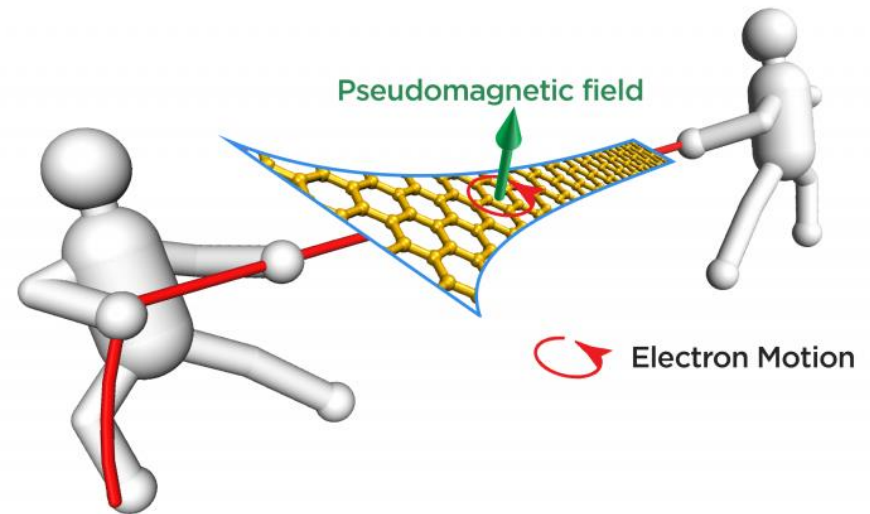
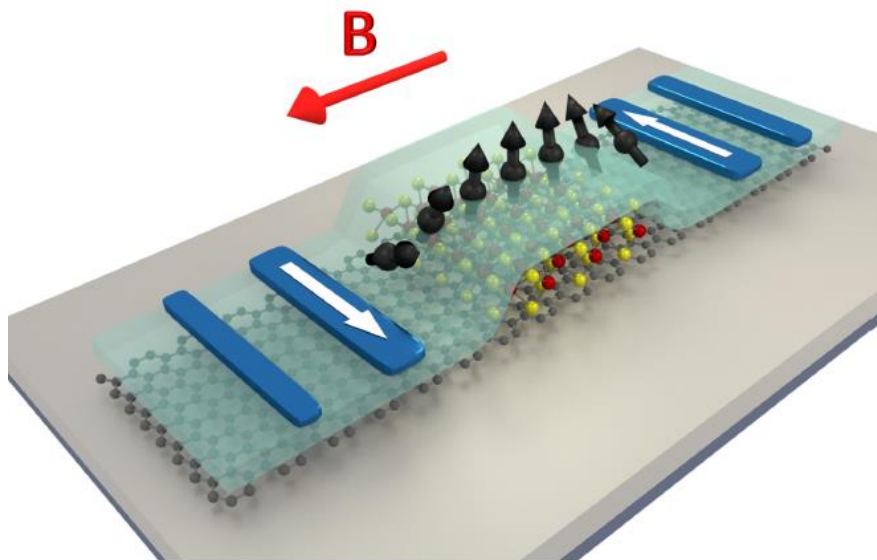


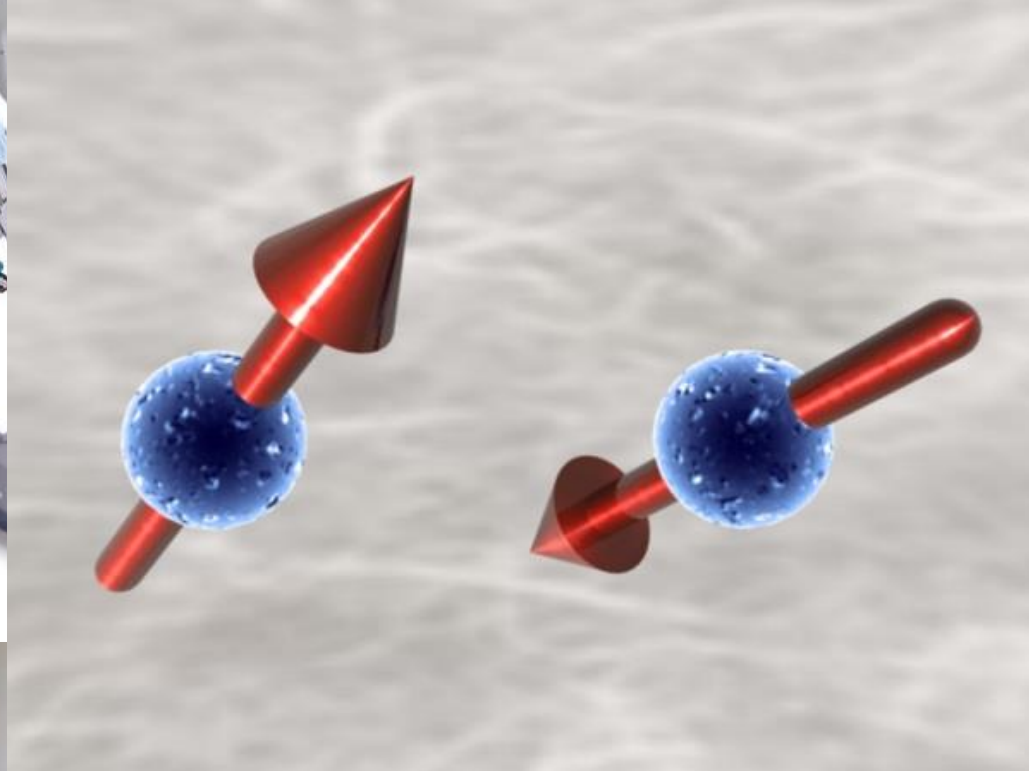
# 2D materials for Spin/Valleytronics Theoretical Perspective

Stephan Roche  **ICREA**



# Spintronics inside !

ROBOTICS/SURGERY



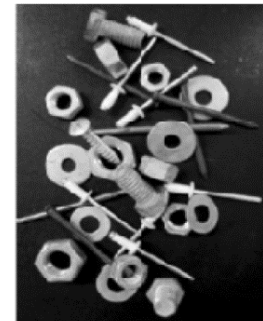
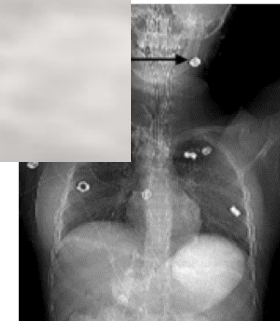
POINT-OF-CARE DIAGNOSTICS



Sensors

WELDING

COMPASS

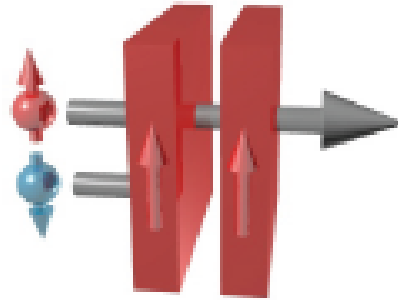
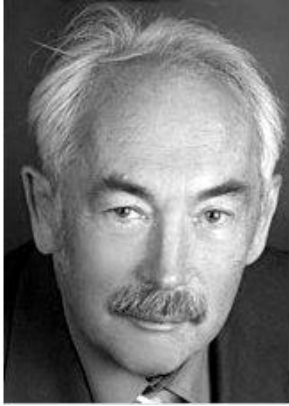
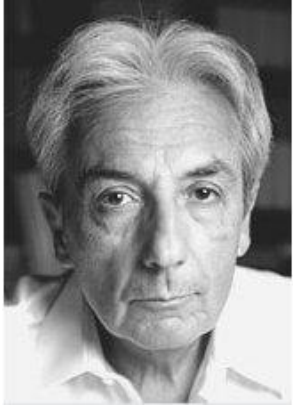


LOCATION OF SHRAPNEL

# Spintronics and its industrial/Societal impact

Albert Fert

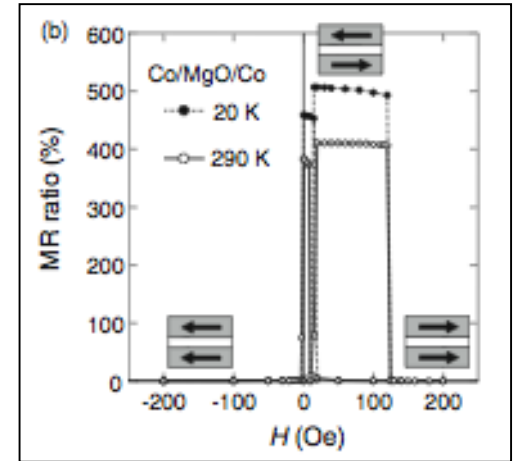
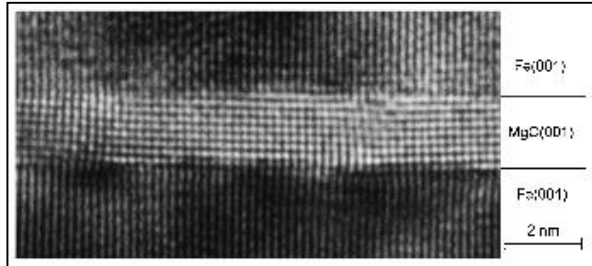
Peter Grünberg



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



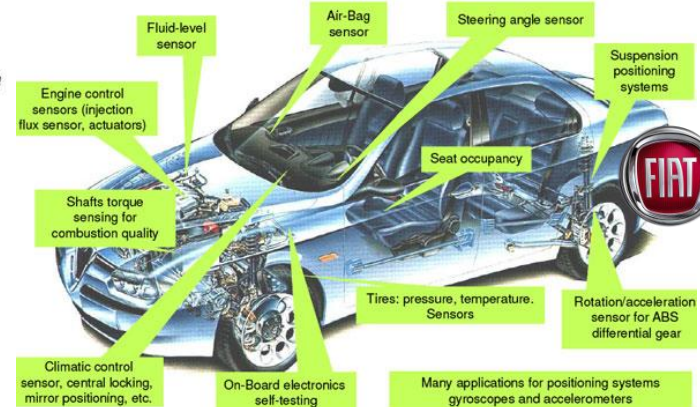
2007 Physics Nobel Laureates



*Magnetic field sensors used to read data in hard disk drives,  
Microelectromechanical systems  
Minimally invasive surgery*

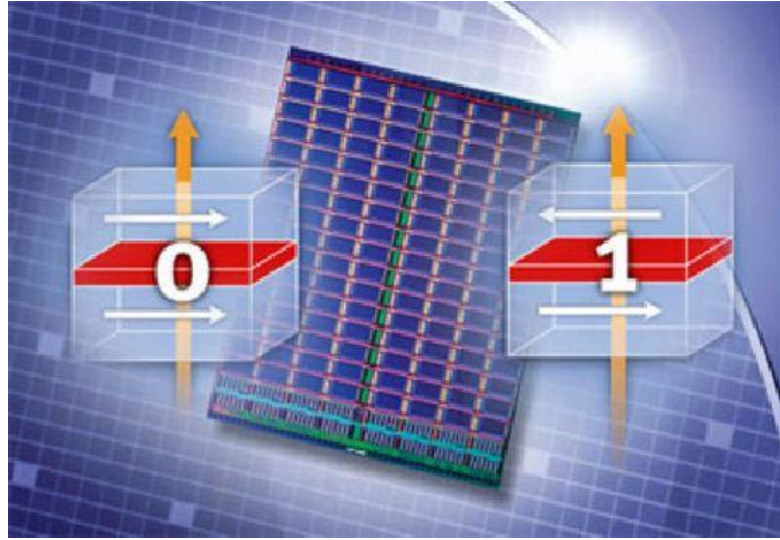


*Automotive sensors for fuel handling system,  
Anti-skid system, speed control & navigation*

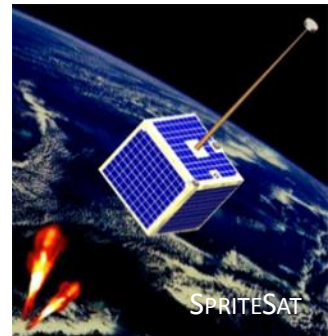


# Data Storage & TMR

## Magnetic junctions and MRAM



MEMORY BUFFER SSD



AEROSPACE



AERONAUTICS



AUTOMOTIVE



RAID SERVERS



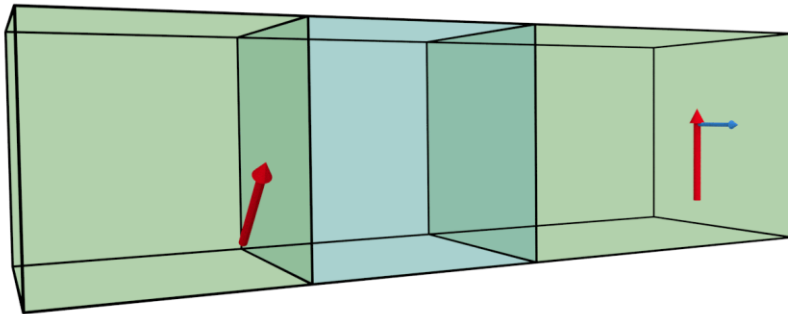
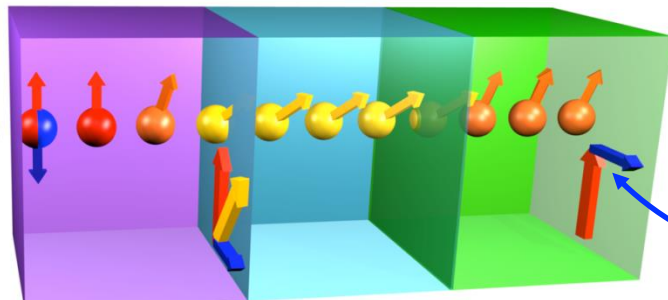
FACTORY AUTOMATIZATION

# Advanced generation of Spin Transfer Torque MRAM

(proposed by Slonczewski, Berger 1996)

## Spin Transfer Torque

Ferro 1    Spacer    Ferro 2



**256Mb in production 2018**



**2016**



**SAMSUNG**

In production  
for 2019

## *Why Spintronics using 2D Materials ?*

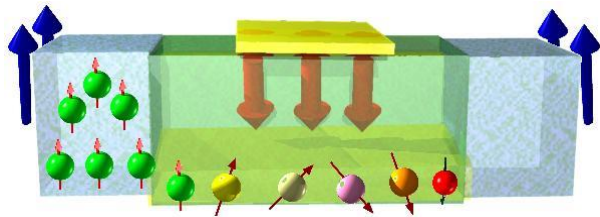
*Proximity effects in 2D Materials-based heterostructures  
(spin dynamics & relaxation, SHE, weak antilocalization,  
QSHE)*

*Generating valley polarized quantum transport  
(valleytronics)*

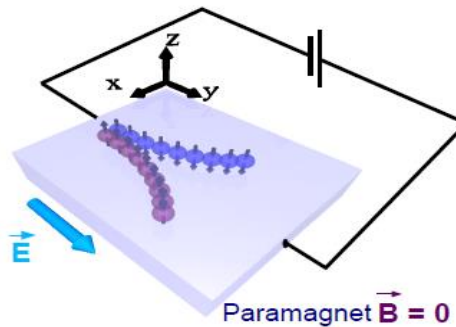
# Spin-based information processing ?

Active devices based on **Spin manipulation** ?

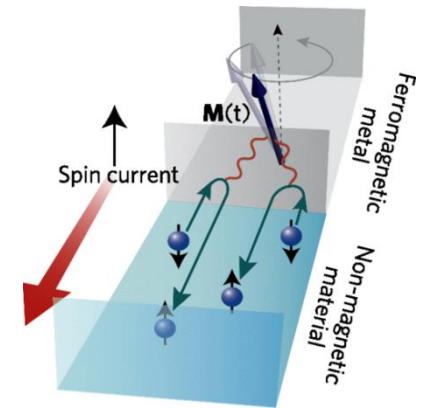
**Datta-Das  
spin transistor**



**Spin Hall Effect/QSHE**



**Spin torques/pumping**

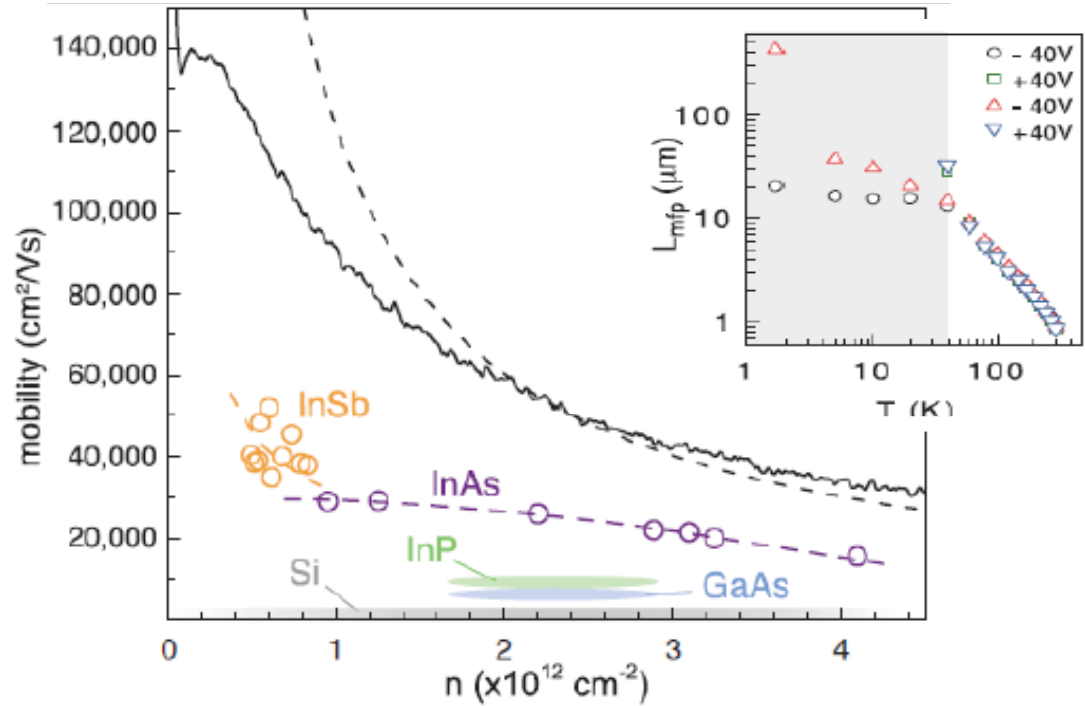
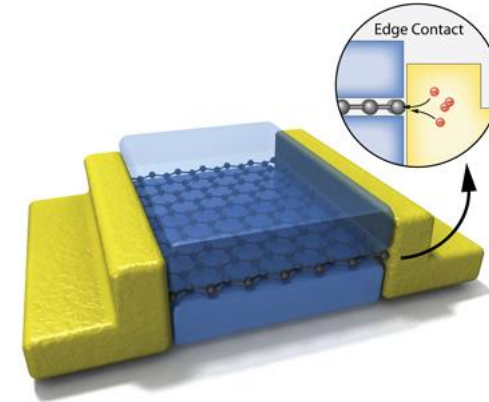
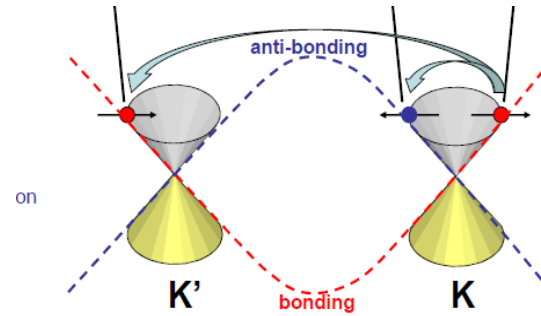


