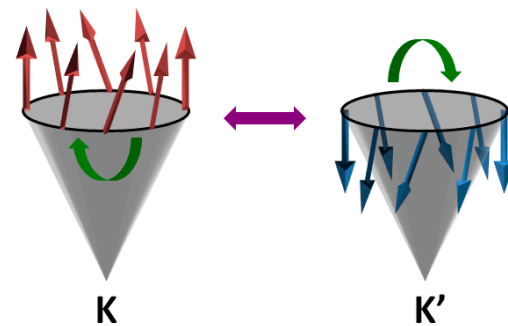
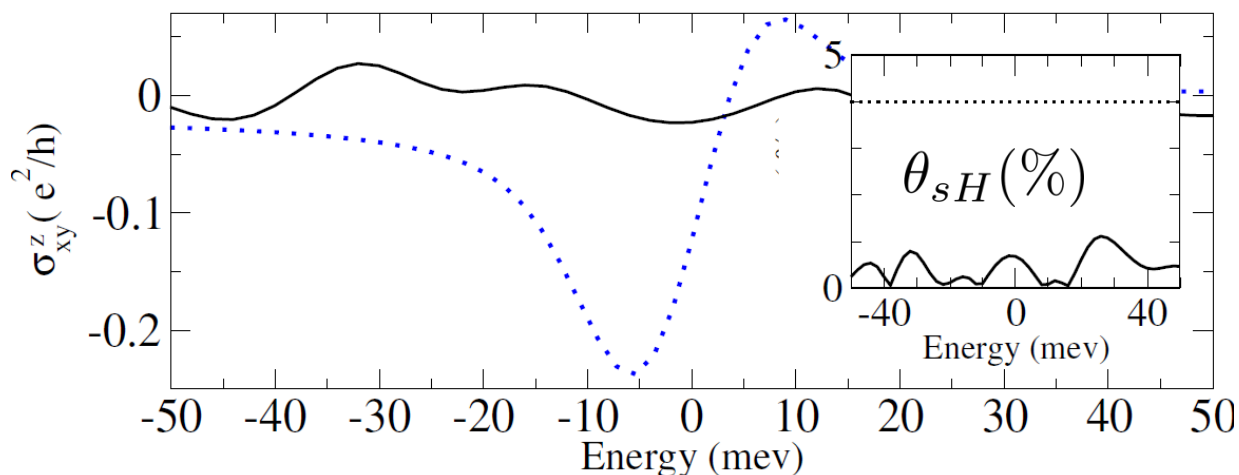