**Need for spin information transport on long distance (room T)  
Spin injection and detection (ferromagnets/non magnetic materials)**

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

# What makes graphene attractive

- Ambipolar/tuneable transport
- **Linear energy dispersion & 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





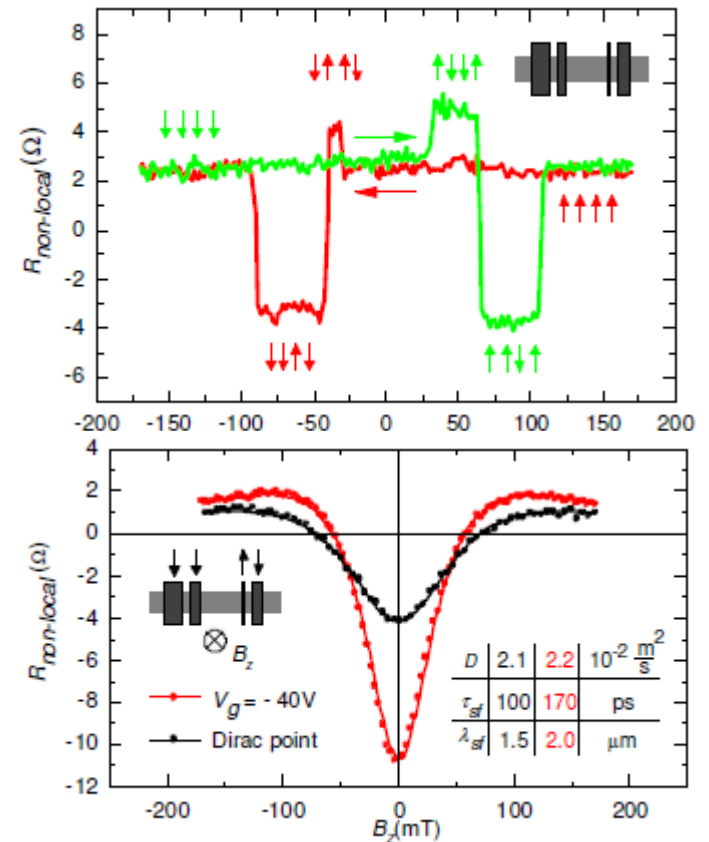
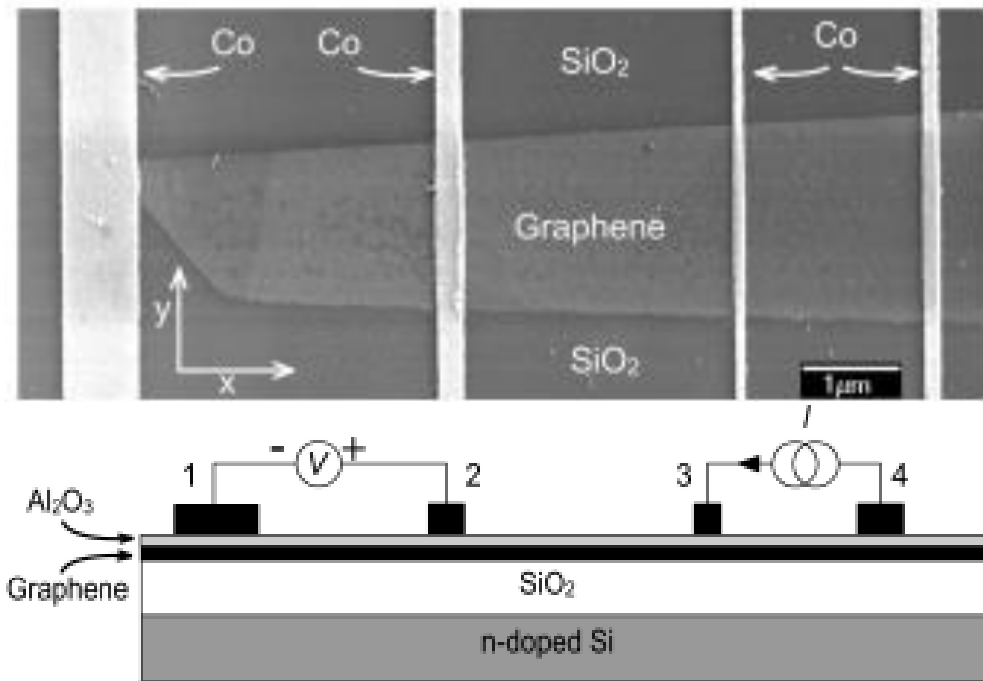
nature

10 years ago !



N. Tombros, ... Bart J. van Wees

Nature 448, 571-574 (2 August 2007)



“non-local” spin valve geometry  
+ Hanle spin precession  
measurements

Spin diffusion length  **$2 \mu m$  (RT)**

# Spin diffusion length in epitaxial graphene

B. Dluback et al, A. Fert  
**Nature Phys. 8,557 (2012)**

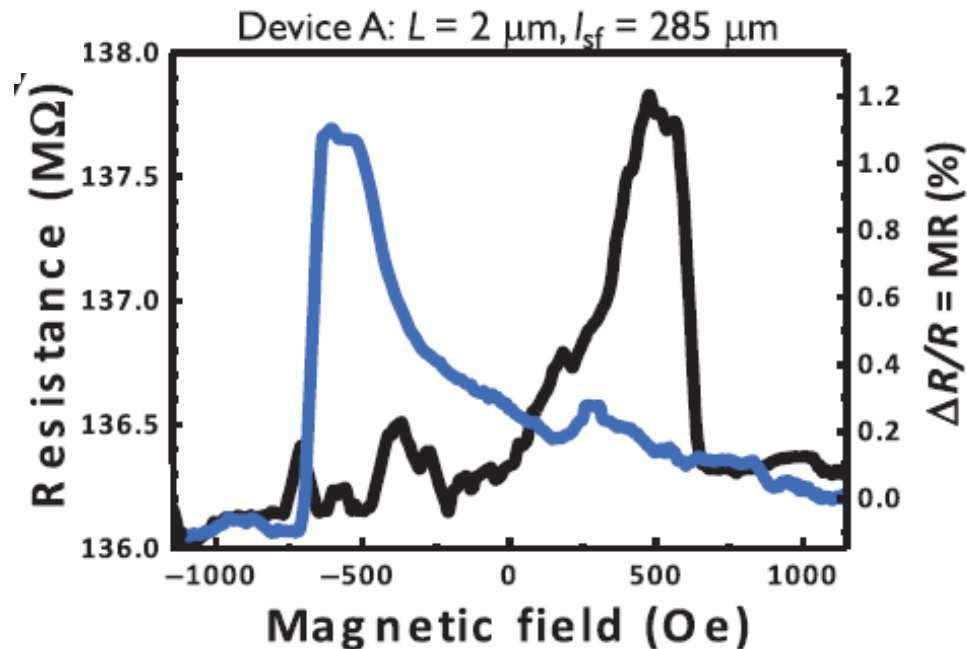
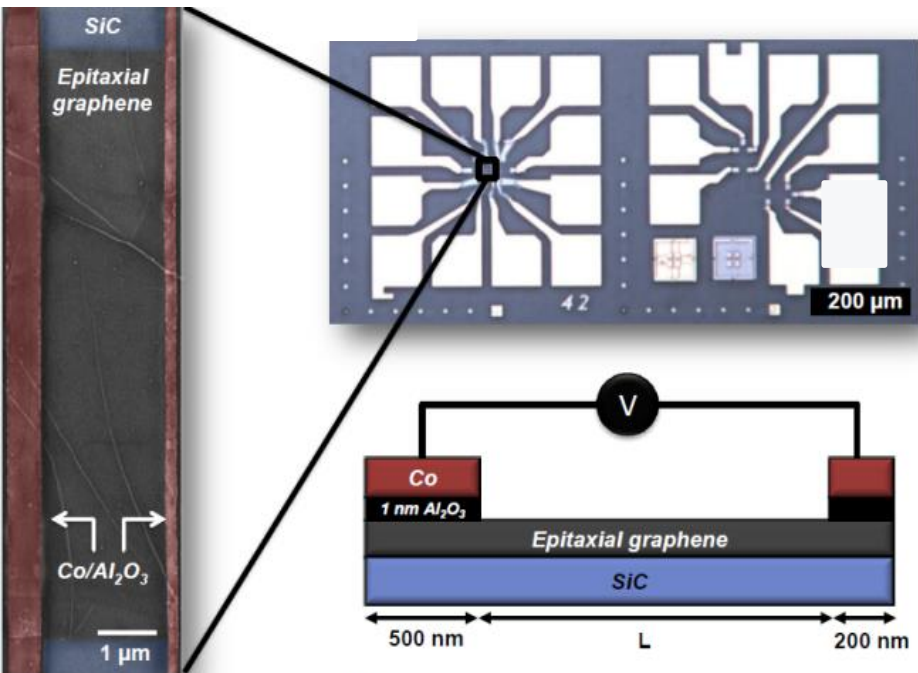


THALES



*2-T magnetoresistance*

*Spin diffusion length up to **100  $\mu\text{m}$** (RT)*



# Graphene Flagship



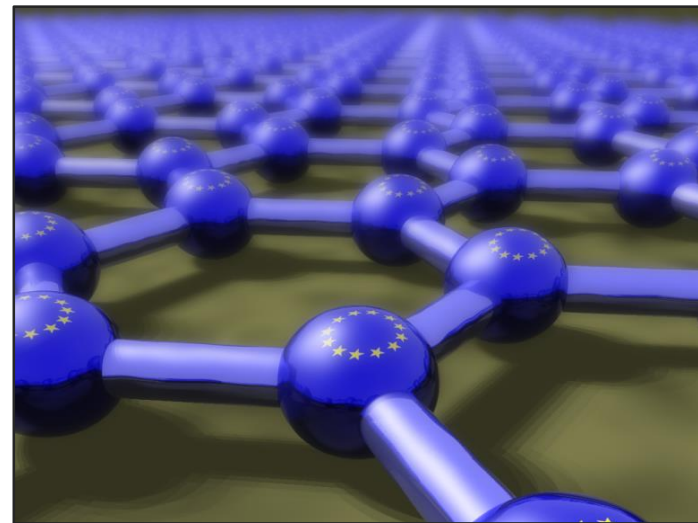
Europe has chosen Graphene Flagship as one of only two FET projects, with

**1,000 million € over 10 years...**

**Launch in 2013**

*“to take graphene and related layered materials from academic laboratories to society, revolutionize multiple industries and create economic growth and new jobs in Europe.”*

- 154 partners with in 17 EU countries with an
- Potential applications include:
  - flexible consumer electronics
  - lighter and more energy efficient airplanes
  - optical devices and artificial retinas
  - functional lightweight components
  - advanced batteries
  - **-spintronics**





university of  
 groningen



**Experimental partners**

Univ. of Groningen [RUG] : **Bart van Wees**

Univ. of Manchester [UNIMAN] : **Irina Grigorieva**

Univ. of Aachen [RWTH] : **Christoph Stampfer, Bernd Beschoten**

Univ. of Basel [UNIBAS]: **Christian Schönenberger**

CNRS/Thales [CNRS]: **Pierre Seneor and Albert Fert**

Chalmers University Technology [CUT]: **Saroj Dash**

Catalan Inst. Nanoscience & Nanotech [ICN<sub>2</sub>]: **Sergio Valenzuela**

NanOSC AB : **Johan Åkerman**



**Theoretical partners:**

Catalan Inst. Nanoscience & Nanotech [ICN<sub>2</sub>]: **Stephan Roche**

Université Catholique de Louvain [UCL]: **Jean Christophe Charlier**

University of Regensburg [UREG] : **Jaroslav Fabian**

Commissariat à l'Énergie Atomique [CEA]: **Mairbek Chshiev, Xavier Waintal**

IMDEA : **Paco Guinea**



Universität Regensburg





*“The global objective of the Graphene Spintronics task force is to establish the **ultimate scientific and technological potential of graphene and graphene related materials for spintronics**, targeting efficient spin injection, transport and detection but also demonstrating spin gating and spin manipulation in graphene spintronic devices and realizing operational devices for information storage and information processing, by engineering device architecture and material transformations”*



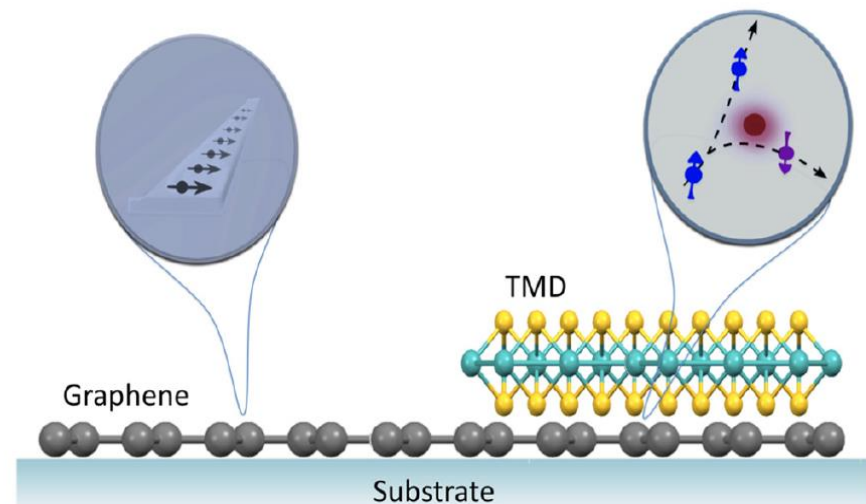
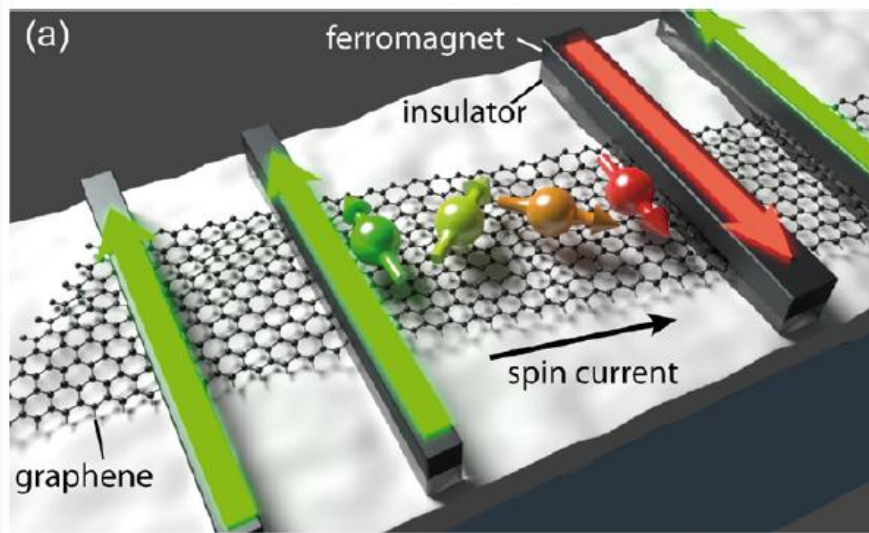
2D Materials

EDITORIAL

## Graphene spintronics: the European Flagship perspective

Stephan Roche<sup>1,2</sup>, Johan Åkerman<sup>3,4,5</sup>, Bernd Beschoten<sup>6</sup>, Jean-Christophe Charlier<sup>7</sup>, Mairbek Chshiev<sup>8,9</sup>, Saroj Prasad Dash<sup>10</sup>, Bruno Dlubak<sup>12</sup>, Jaroslav Fabian<sup>11</sup>, Albert Fert<sup>12</sup>, Marcos Guimarães<sup>13,19</sup>, Francisco Guinea<sup>14,15</sup>, Irina Grigorieva<sup>14</sup>, Christian Schönberger<sup>16</sup>, Pierre Seneor<sup>12</sup>, Christoph Stampfer<sup>17</sup>, Sergio O Valenzuela<sup>1,2</sup>, Xavier Waintal<sup>9,18</sup> and Bart van Wees<sup>19</sup>

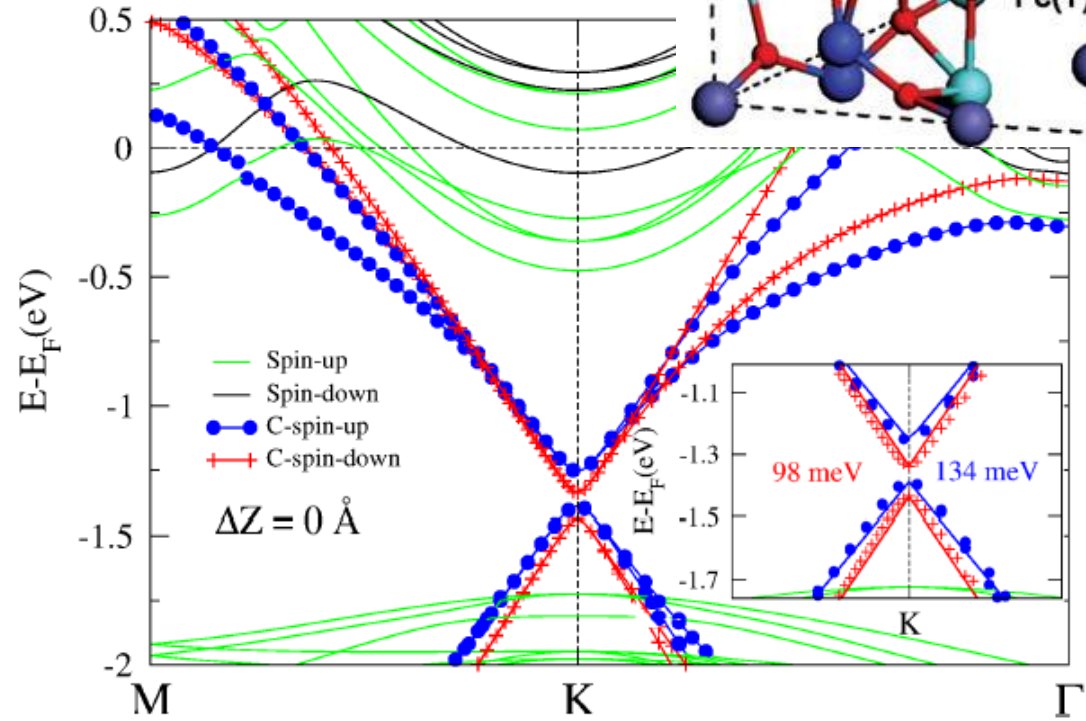
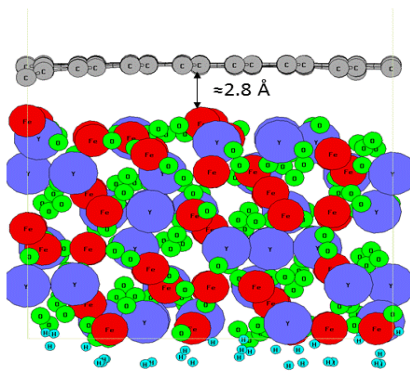
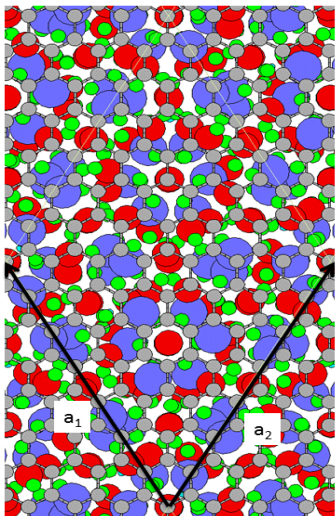
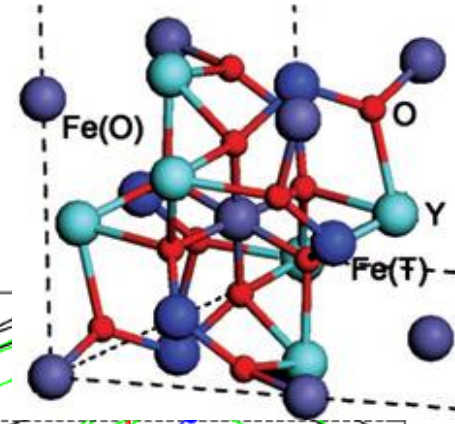
*2D Mater.* 2 (2015) 030202