Spin Hall Effect

in disordered graphene/TMDC interfaces

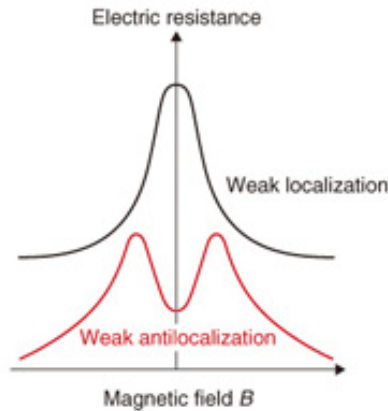
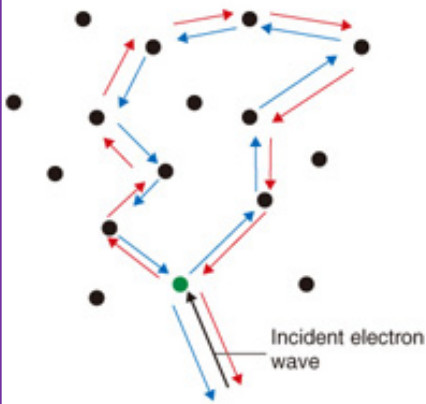
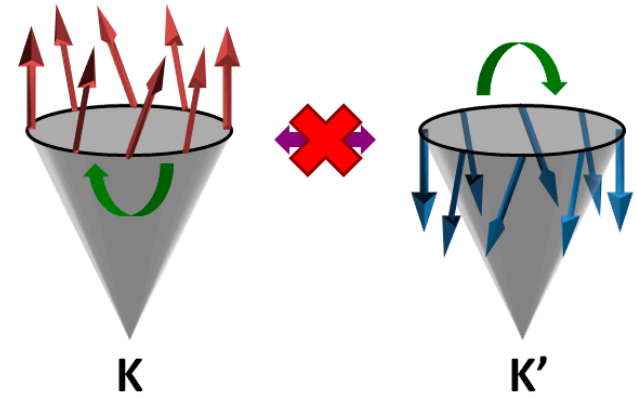
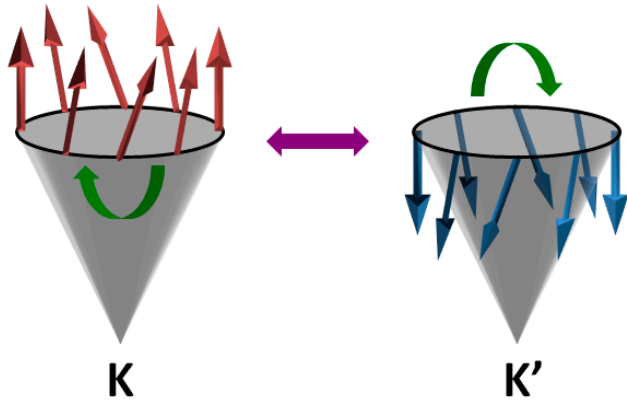


$$\theta_{sH}(\%) \simeq 4\%$$



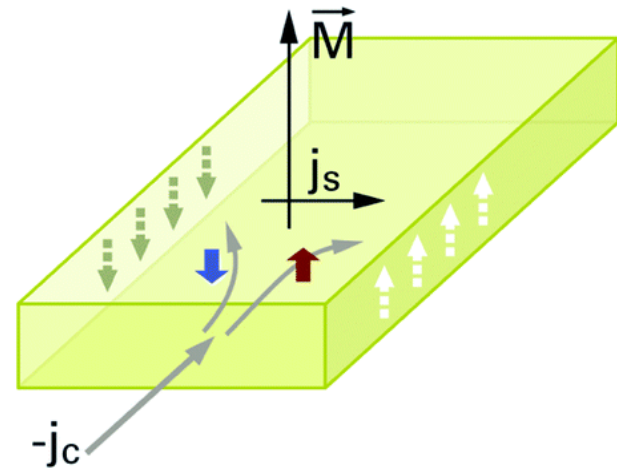
$$\theta_{sH}(\%) \ll 1\%$$

Weak antilocalization vs Spin Hall Effect



(a) Generation mechanism

(b) Magneto-resistance effect



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

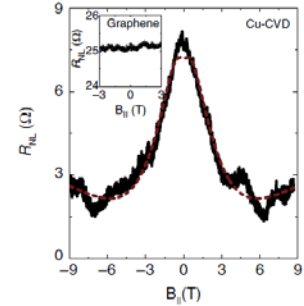
$$\frac{\tau_{s,\perp}}{\tau_{s,\parallel}} = 1/2$$

SHE induced by metallic ad-atoms onto graphene

ARTICLE

Received 17 Apr 2014 | Accepted 18 Jul 2014 | Published 1 Sep 2014

DOI: 10.1038/ncomms5748



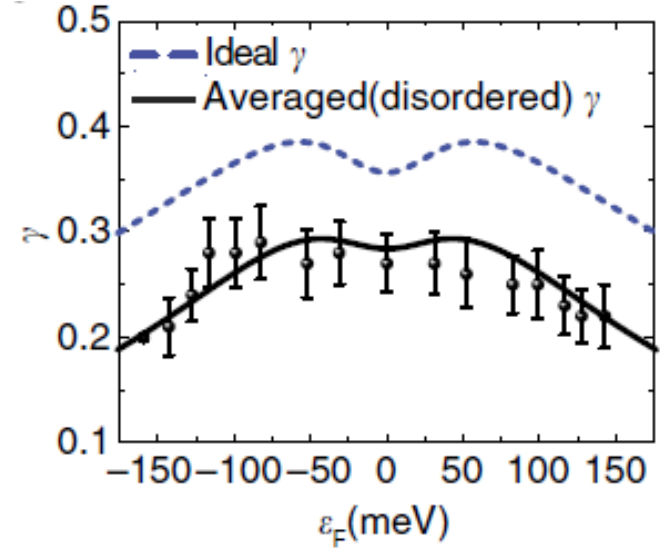
Giant spin Hall effect in graphene grown by chemical vapour deposition

Jayakumar Balakrishnan^{1,2,*}, Gavin Kok Wai Koon^{1,2,3,*}, Ahmet Avsar^{1,2}, Yuda Ho^{1,3}, Jong Hak Lee^{1,2}, Manu Jaiswal^{1,2,†}, Seung-Jae Baeck⁴, Jong-Hyun Ahn⁴, Aires Ferreira^{1,2,5}, Miguel A. Cazalilla^{2,6}, Antonio H. Castro Neto^{1,2} & Barbaros Özyilmaz^{1,2,3}

Table 1 | Graphene decorated with metallic adatoms.

Adatom	Mobility ($\text{cm}^2\text{V}^{-1}\text{s}^{-1}$)	λ_s (μm)	γ	Δ (meV)
Cu-CVD	11,000	1.9	0.17	14.4
Cu-EPG	9,000	1.1	0.27	17.4
Au-EPG	15,000	2.0	0.15	18.0

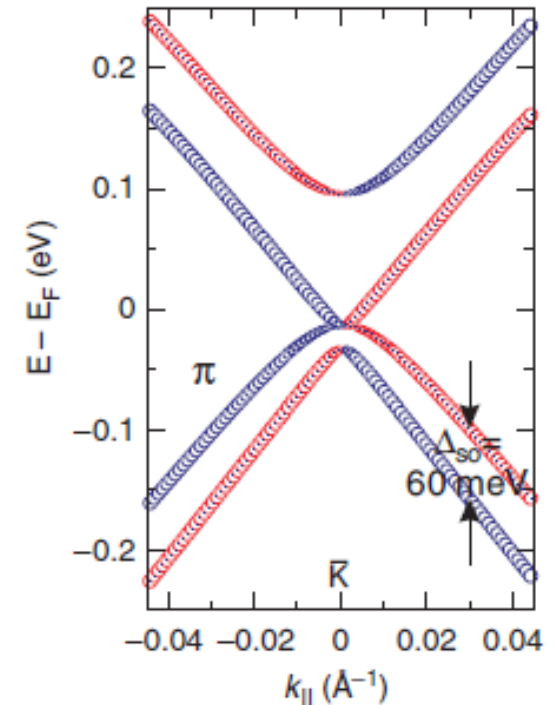
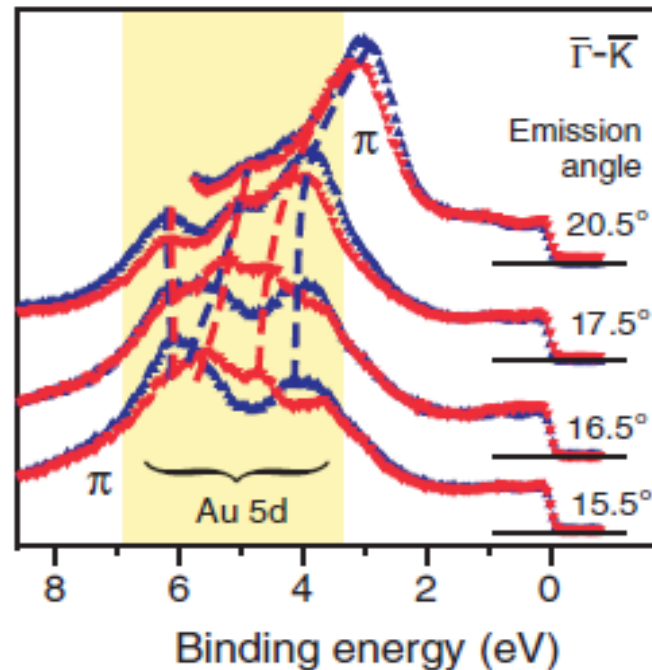
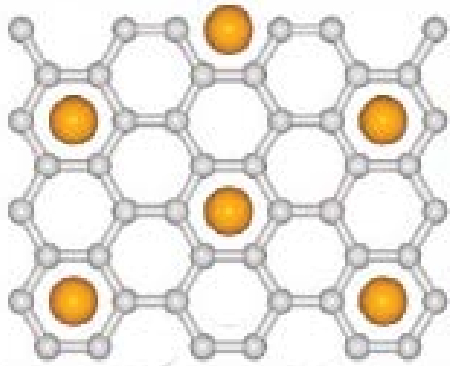
CVD, chemical vapour deposition; EPG, exfoliated pristine graphene.
The extracted values for Δ assume predominant intrinsic SOC (see main text).