# Graphene/Magnetic insulators

## Graphene/EuO and Graphene/Y<sub>3</sub>Fe<sub>5</sub>O

*Spin filtering and exchange splitting Gaps*



**Exchange splitting  
(G/YIG) = 40 meV**

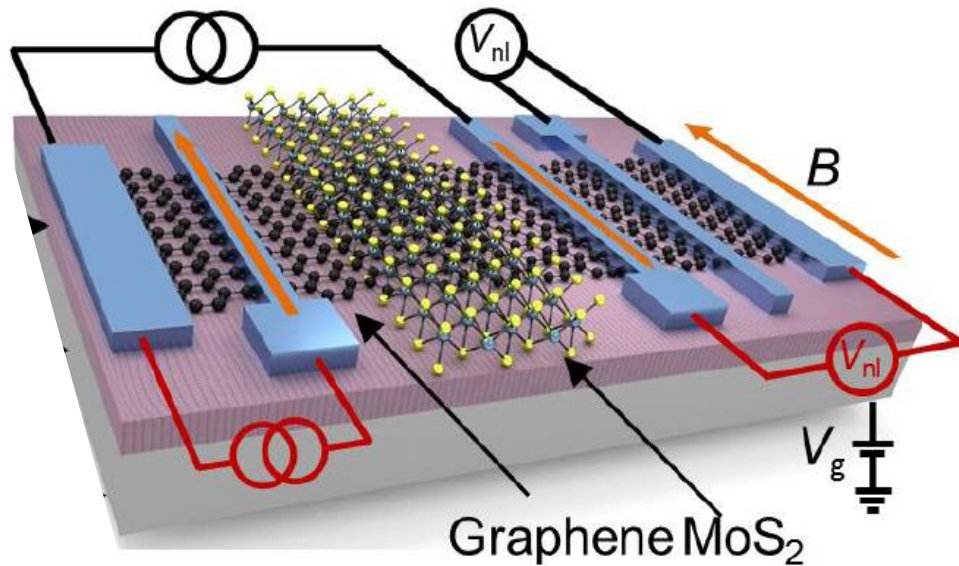
Yang, Hallal, Waintal, Roche, Chshiev, **PRL 110, 046603 (2013)**

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

# All-Electrical Spin-FET

Gate control of spin information (switch ON/OFF)

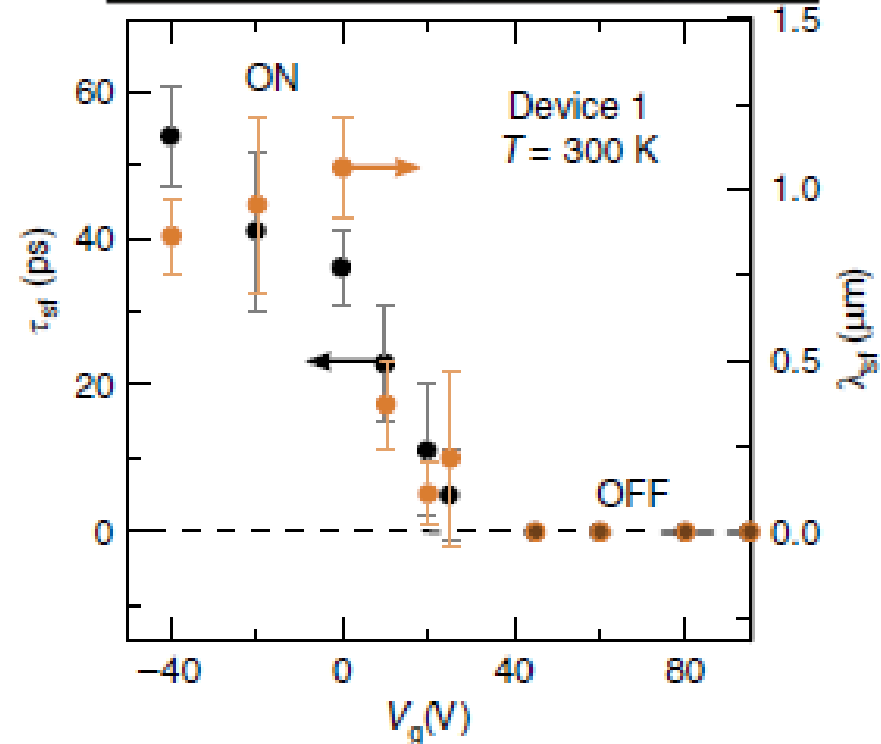
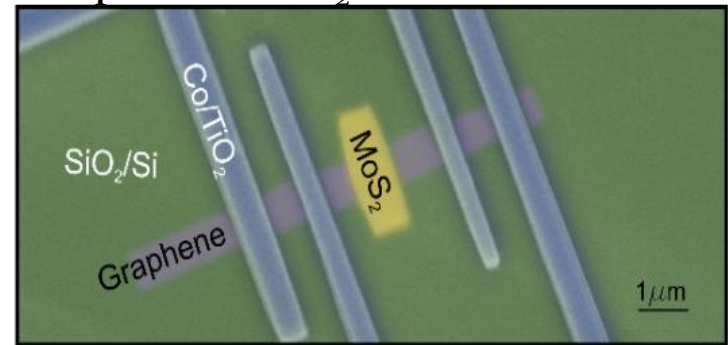
W. Yan, O. Txoperena, R. Llopis, H. Dery, L. E. Hueso & F. Casanova,  
**Nature Comm. 7, 13372 (2016)**



Room Temperature

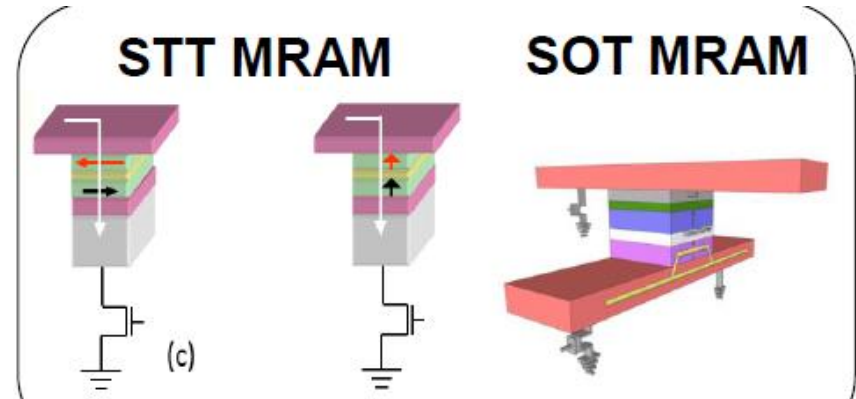
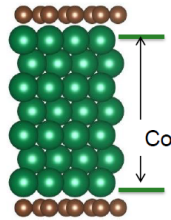
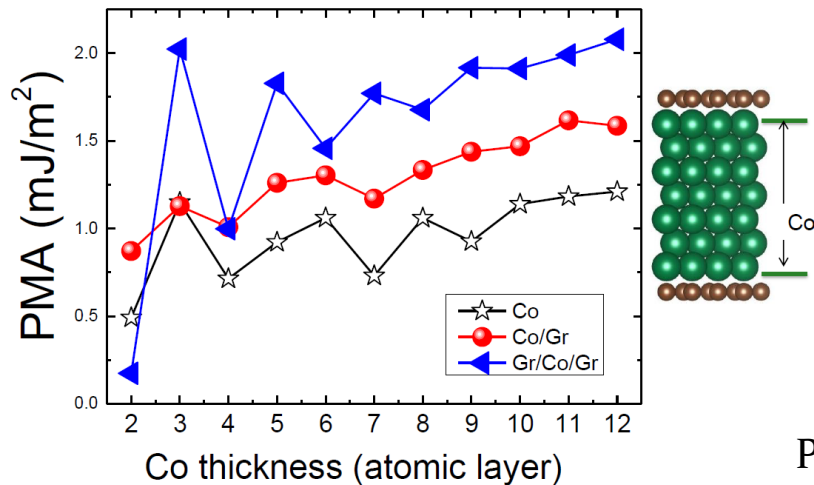
A. Dankert & S. P. Dash,  
**Nature Comm. 8, 16093 (2017)**

Graphene/MoS<sub>2</sub> heterostructures





# 2D Materials for STT-MRAM technologies

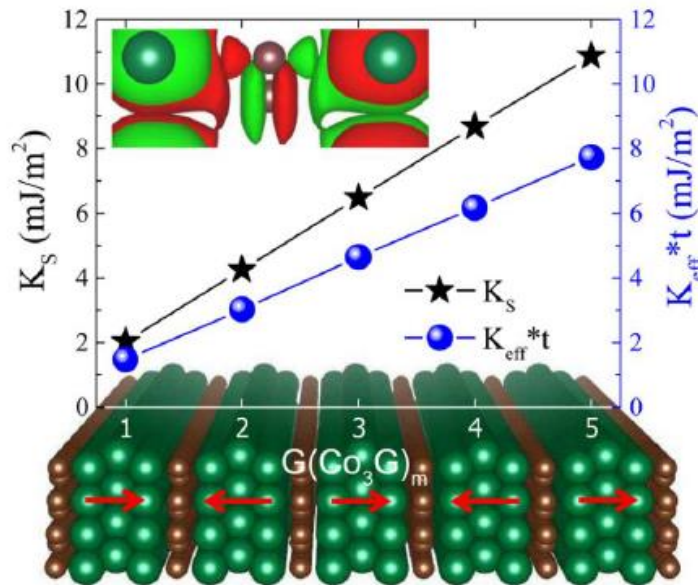


Perpendicular Magnetic Anisotropy in FM/Ox and FM/Graphene interfaces :

*Strongly enhanced PMA of Co realized by graphene coating*

Layer and orbital resolved contributions unveil the PMA mechanisms

*Superlattice structures to obtain Giant PMA*

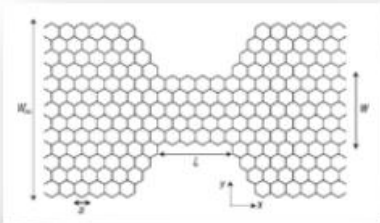


$$K_{eff} = \frac{K_s}{t_{Co}} - E_{demag}$$



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

# Opportunities “in the valley”



PRL 99, 236809 (2007)

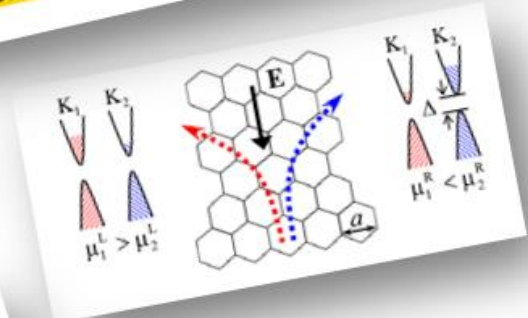
PHYSICAL REVIEW LETTERS

## Valley-Contrasting Physics in Graphene: Magnetic Moment and Topological Transport

Di Xiao,\* Wang Yao,\* and Qian Niu

Department of Physics, The University of Texas, Austin, Texas 78712-0264, USA  
(Received 11 September 2007; published 7 December 2007)

We investigate physical properties that can be used to distinguish the valley degree of freedom in systems where inversion symmetry is broken, using graphene systems as examples. We show that the pseudospin associated with the valley index of carriers has an intrinsic magnetic moment. In close analogy with the Bohr magneton for the electron spin, there is also a valley dependent Berry phase effect that can result in a valley contrasting Hall transport, with carriers in different valleys turning into opposite directions transverse to an in-plane electric field. These effects can be used to generate and detect valley polarization by magnetic and electric means, forming the basis for the valley-based electronics applications.

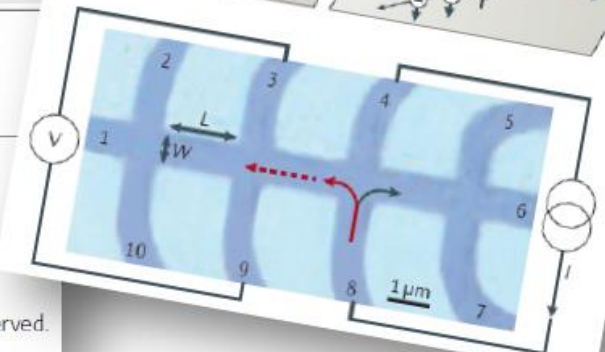
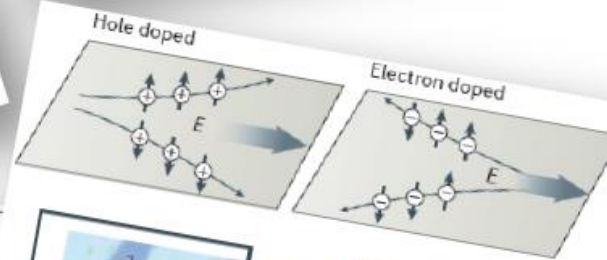
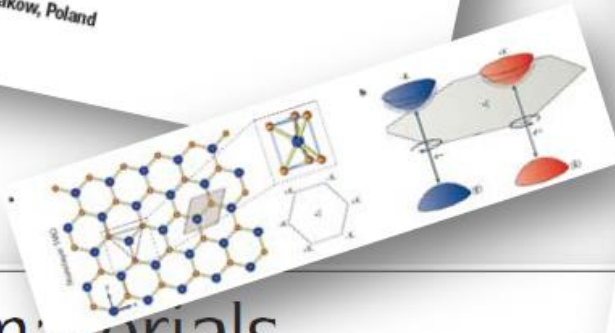
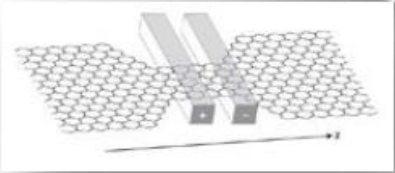


LETTERS

## Valley filter and valley valve in graphene

A. RYCERZ<sup>1,2</sup>, J. TWORZYDŁO<sup>3</sup> AND C. W. J. BEENAKKER<sup>1\*</sup>

<sup>1</sup>Instituut-Lorentz, Universiteit Leiden, PO Box 9506, 2300 RA Leiden, The Netherlands  
<sup>2</sup>Marian Smoluchowski Institute of Physics, Jagiellonian University, Reymonta 4, 30-059 Kraków, Poland  
<sup>3</sup>Institute of Theoretical Physics, Warsaw University, Hoza 69, 00-681 Warsaw, Poland  
e-mail: beenakker@lorentz.leidenuniv.nl



## Valleytronics in 2D materials

John R. Schaibley<sup>1</sup>, Hongyi Yu<sup>2</sup>, Genevieve Clark<sup>3</sup>, Pasqual Rivera<sup>1</sup>, Jason S. Ross<sup>3</sup>, Kyle L. Seyler<sup>1</sup>, Wang Yao<sup>2</sup> and Xiaodong Xu<sup>1,3</sup>

NATURE REVIEWS | MATERIALS

# « Low » Energy Excitations in clean Graphene

*No intervalley/spin mixing - (low disorder & SOC)*

## 8-components Matrix

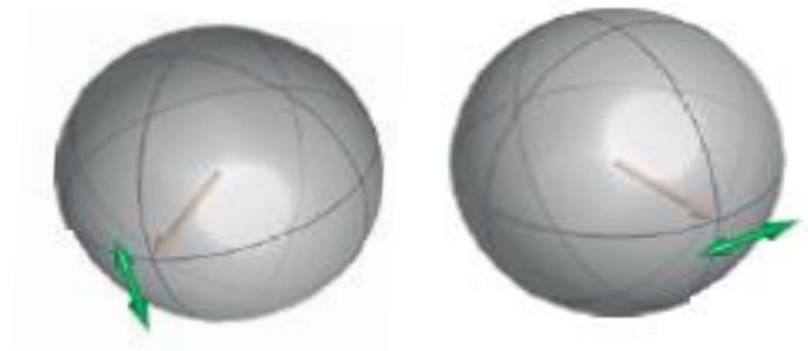
$$\begin{pmatrix}
 0 & p_x - ip_y & 0 & 0 & 0 & 0 & 0 & 0 \\
 p_x - ip_y & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & -p_x + ip_y & 0 & 0 & 0 & 0 \\
 0 & 0 & -p_x + ip_y & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & 0 & p_x - ip_y & 0 & 0 \\
 0 & 0 & 0 & 0 & p_x - ip_y & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & 0 & 0 & 0 & -p_x + ip_y \\
 0 & 0 & 0 & 0 & 0 & 0 & -p_x + ip_y & 0
 \end{pmatrix}
 \begin{pmatrix}
 \Psi_{A,+}^{\uparrow} \\
 \Psi_{B,+}^{\uparrow} \\
 \Psi_{A,-}^{\uparrow} \\
 \Psi_{B,-}^{\uparrow} \\
 \Psi_{A,+}^{\downarrow} \\
 \Psi_{B,+}^{\downarrow} \\
 \Psi_{A,-}^{\downarrow} \\
 \Psi_{B,-}^{\downarrow}
 \end{pmatrix}$$

Three internal degrees of freedom

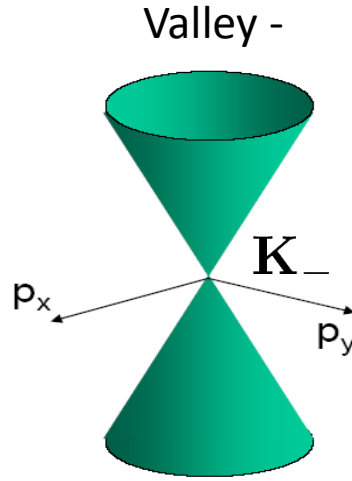
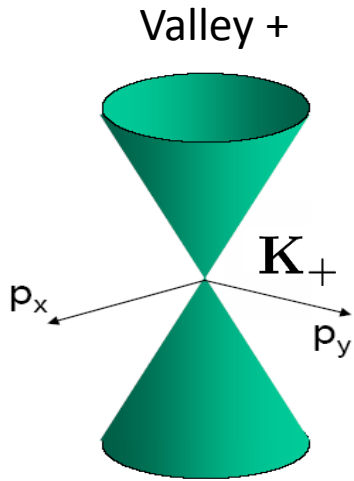
**Spin**