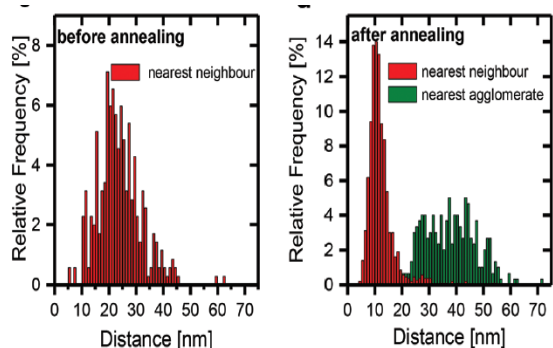
intrinsic-like spin-orbit interaction
(20meV), Elliot-Yafet and skew scattering

Giant Rashba Splitting in graphene hybridized with Au-adatoms

D. Marchenko et al, **Nature Comm. 3 (1232), 2012**

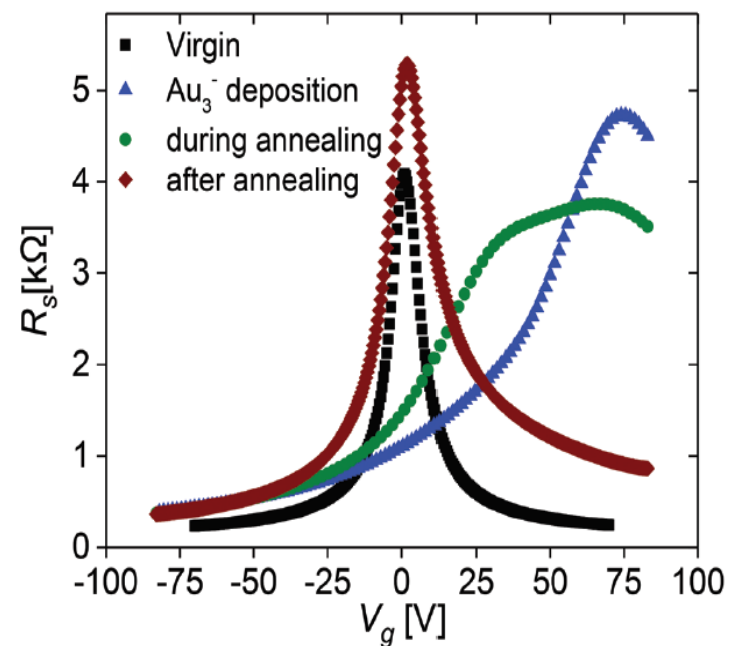
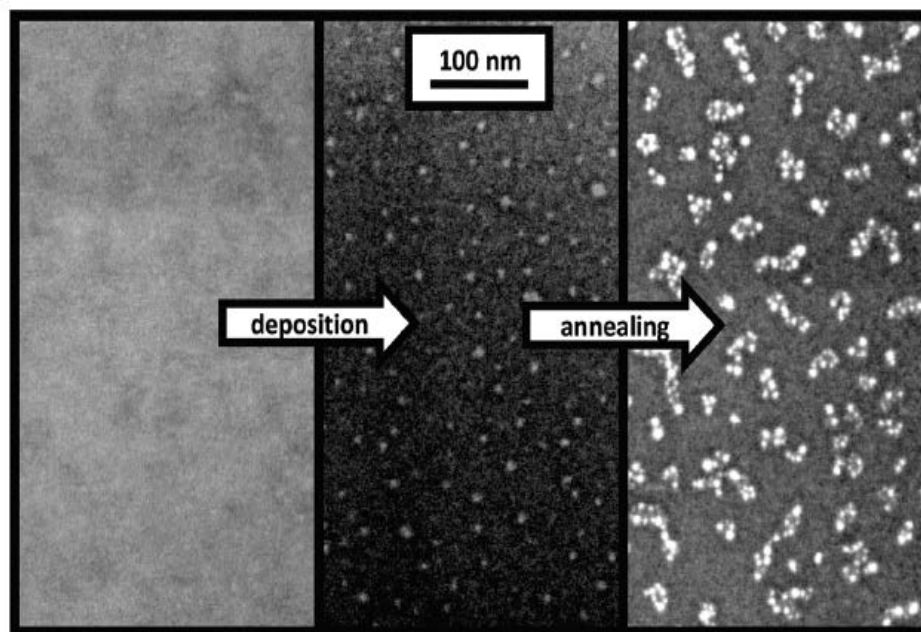