**Valley index**

**Sublattice pseudospin**



# 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**

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

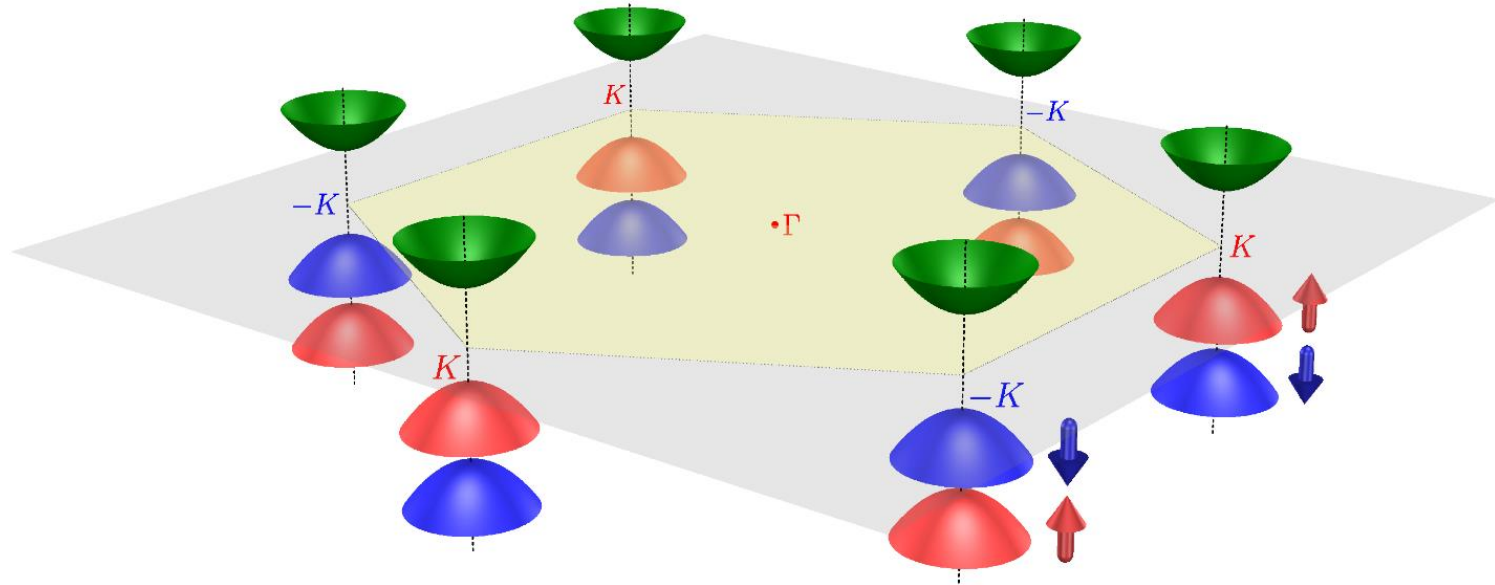
$$\Psi_{\vec{p}} = \frac{1}{\sqrt{2}} \left( \Psi_{\vec{p}}(A) \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \Psi_{\vec{p}}(B) \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right) = \frac{1}{\sqrt{2}} \begin{pmatrix} s e^{i\theta_p/2} \\ e^{-i\theta_p/2} \end{pmatrix}$$

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

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

# Transition Metal dichalcogenides (monolayer)

**Broken  
inversion  
symmetry**



D. Xiao et al.

**PRL 108, 196802 (2012)**

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

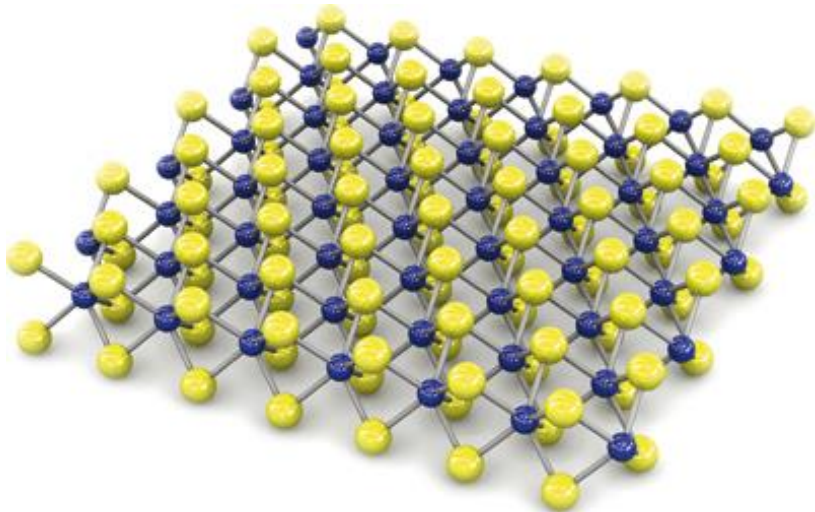
***Massive Dirac Fermion model***  
*Partially filled d-orbitals (metal)*

*Gap*  $\sim 2$  eV

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

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

***Spin-valley locking***



# Interlinking optics with Valleytronics & Spintronics

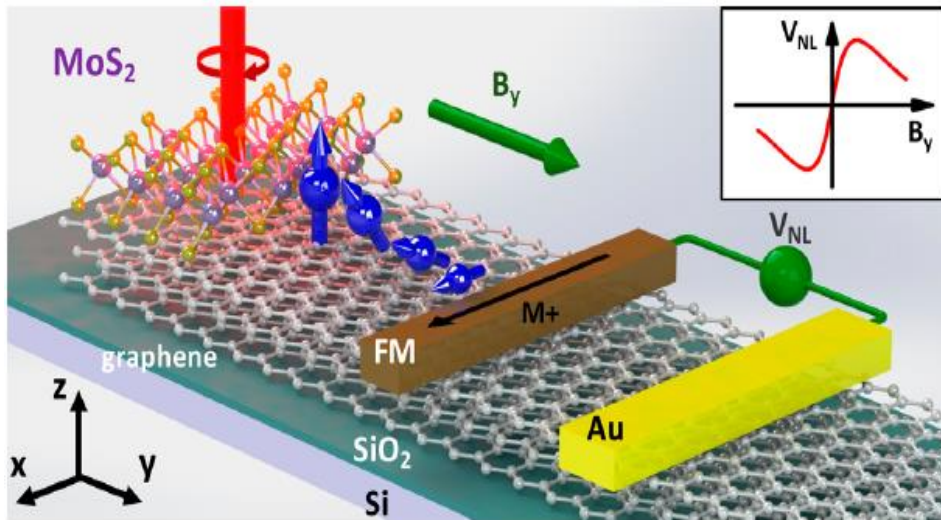
NANO LETTERS

Letter

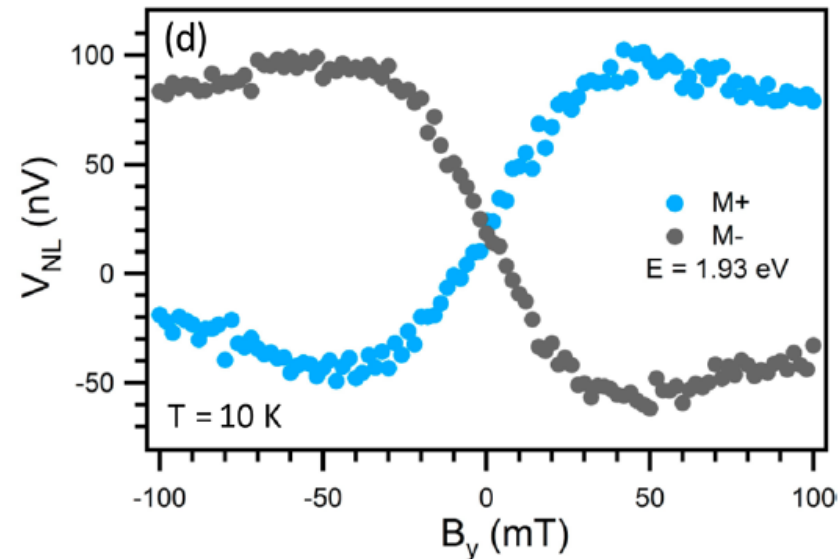
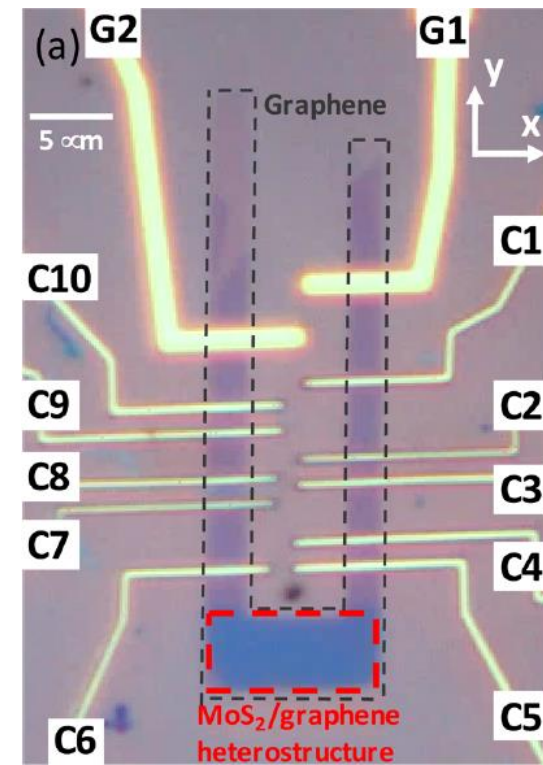
pubs.acs.org/NanoLett

## Opto-Valleytronic Spin Injection in Monolayer MoS<sub>2</sub>/Few-Layer Graphene Hybrid Spin Valves

Yunqiu Kelly Luo,<sup>†</sup> Jinsong Xu,<sup>†</sup> Tiancong Zhu,<sup>†</sup> Guanzhong Wu,<sup>†</sup> Elizabeth J. McCormick,<sup>†</sup> Wenbo Zhan,<sup>†</sup> Mahesh R. Neupane,<sup>‡</sup> and Roland K. Kawakami<sup>\*,†,Ⓞ</sup>



**Multifunctional 2D  
spintronic/valleytronic devices**



# OUTLINE

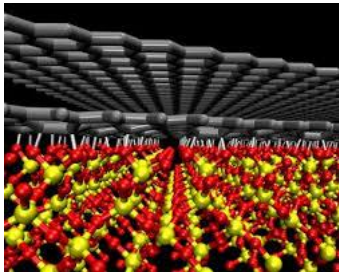
*Why Spintronics using 2D Materials ?*

*Proximity effects in 2D Materials-based heterostructures  
(spin dynamics & relaxation, SHE, weak antilocalization,  
QSHE)*

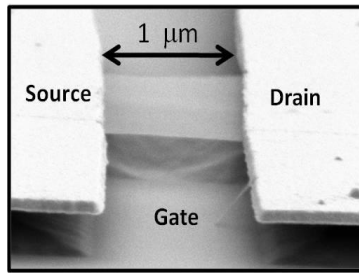
*Generating valley polarized quantum transport  
(valleytronics)*

# Experimental spin lifetime features

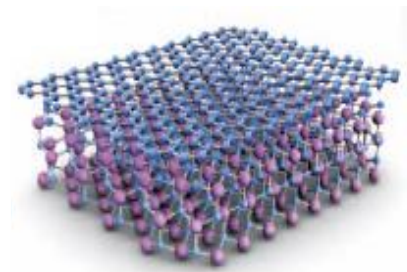
*Graphene  
on SiO<sub>2</sub>*



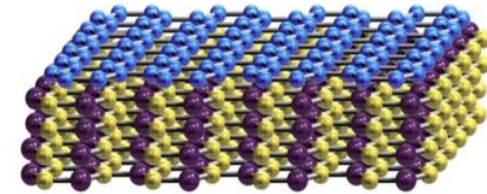
*Suspended  
Graphene*



*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**

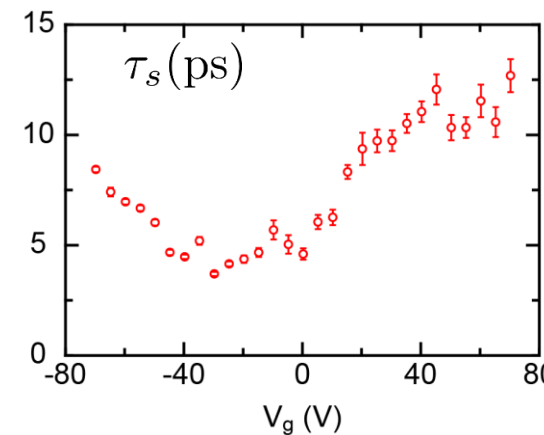
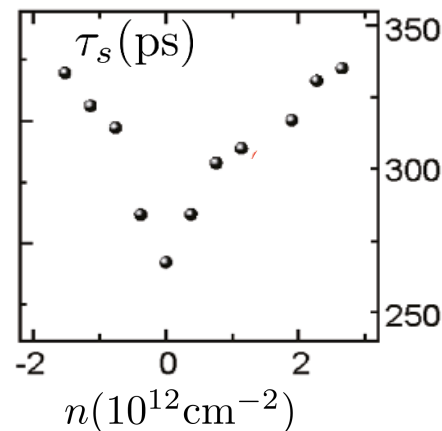
$$\tau_s \sim 0.1 - 10 \text{ ns}$$

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)

Drögeler et al. *Nano Lett.* **16** (6), 3533 (2016)





# Tight-binding Modelling

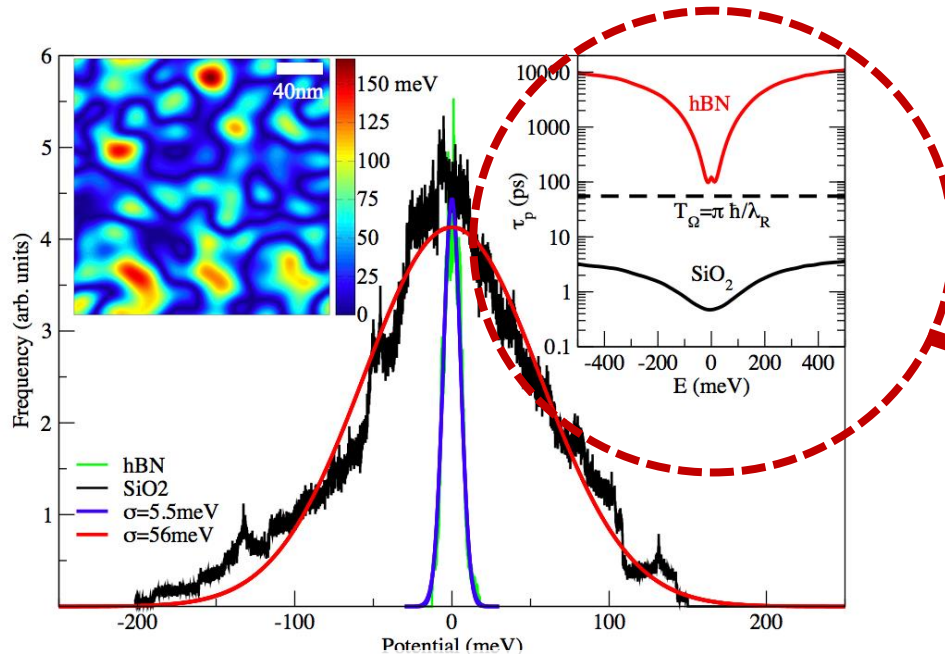
$$\mathcal{H} = -\gamma_0 \sum_{\langle ij \rangle} c_i^\dagger c_j + \sum_{\langle i \rangle} V_i c_i^\dagger c_i + iV_R \sum_{\langle ij \rangle} c_i^\dagger \vec{z} \cdot (\vec{s} \times \vec{d}_{ij}) c_j$$

## Screened Coulomb potential

Long range (Gaussian) potential

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

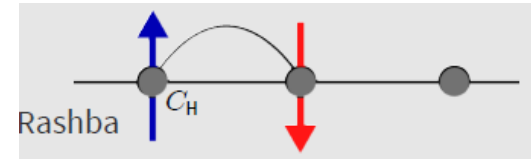
Shaffique Adam et al **Phys. Rev. B** 84, 235421 (2011)



Onsite energy distribution of the  $\pi$ -orbitals with standard deviation for hBN (5meV) & SiO<sub>2</sub> (56meV)

## Rashba SOC

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

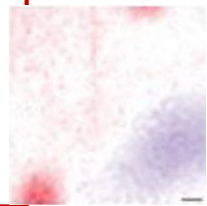
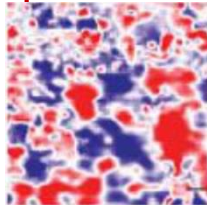


**Graphene on SiO<sub>2</sub>**


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

**Graphene on hBN**

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



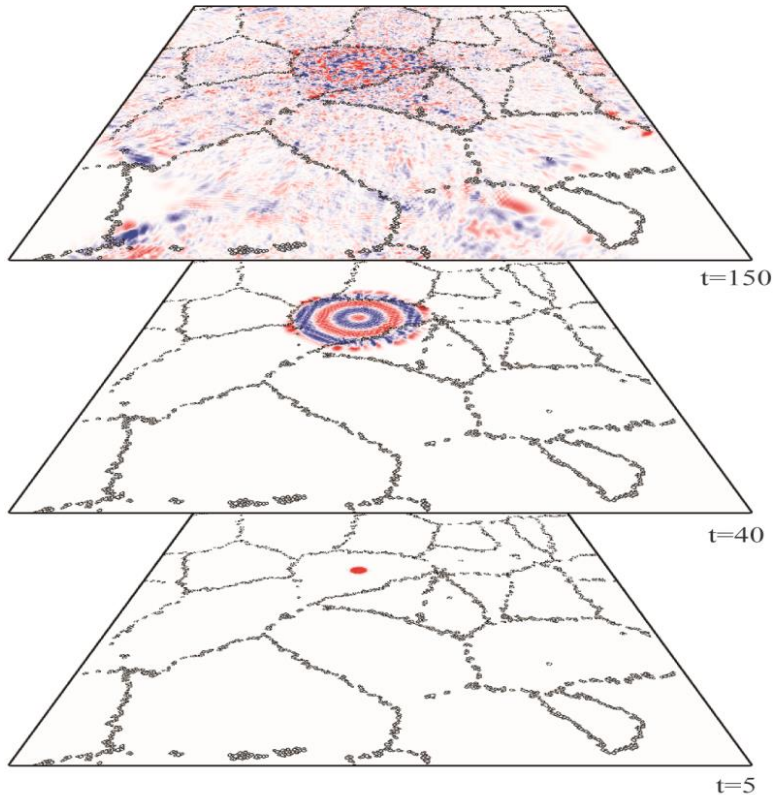
# Spin dynamics of propagating wavepacket


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

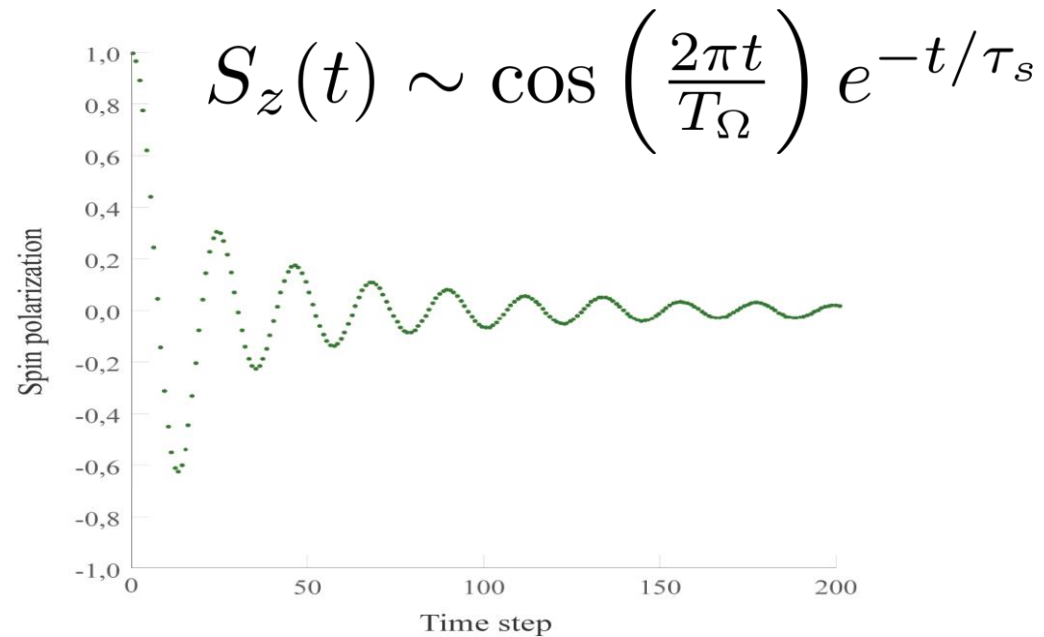
$$s_i(t) = |\Psi_i^{\uparrow}(t)|^2 - |\Psi_i^{\downarrow}(t)|^2$$

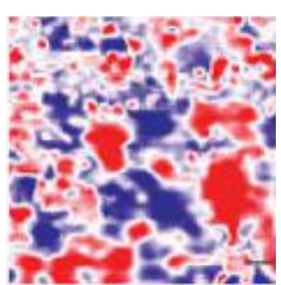
(time-dependent)

Local spin density in real space



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

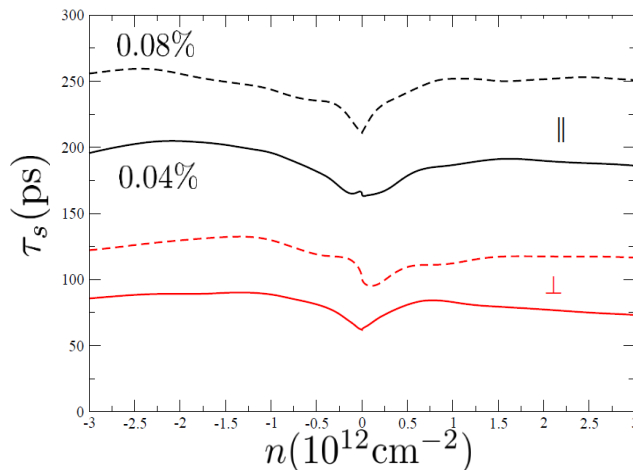
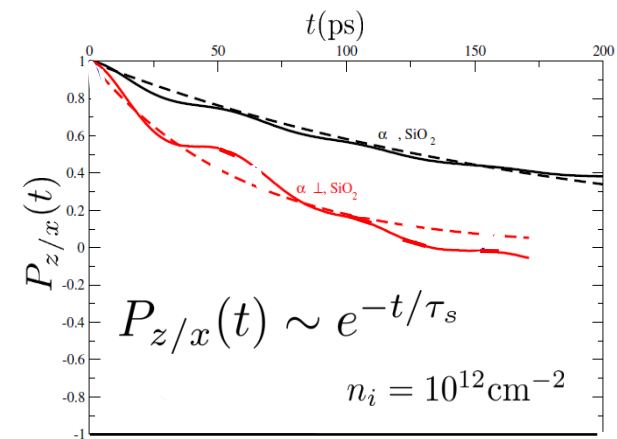




# Graphene on SiO<sub>2</sub>

electron-hole puddles drive the relaxation

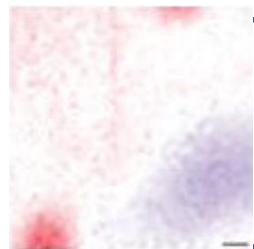
$$\tau_p^{\text{SiO}_2} / T_\Omega \ll 1$$



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

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

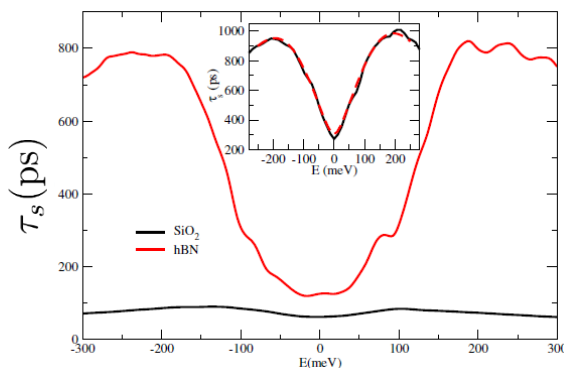
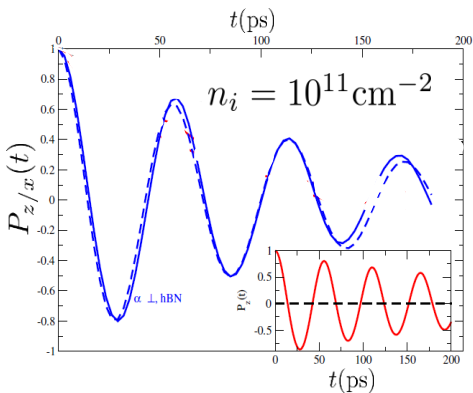
**Dyakonov-Perel**  
relaxation mechanism



# Graphene on hBN

electron-hole puddles drive the relaxation

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



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

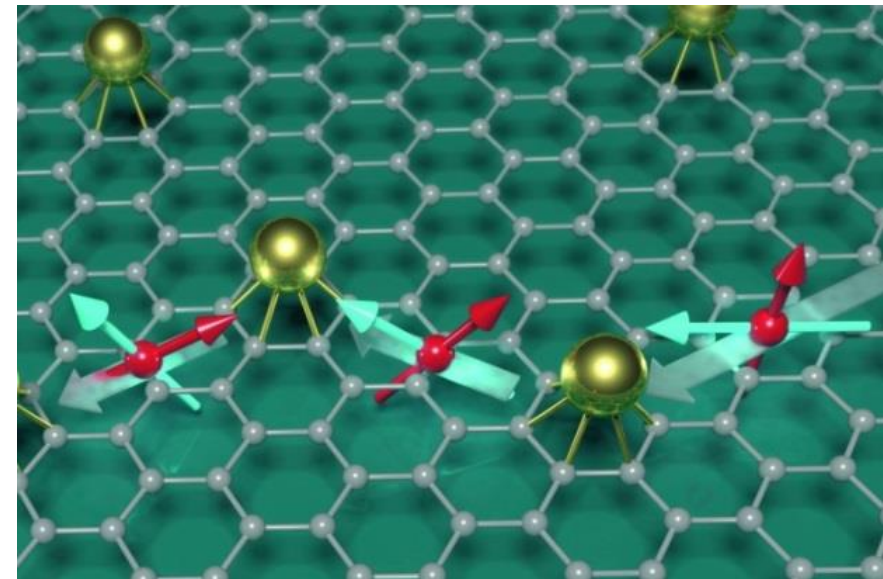
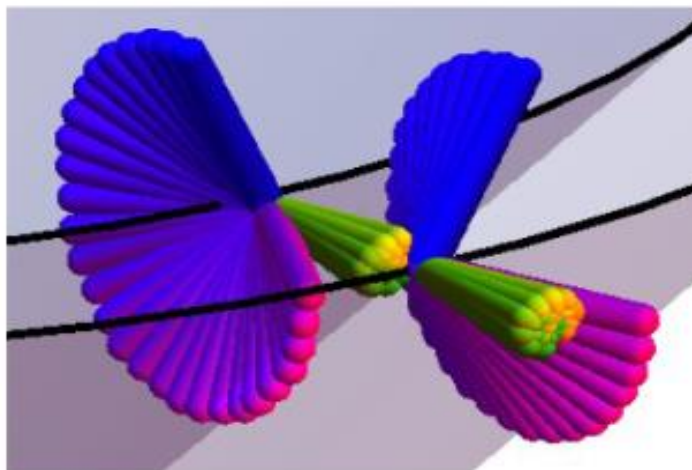
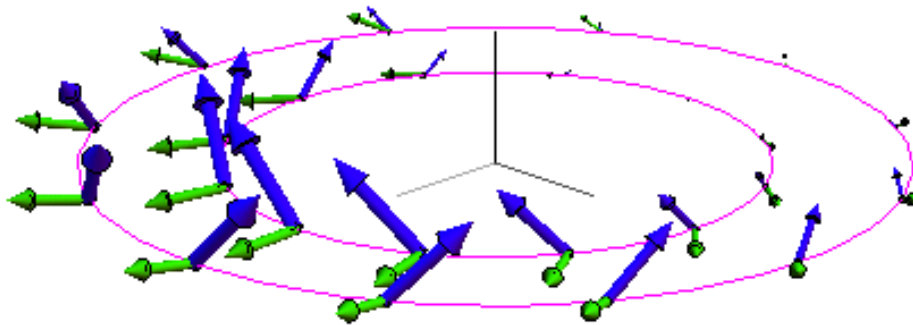
$$\tau_s \simeq 1 - 10 \text{ ns}$$

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

**Dephasing**  
relaxation  
mechanism

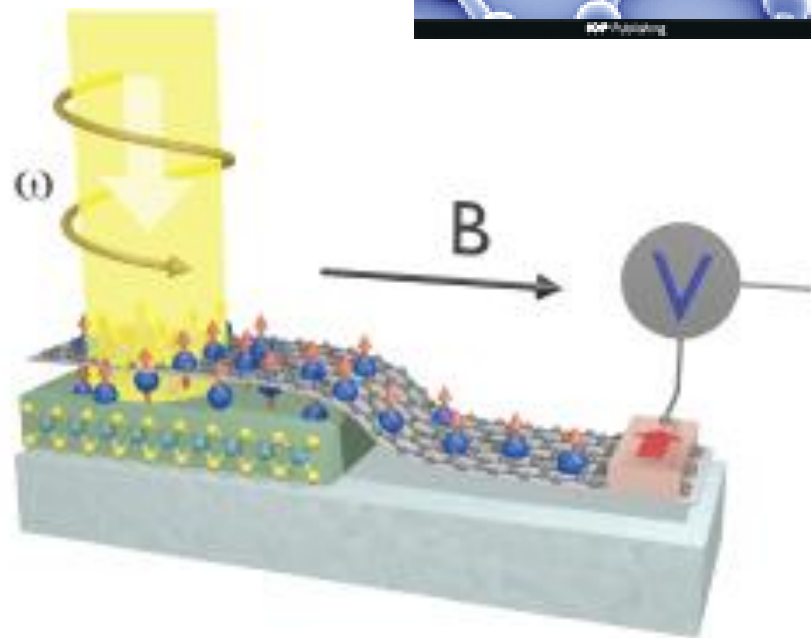
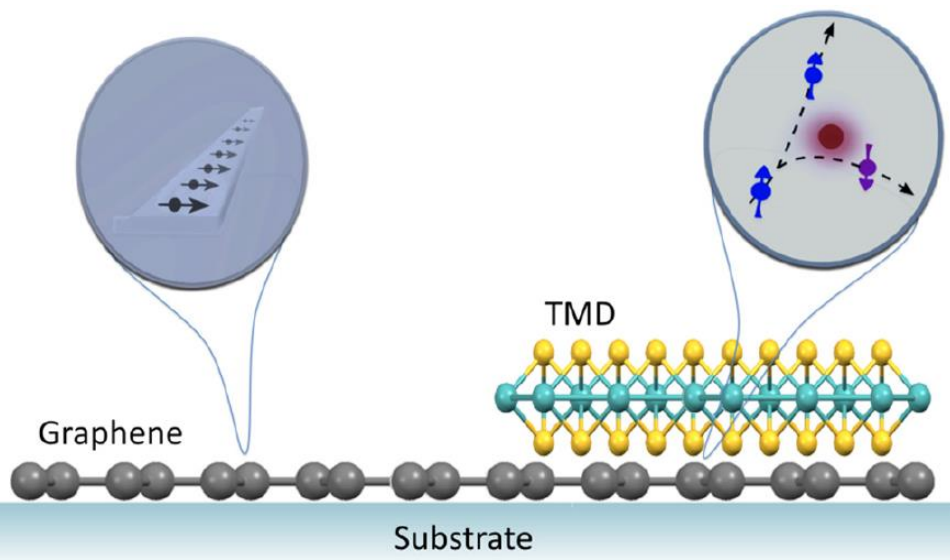
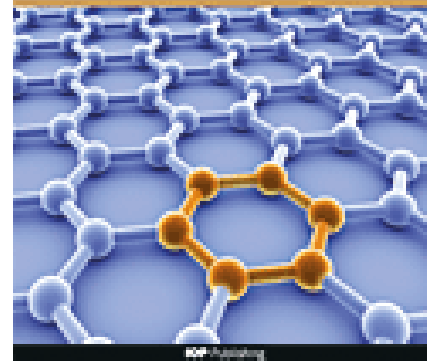
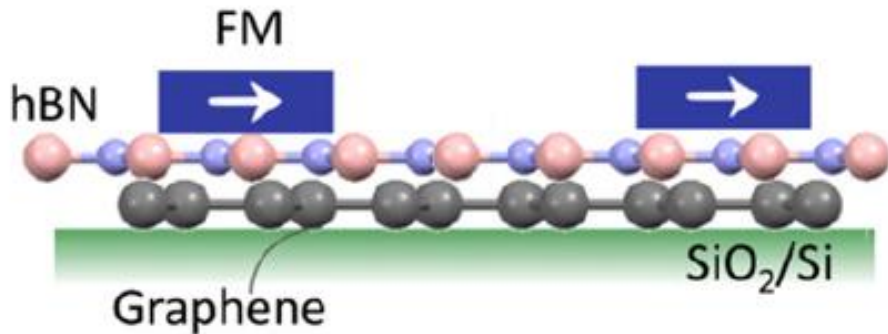
# Pseudospin-driven spin relaxation mechanism in graphene

Dinh Van Tuan<sup>1,2</sup>, Frank Ortmann<sup>1,3,4</sup>, David Soriano<sup>1</sup>, Sergio O. Valenzuela<sup>1,5</sup> and Stephan Roche<sup>1,5\*</sup>



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

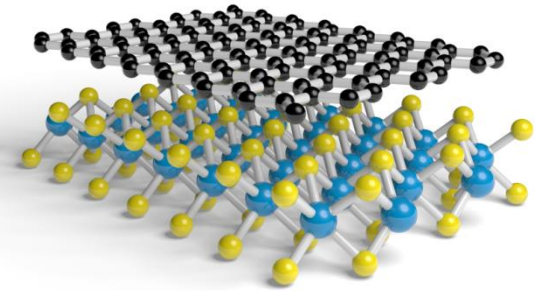
# Hybrid devices of graphene and other 2D materials



*2D Mater.* 2 (2015) 030202

Martin Gmitra and Jaroslav Fabian  
Phys. Rev. B 92, 155403 (2015)

# Realistic Model of Graphene/TMDC with interface disorder



DFT-TB model from

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

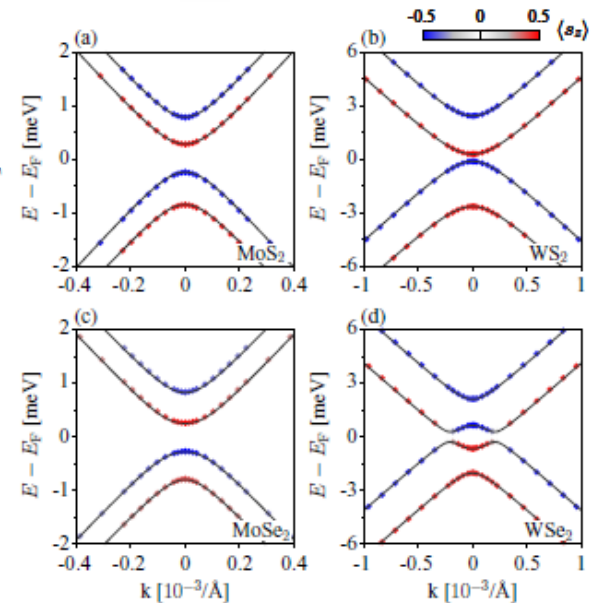
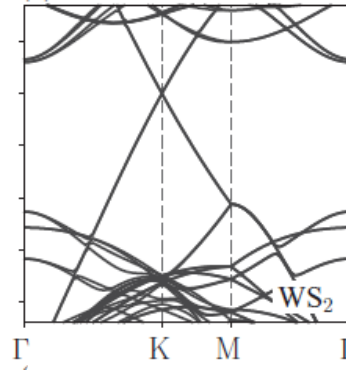
PRB 93, 155104 (2016)

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

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

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

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

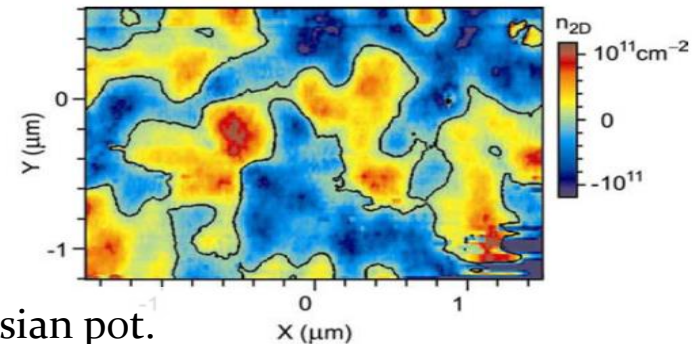


Random distribution of  $n_p$  electron-hole puddles

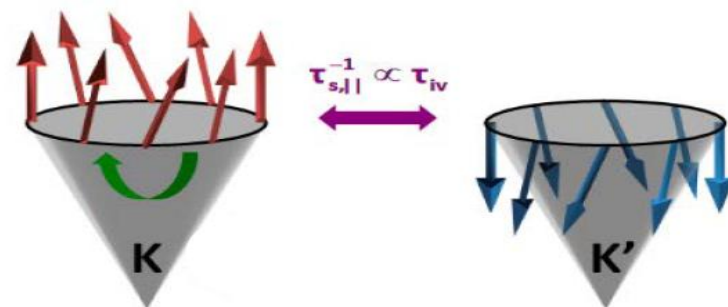
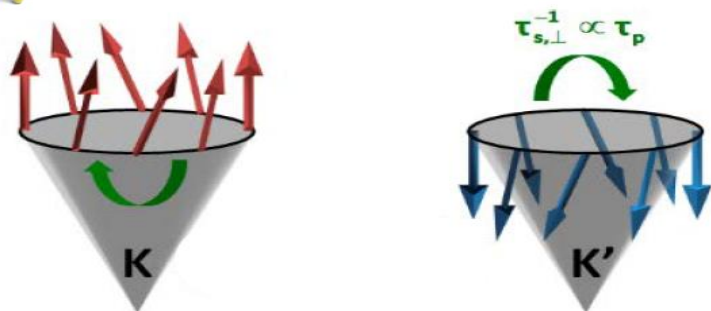
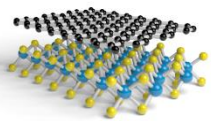
S. Adam et al. PRB 84, 235421 (2011)

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

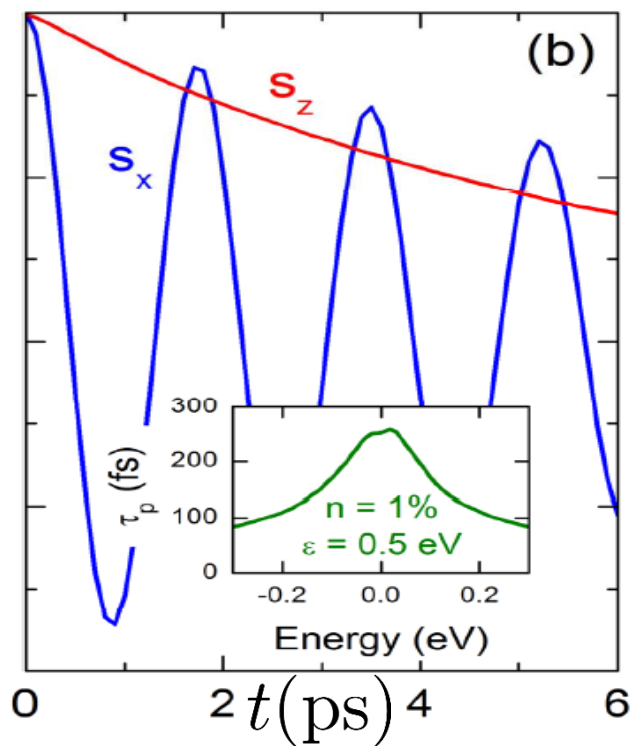
$u_n \in [-U_p, U_p]$   $\mathbf{R}_n$  is the position of the center of the Gaussian pot.