Au intercalation at the graphene–Ni interface creates a **giant spin–orbit splitting (60 meV)**



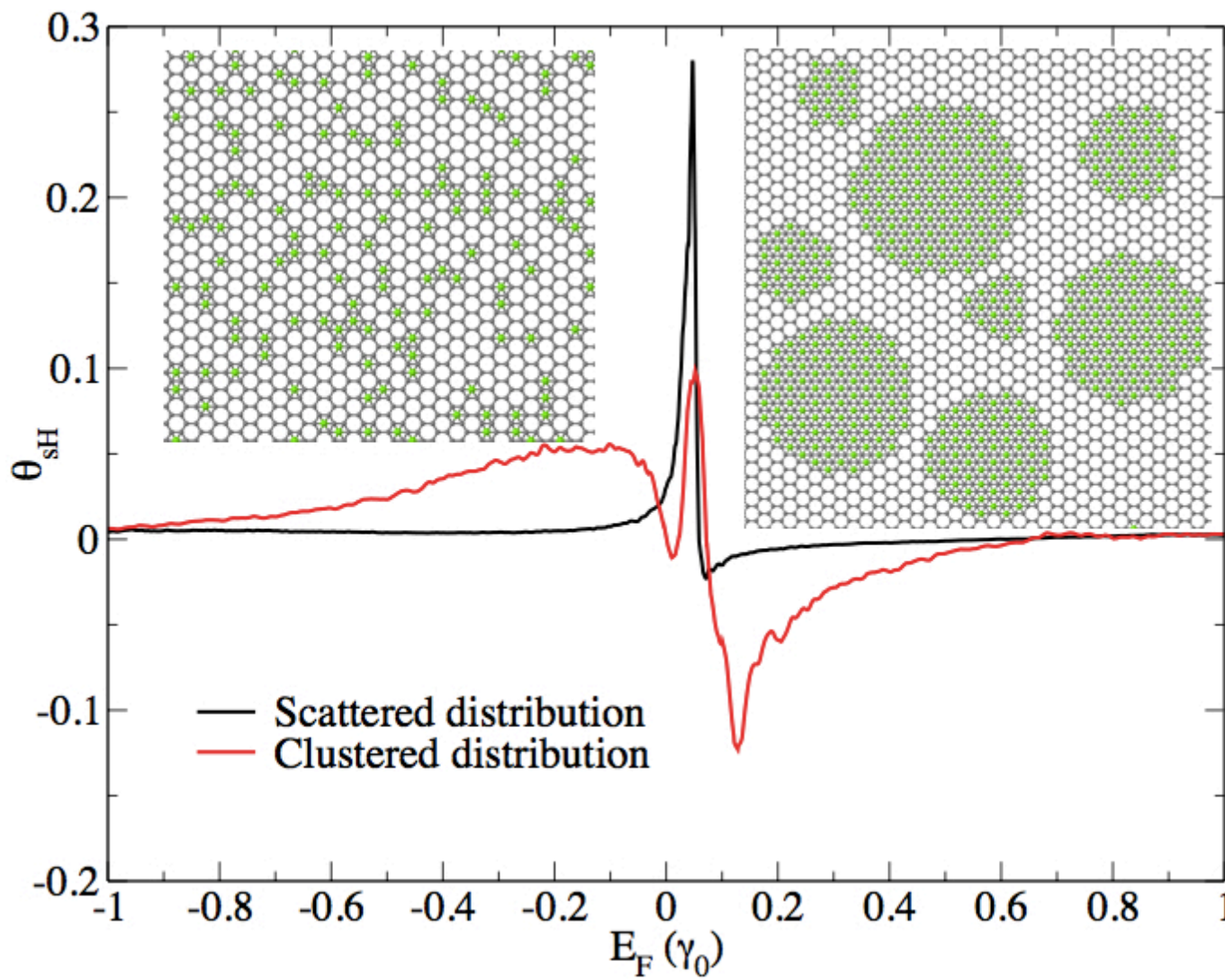
Decorating graphene with size-selected few-atom clusters: a novel approach to investigate graphene–adparticle interactions†