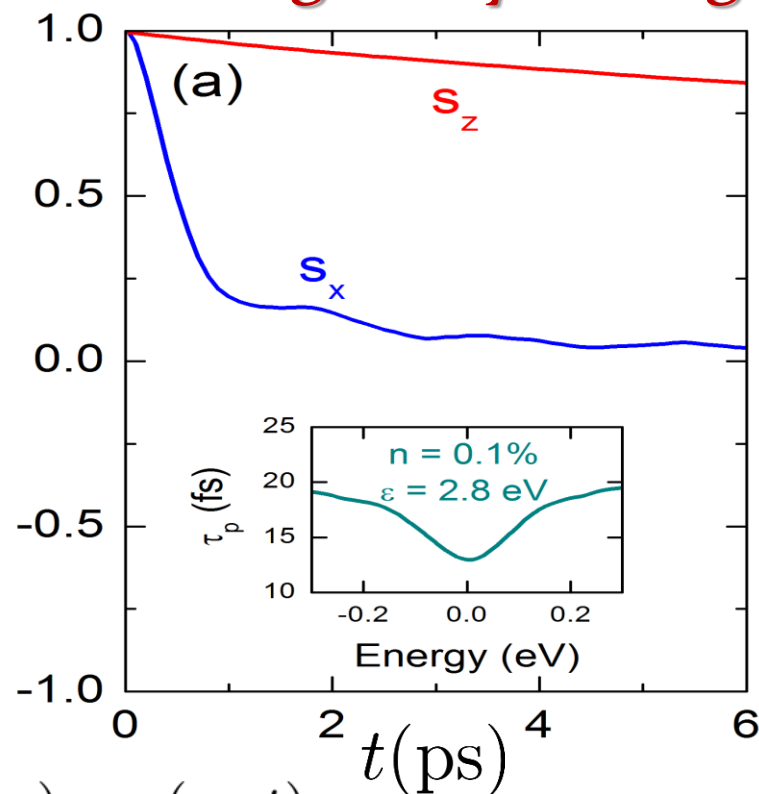
# Spin dynamics (Graphene/TMDC+ el-h puddles)



## Intravalley scattering



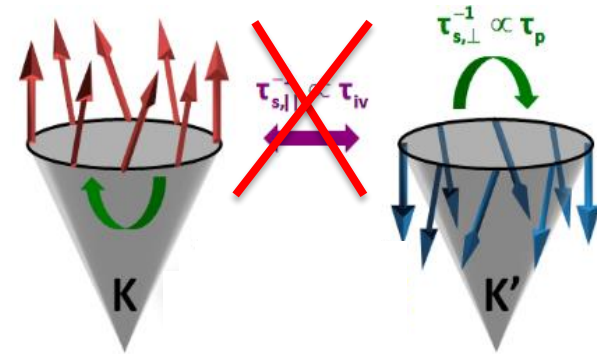
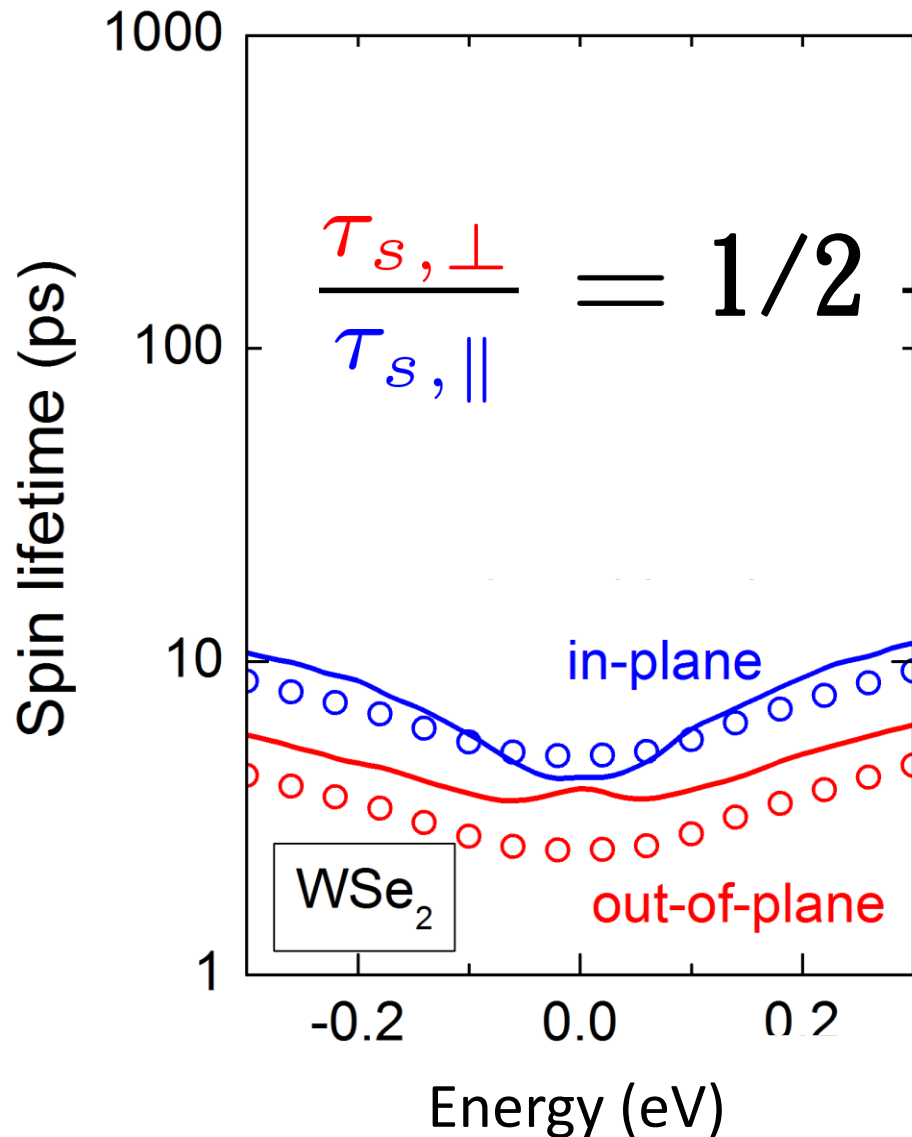
## Strong valley mixing



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

# High-quality Graphene/TMDC

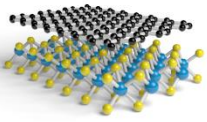
*Absence of valley mixing (Dyakonov-Perel)*



Weak anisotropy as in conventional *Rashba disordered systems*

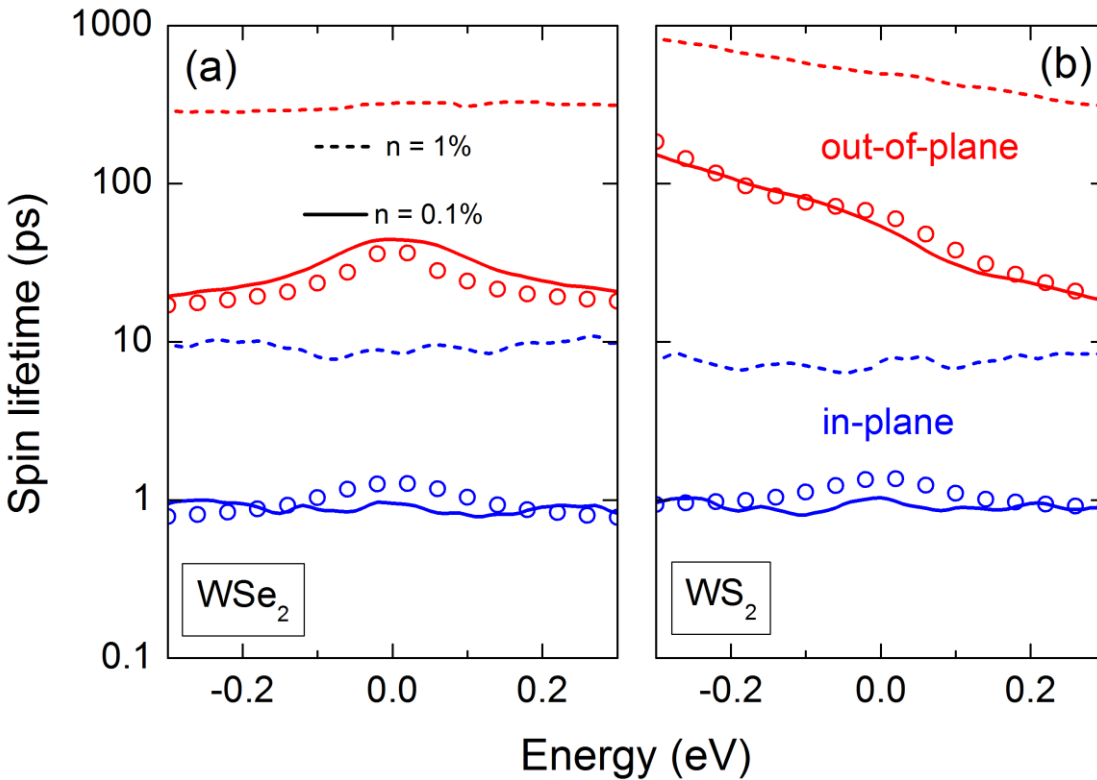
*Dyakonov-Perel regime (single valley approximation)*





# Giant spin lifetimes anisotropy

in low quality Graphene/TMDC (*strong valley mixing*)



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

Lifetime values

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

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

Dyakonov-Perel mechanism

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

## Symbols:

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

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

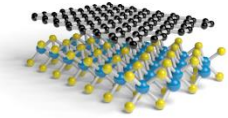
$$\overline{\omega_\alpha(t) \omega_\beta(t')} = \delta_{\alpha\beta} \overline{\omega_\alpha^2} e^{-|t-t'|/\tau_{c,\alpha}},$$

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

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

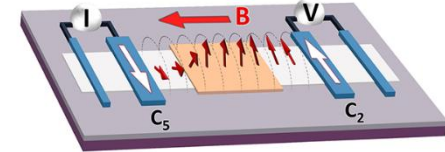
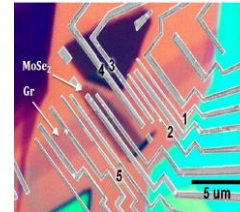
# Theoretical prediction confirmed !!!

AW. Cummings, J.H. García, J. Fabian, S. Roche,  
**Phys. Rev. Lett 119, 206601 (2017)**



NANO LETTERS

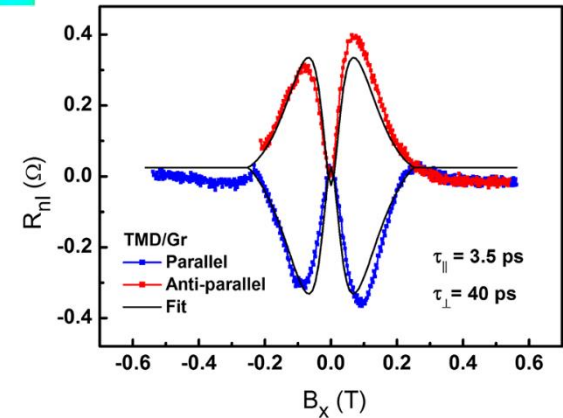
Cite This: *Nano Lett.* XXXX, XXX, XXX-XXX



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

Talieh S. Ghiasi,<sup>\*</sup> Josep Ingla-Aynés, Alexey A. Kaverzin, and Bart J. van Wees

Physics of Nanodevices, Zernike Institute for Advanced Materials, University of Groningen, Groningen, 9747 AG, The Netherlands



nature physics

ARTICLES

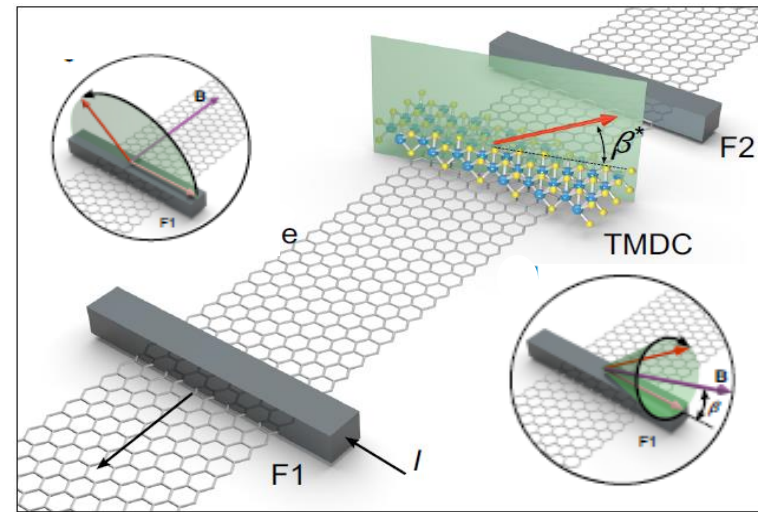
<https://doi.org/10.1038/s41567-017-0019-2>

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

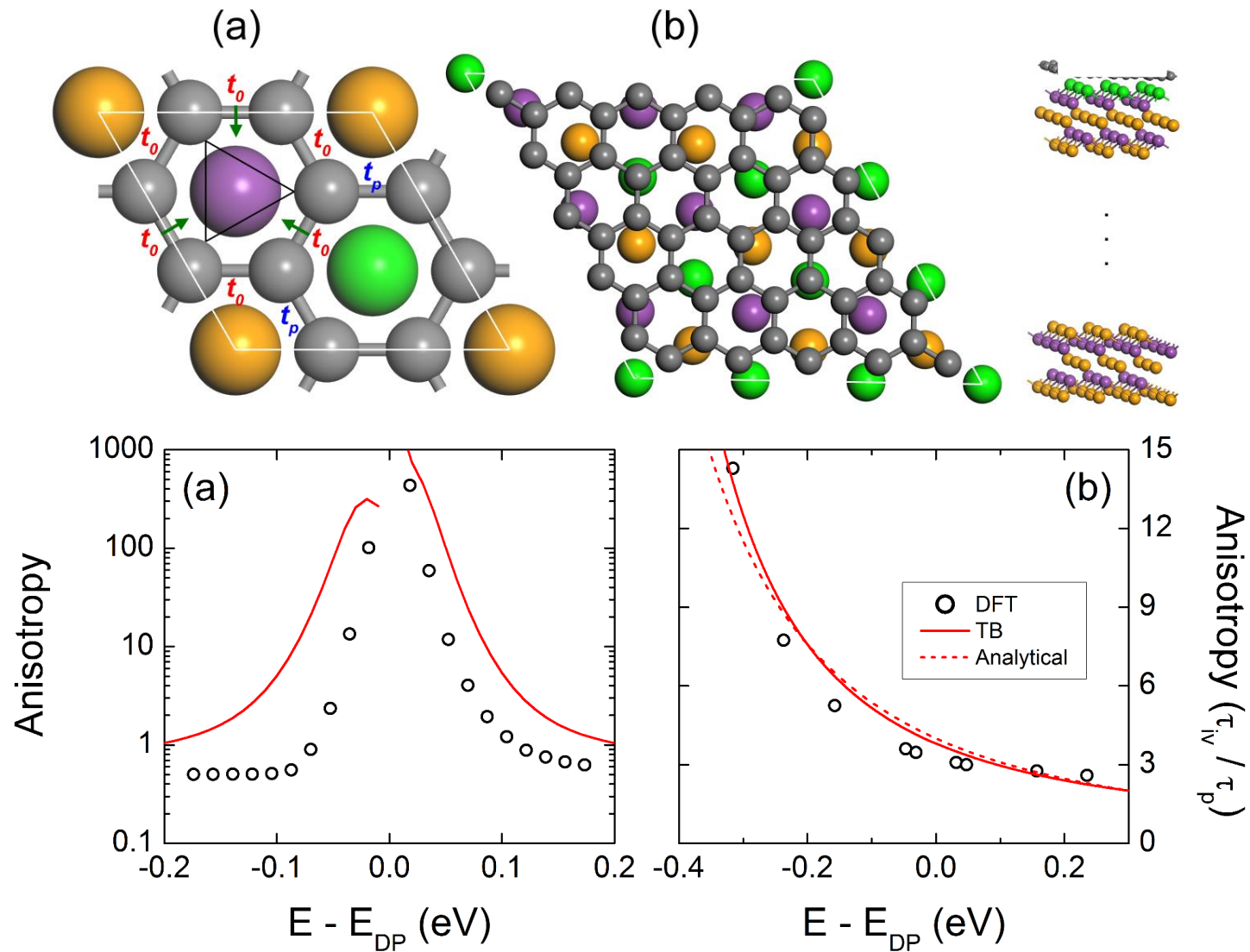
L. Antonio Benítez<sup>1,2\*</sup>, Juan F. Sierra<sup>1</sup>, Williams Savero Torres<sup>1</sup>, Aloïs Arrighi<sup>1,2</sup>, Frédéric Bonell<sup>1</sup>, Marius V. Costache<sup>1</sup> and Sergio O. Valenzuela<sup>1,3\*</sup>



GRAPHENE FLAGSHIP



# Tunable spin lifetimes in Graphene/Bi<sub>2</sub>Se<sub>3</sub>

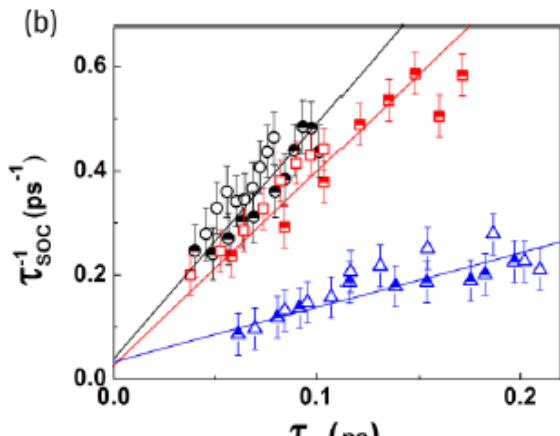
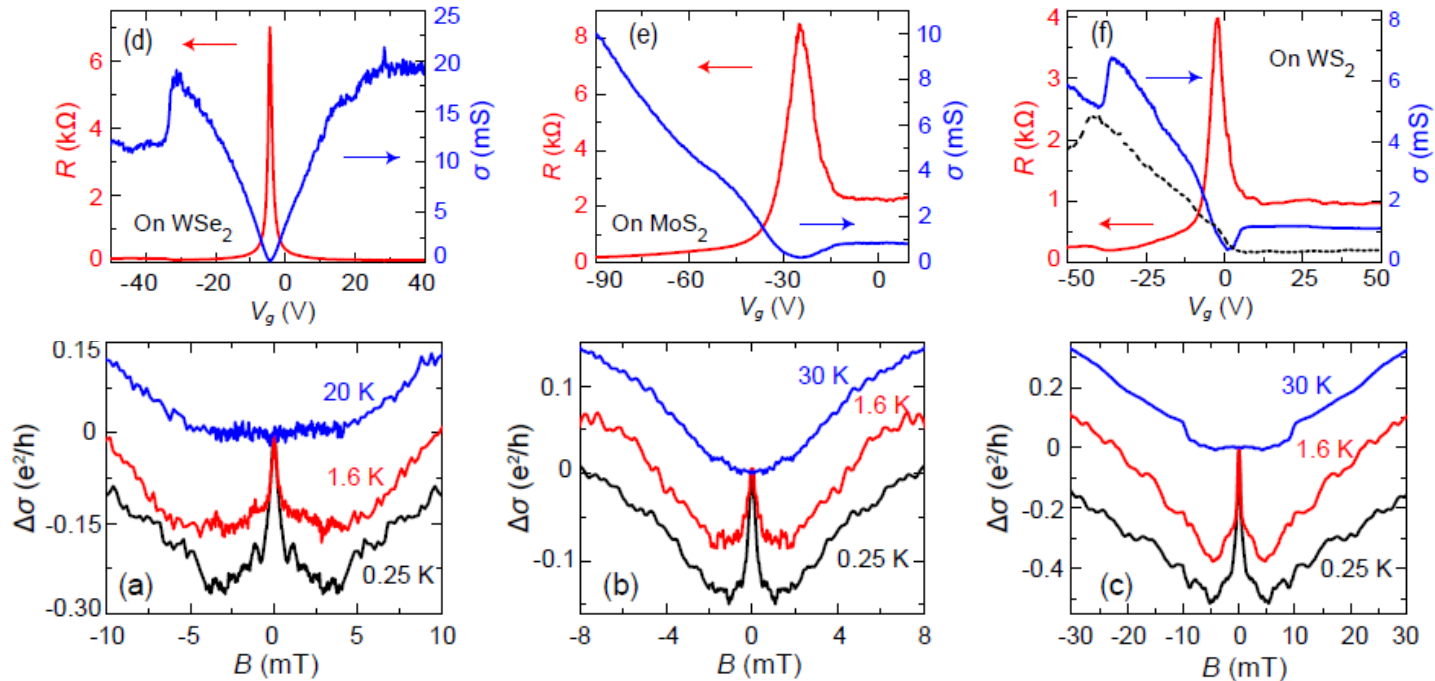
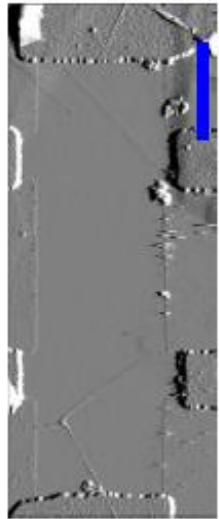


K. Song, D. Soriano, A. W. Cummings, R. Robles, P. Ordejón, and S. Roche

**Nano Lett.** Article ASAP- DOI: [10.1021/acs.nanolett.7b05482](https://doi.org/10.1021/acs.nanolett.7b05482)

# SOC-proximity effect & Weak antilocalization

Wang et al, **Phys. Rev. X** 6, 041020 (2016)

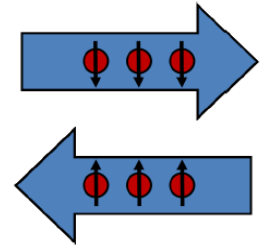


From the fits the scaling of spin scattering times versus Momentum scattering time yields  
**DYAKONOV PEREL mechanism**

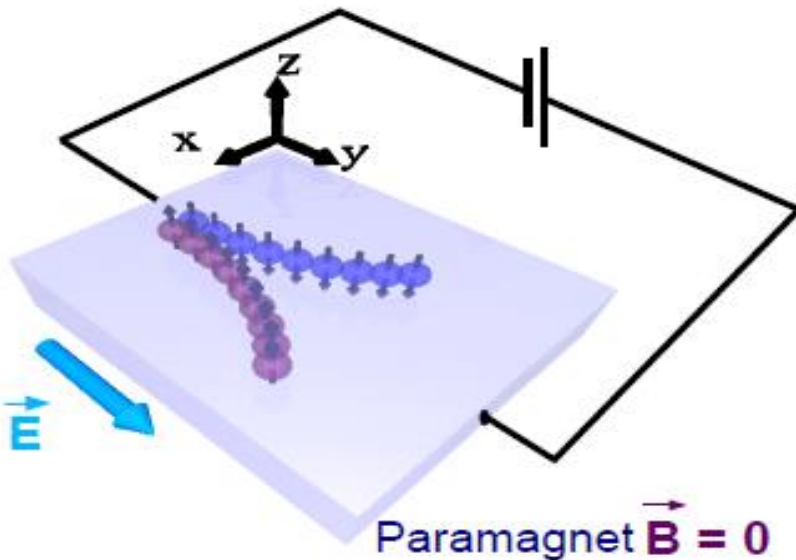
B. Yang et al. **Phys. Rev. B** 96, 041409(RC) (2017)

# Spin Hall Effect

M.I. Dyakonov and V.I. Perel (1971)



Appearance of **spin accumulation** on the lateral surfaces of an electric current-carrying sample  
(*signs of the spin directions being opposite on the opposing boundaries*)



**Strong spin-orbit coupling materials**  
("effective magnetic field")

**Interest !**  
Manipulate Spin  
by electrical means  
Without the use of  
ferromagnetic  
materials or real  
magnetic fields

Direct electronic measurement of the spin  
Hall effect

S.O. Valenzuela\* and M. Tinkham *Nature* 442, 176-179 (2006)

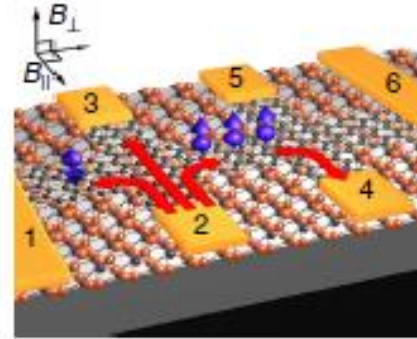
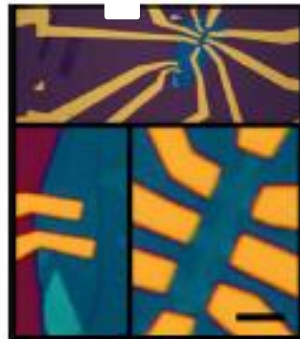
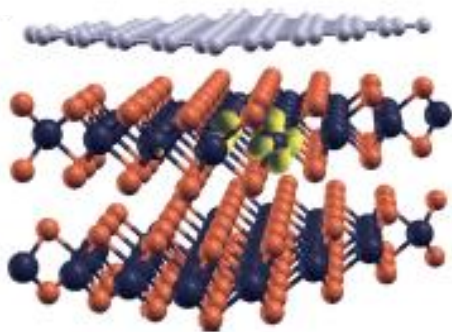
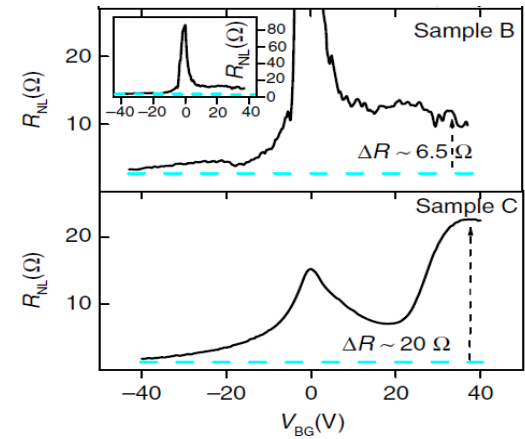
Department of Physics, Harvard University, Cambridge, MA  
02138, USA.

ARTICLE

Received 10 Mar 2014 | Accepted 31 Jul 2014 | Published 26 Sep 2014

# Spin-orbit proximity effect in graphene

A. Avsar<sup>1,2</sup>, J.Y. Tan<sup>1,2</sup>, T. Taychatanapat<sup>1,2</sup>, J. Balakrishnan<sup>1,2</sup>, G.K.W. Koon<sup>1,2,3</sup>, Y. Yeo<sup>1,2</sup>, J. Lahiri<sup>1,2</sup>, A. Carvalho<sup>1,2</sup>, A.S. Rodin<sup>4</sup>, E.C.T. O'Farrell<sup>1,2</sup>, G. Eda<sup>1,2</sup>, A.H. Castro Neto<sup>1,2</sup> & B. Özyilmaz<sup>1,2,3</sup>



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

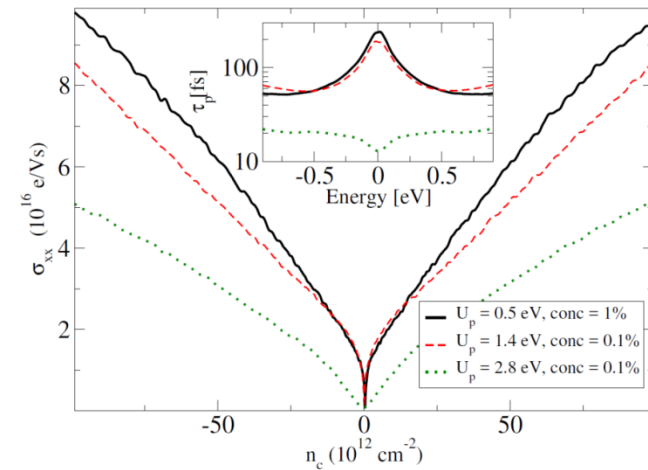
*“Graphene acquires spin-orbit coupling up to **17 meV**, three orders of magnitude higher than its intrinsic value, without modifying the structure of the graphene.*

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

# Localization effects for graphene/WS<sub>2</sub> + el-h puddles

Scaling theory of localization

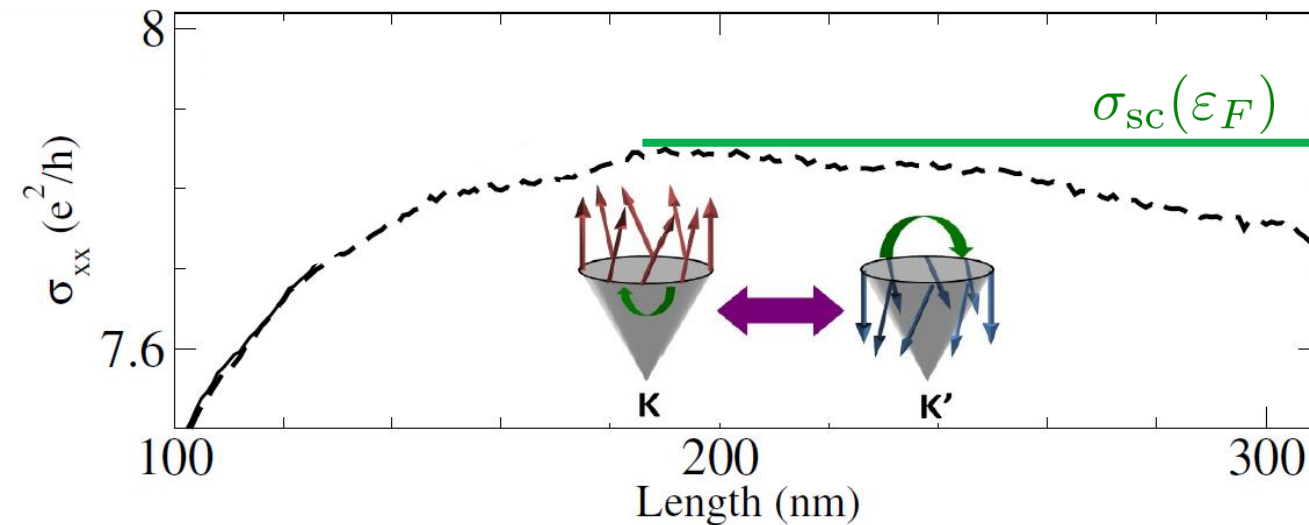
$$\sigma_{xx}(\varepsilon_F) = \sigma_{sc}(\varepsilon_F) + \delta\sigma(\varepsilon_F)$$



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

Case of strong scatterers (puddles) and large intervalley scattering

**SOC switch OFF**



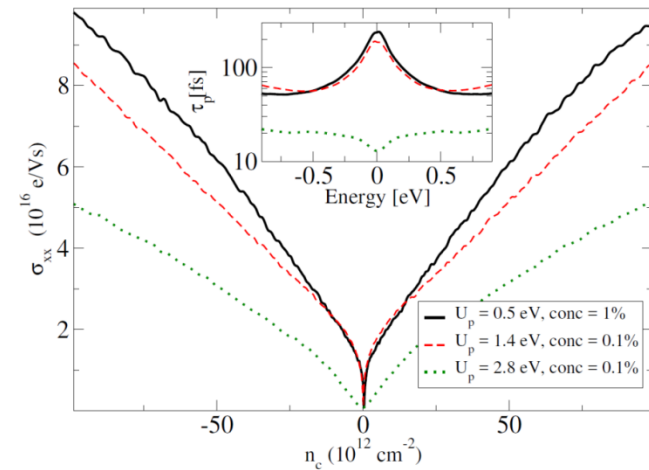
$$\delta\sigma = -\frac{2e^2}{\pi h} \log(L/\ell_e)$$

**Weak localization**

# Localization effects for graphene/WS<sub>2</sub> + el-h puddles

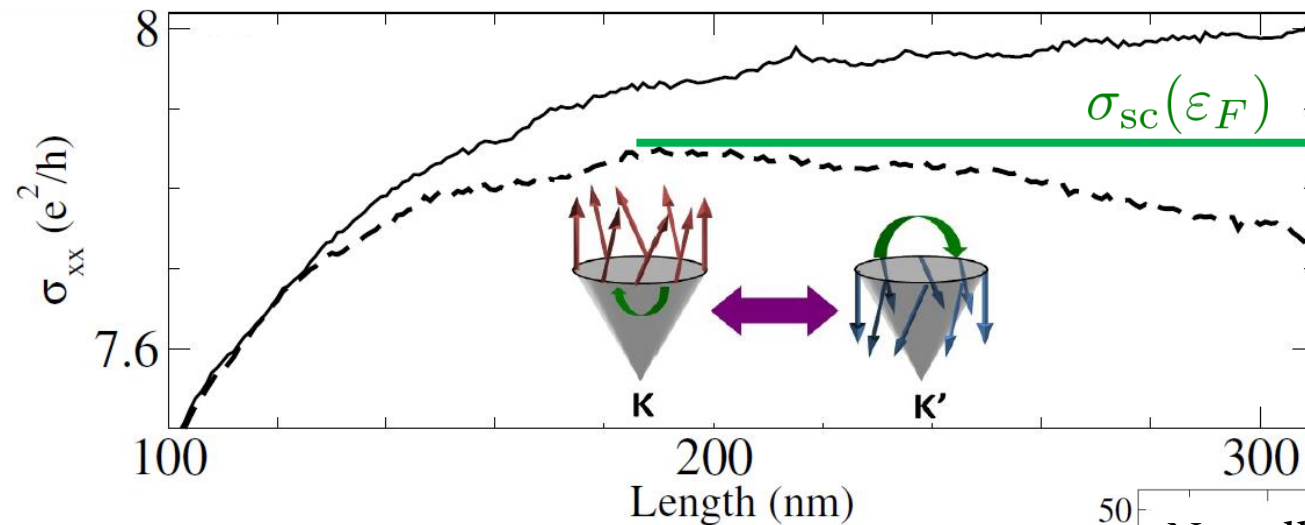
Scaling theory of localization

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



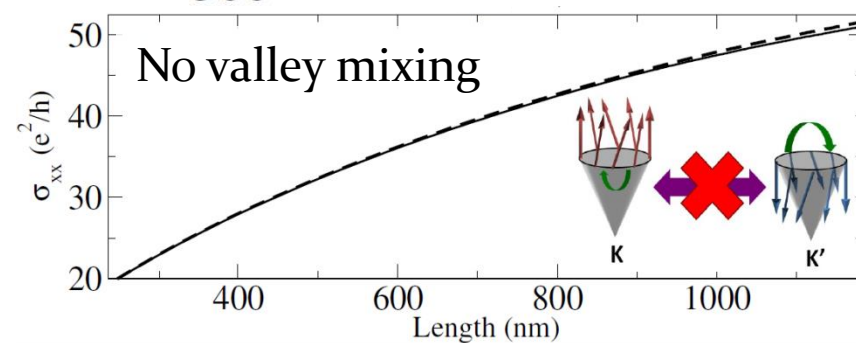
Case of strong scatterers (puddles) and large intervalley scattering

**SOC switch ON**



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

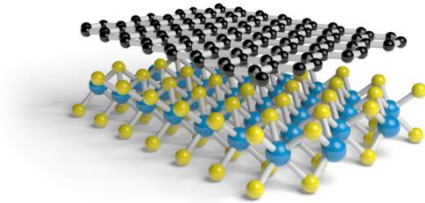
**Weak Antilocalization**





# Spin Hall Effect for Graphene /TMDC heterostructures

## Intrinsic mechanism

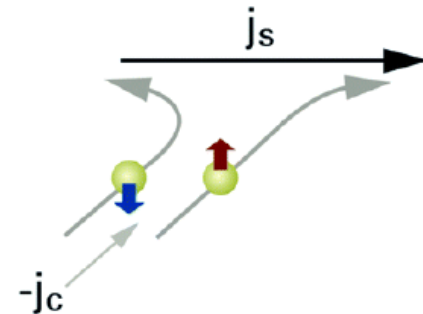


Driven by the translational invariant spin-orbit coupling fields (effective B fields)

Rashba+ intrinsic + Pseudospin Inversion

Asymmetry terms...