Jeroen E. Scheerder,^a Thomas Picot,^a Nicolas Reckinger,^b Tomas Sneyder,^a Vyacheslav S. Zharinov,^a Jean-François Colomer,^b Ewald Janssens^a and Joris Van de Vondel^a



Spin Hall angles

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



$$\theta_{\text{sH}}^{\text{max}} \sim 0.1 - 0.3$$

(Zero-temperature)

Impact of segregation
varies with energy

For same cluster density
and distribution

***Intrinsic SOC gives
rise to larger SHA
than Rashba-SOC***

Far from dilute limit!!!

SHA not expected to
be larger for much lower
density...

Multiple Quantum Phases in Graphene with Enhanced Spin-Orbit Coupling: From the Quantum Spin Hall Regime to the Spin Hall Effect and a Robust Metallic State

Alessandro Cresti,^{1,2} Dinh Van Tuan,^{3,4} David Soriano,³ Aron W. Cummings,³ and Stephan Roche^{3,5}

¹*Univ. Grenoble Alpes, IMEP-LAHC, F-38000 Grenoble, France*

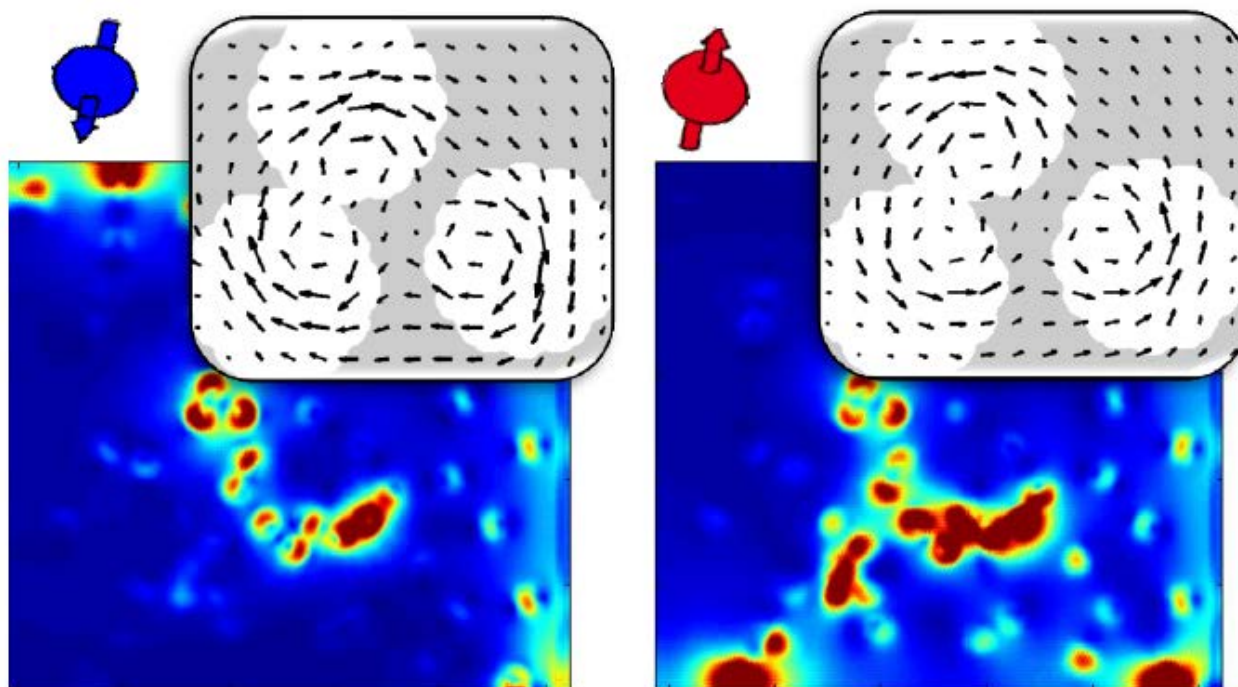
²*CNRS, IMEP-LAHC, F-38000 Grenoble, France*

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(Received 21 December 2013; published 9 December 2014)



Non-local transport & topological effects

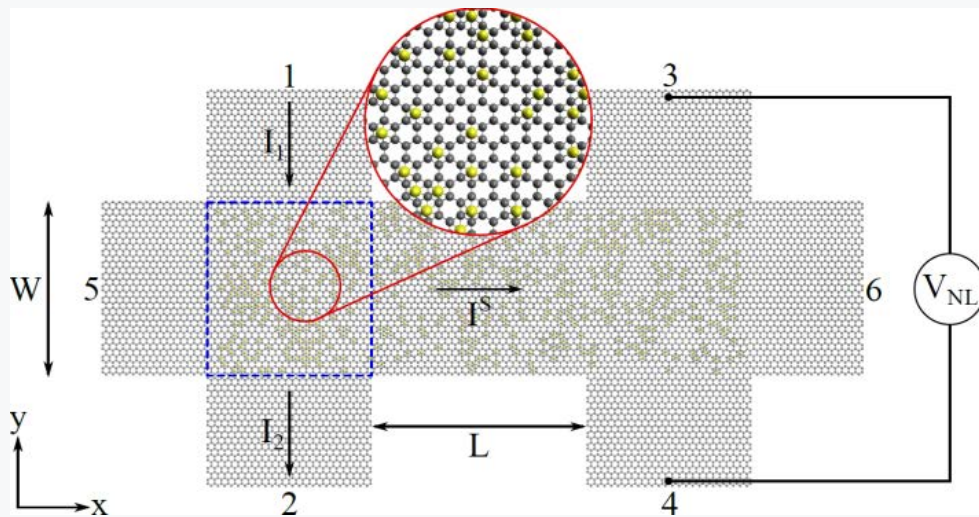
PRL 117, 176602 (2016)

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*
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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)



$$\theta_{\text{SH}} = I_5^S / I_1$$



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University of Delaware, USA

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David Soriano



Marc Vila

Spintronics Coworkers



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(Univ. Regensburg)



Xavier Waintal
(CEA)



Sergio Valenzuela
(ICN2)

“Introduction to Graphene-Based Nanomaterials From electronic structure to Quantum Transport”



<http://www.introductiontographene.org/>

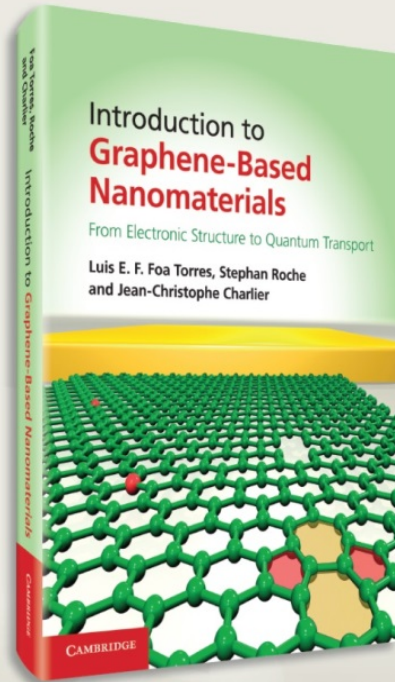
Introduction to Graphene-Based Nanomaterials

From Electronic Structure to Quantum Transport

Luis E. F. Foa Torres, Universidad Nacional de Córdoba, Argentina
Stephan Roche, Catalan Institute of Nanotechnology - ICN
Jean-Christophe Charlier, Université Catholique de Louvain, Belgium

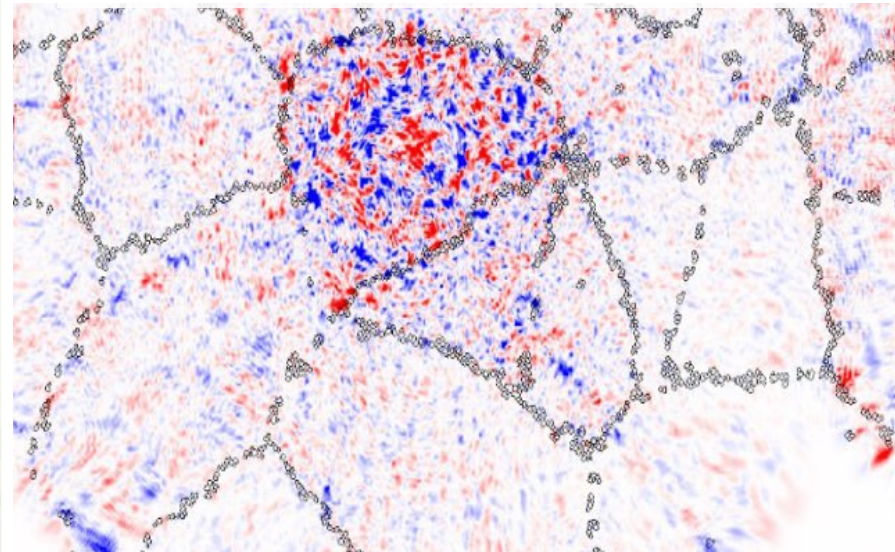
Beginning with an introduction to carbon-based nanomaterials, their electronic properties, and general concepts in quantum transport, this detailed primer describes the most effective theoretical and computational methods and tools for simulating the electronic structure and transport properties of graphene-based systems. Transport concepts are clearly presented through simple models, enabling comparison with analytical treatments, and multiscale quantum transport methodologies are introduced and developed in a straightforward way, demonstrating a range of methods for tackling the modelling of defects and impurities in more complex graphene-based materials. The authors also discuss the practical applications of this revolutionary nanomaterial, contemporary challenges in theory and simulation, and longterm perspectives. Containing numerous problems for solution, real-life examples of current research, and accompanied online by further exercises, solutions and computational codes, this is the perfect introductory resource for graduate students and researchers in nanoscience and nanotechnology, condensed matter physics, materials science and nanoelectronics.

- Provides a deep exploration of quantum transport in disordered graphene-based materials
- Covers all members of the sp² family (nanotubes, graphene ribbons, monolayer and multilayer graphene) as well as some chemical derivatives
- An excellent starting point for new researchers in the field



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Thank you!