## Extrinsic mechanism



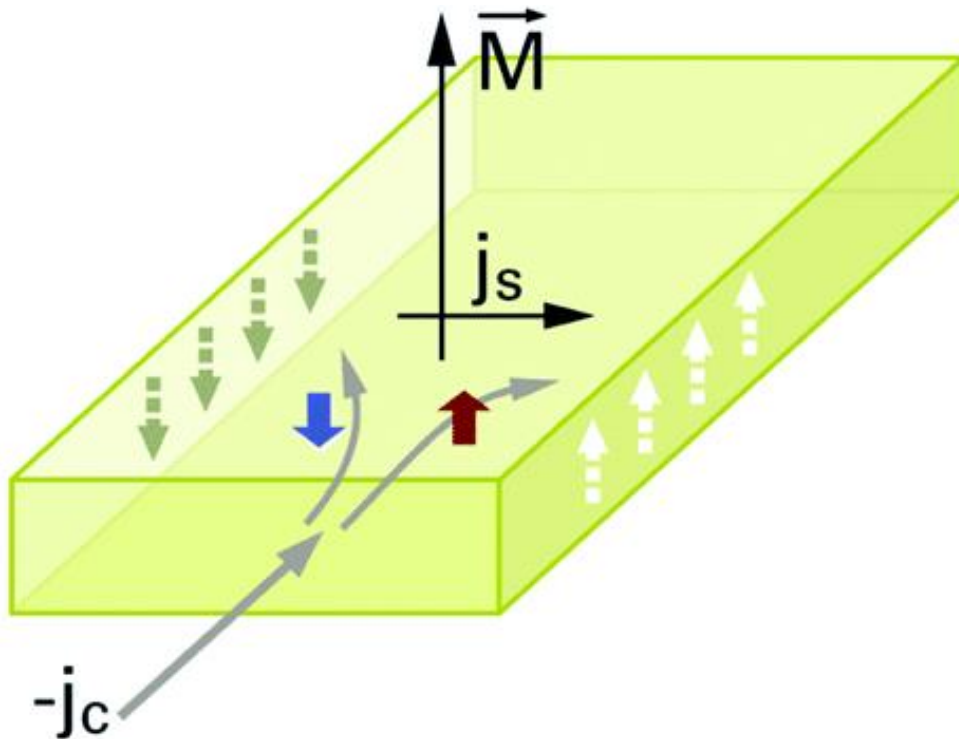
If impurities introduce local changes of SOC here **electron-hole puddles** (disorder)

# Spin Hall Kubo conductivity in clean 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

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

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

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

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

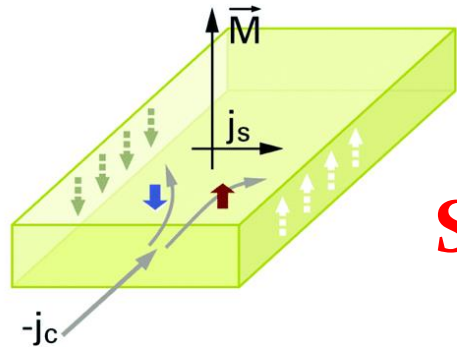
$$\mu_{mn} = \frac{4}{\Delta E^2} \mathcal{I}m[\text{Tr}[J_x^z T_n(\hat{H}) v_y T_m(\hat{H})]]$$

The trace in  $\mu_{mn}$  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**

# Spin Hall Kubo conductivity in clean graphene/TMDC interfaces

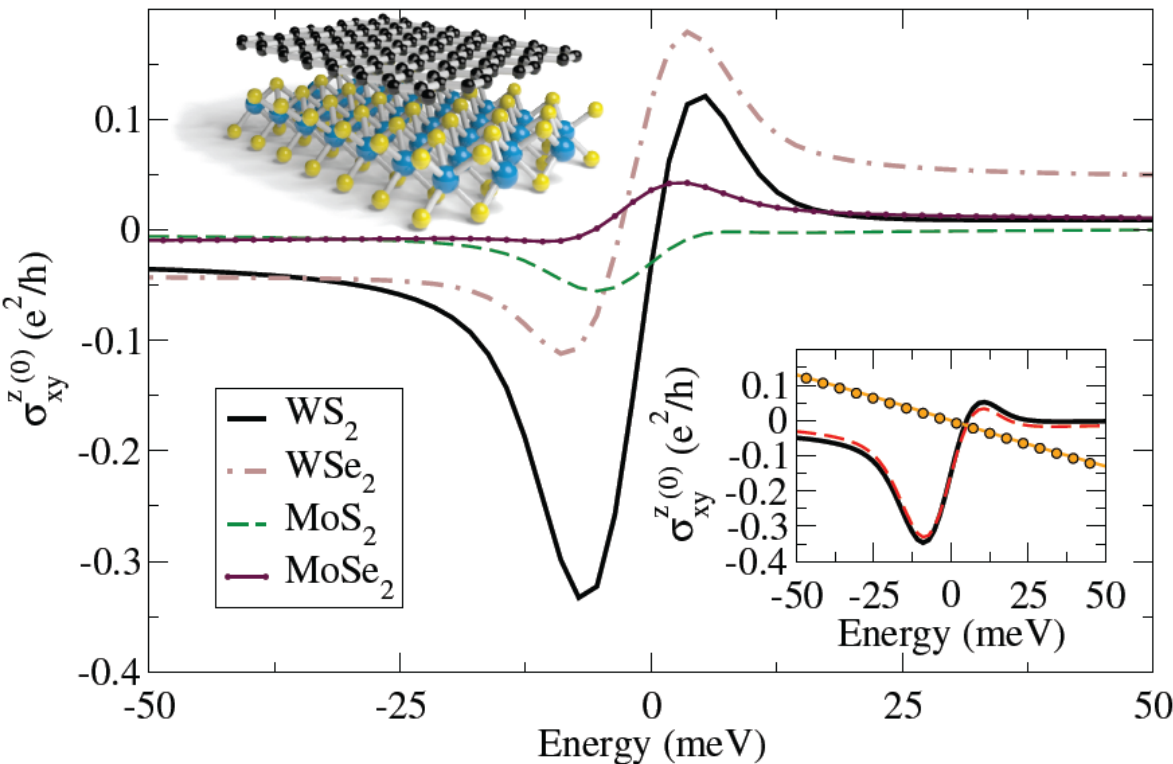


$\theta_{sH}$

**Spin Hall angle**

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

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



Dissipative SHE

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

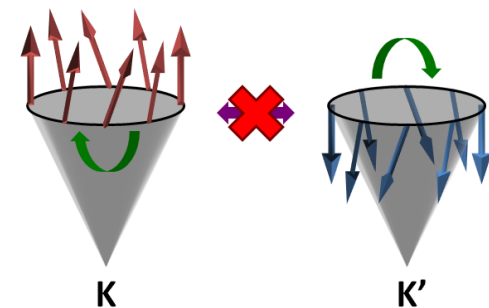
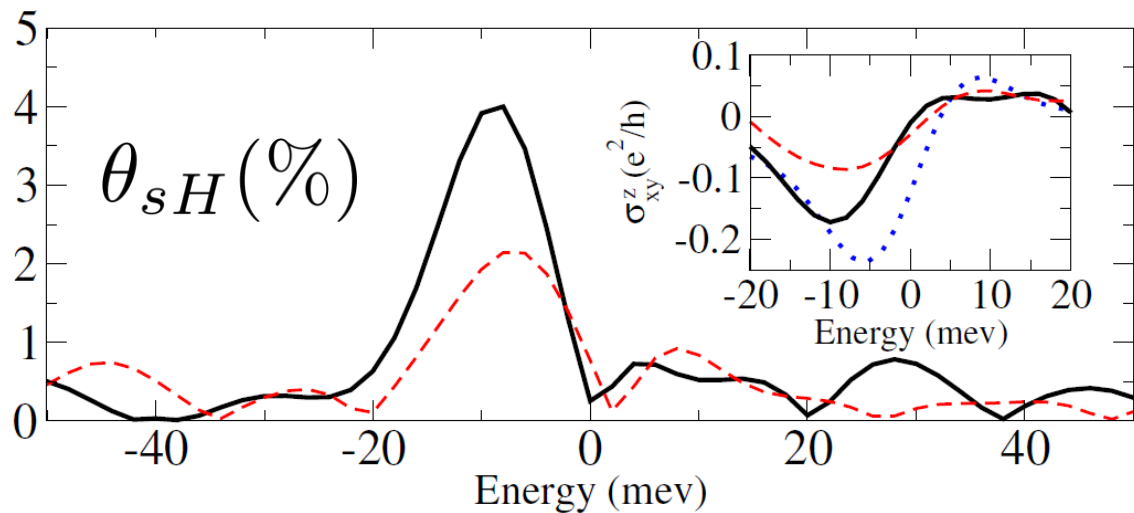
Clean case :

***“intrinsic SHE”***

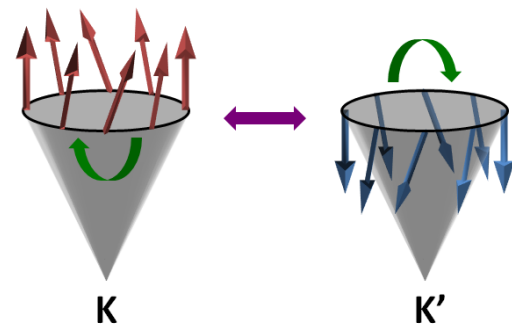
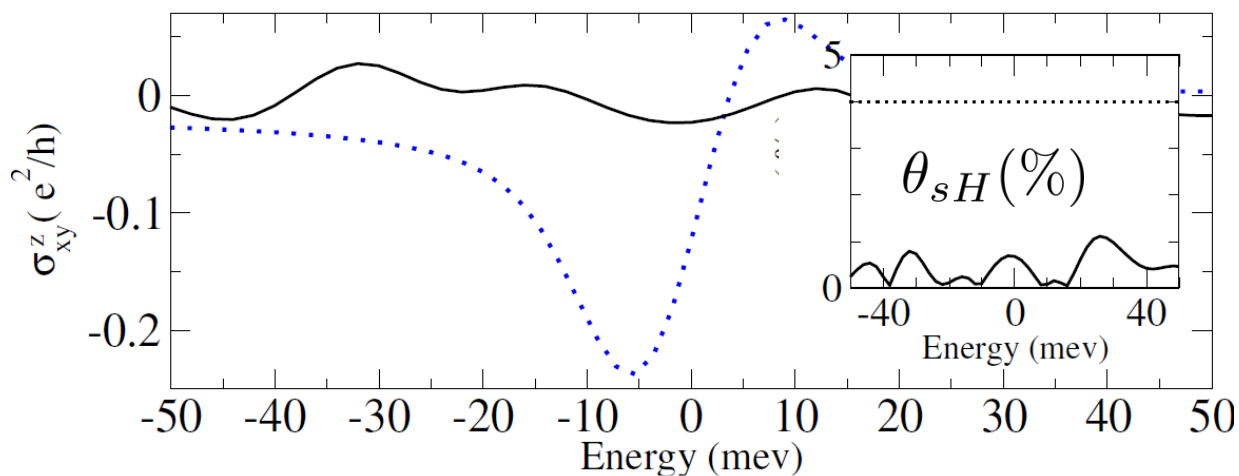
**WS<sub>2</sub>** leads to larger Spin Hall conductivity (larger SHA)

# Spin Hall Effect

in disordered graphene/TMDC interfaces

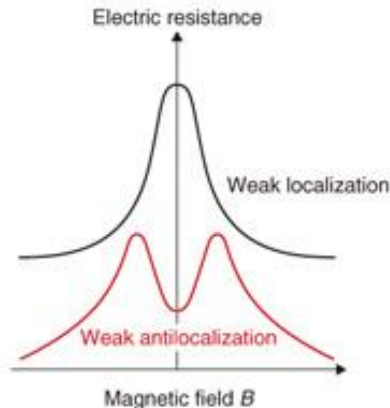
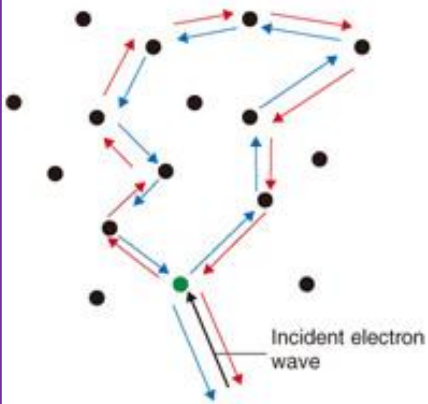
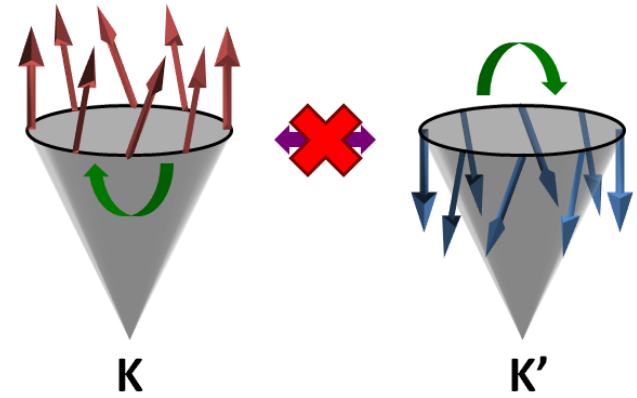
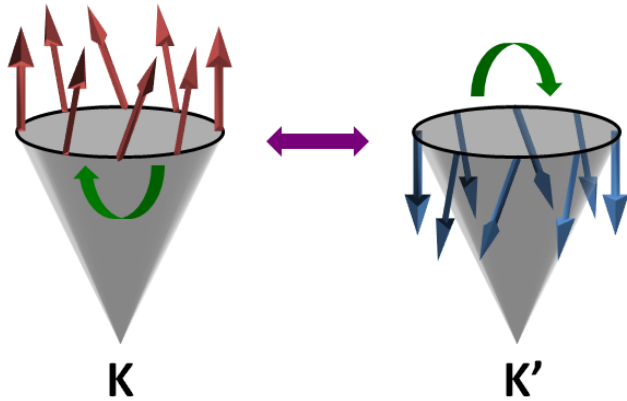


$$\theta_{sH} (\%) \simeq 4\%$$



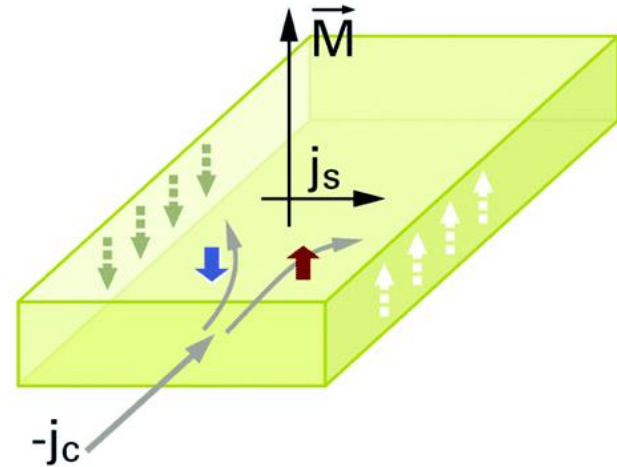
$$\theta_{sH} (\%) \ll 1\%$$

# Weak antilocalization vs Spin Hall Effect



(a) Generation mechanism

(b) Magneto-resistance effect



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

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

# OUTLINE

*Why Spintronics using 2D Materials ?*

*Proximity effects in 2D Materials-based heterostructures  
(spin dynamics & relaxation, SHE, weak antilocalization,  
QSHE)*

*Generating valley polarized quantum transport  
(valleytronics)*

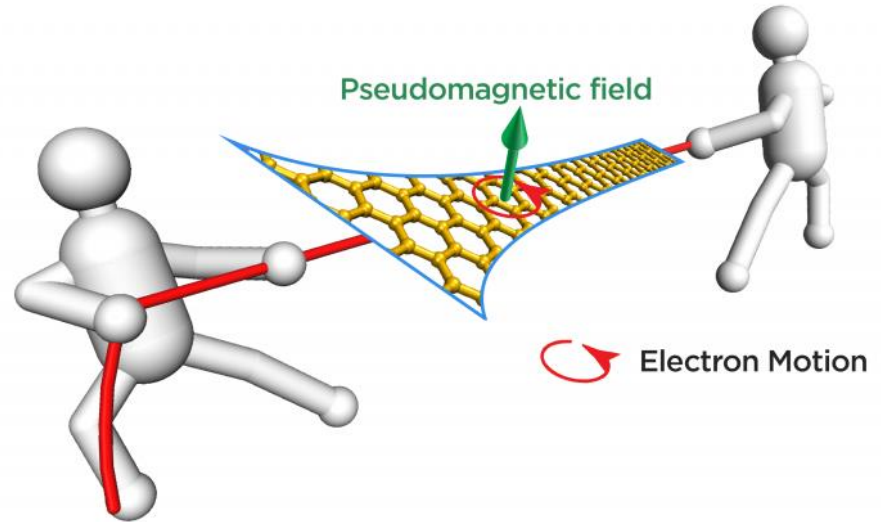
# Lattice deformation strain & pseudomagnetic fields

F. Guinea, M. I. Katsnelson,  
and A. K. Geim

**Nat. Phys. 6, 30 (2010)**

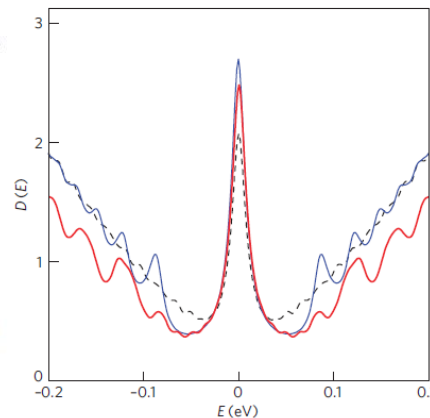
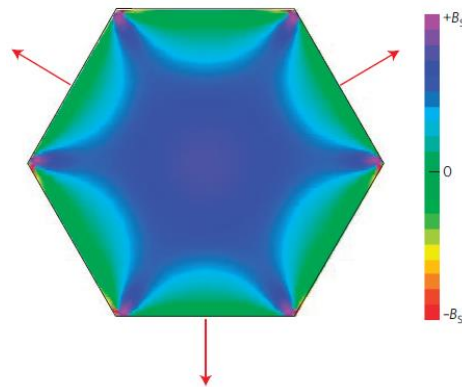
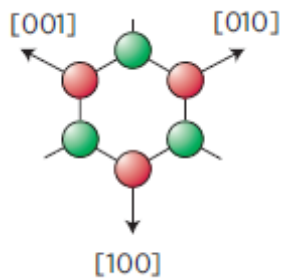
Strained superlattices  
**Gap opening & QHE**

$$\mathbf{B}_{strain} = \nabla \times \mathbf{A}$$



The strain-induced, pseudomagnetic field (idem for gauge-field vector potential) **has opposite signs for graphene's two valleys K and K' (no TRS breaking)**

Distribution of strain (triangular symmetry) results in a **strong uniform pseudomagnetic field**



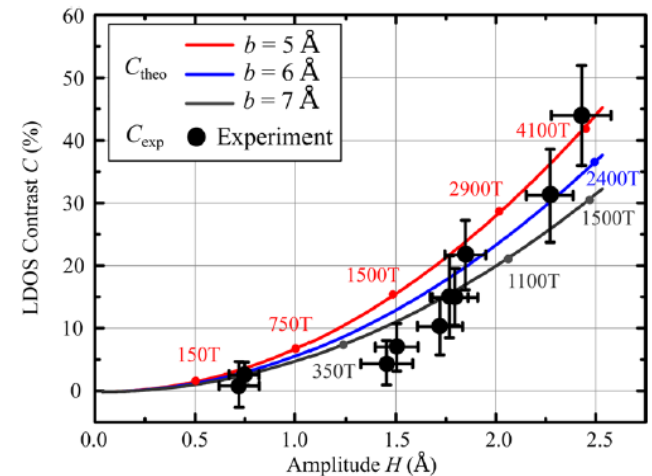
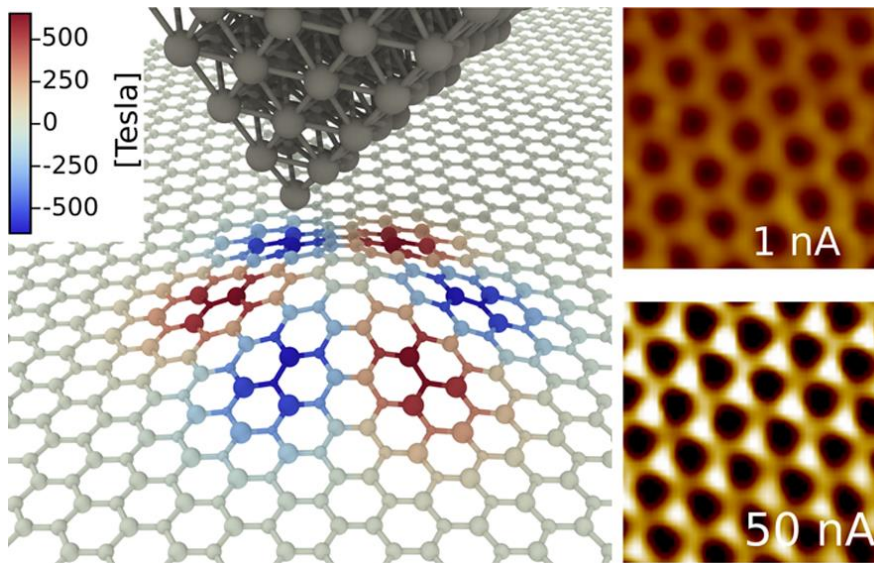
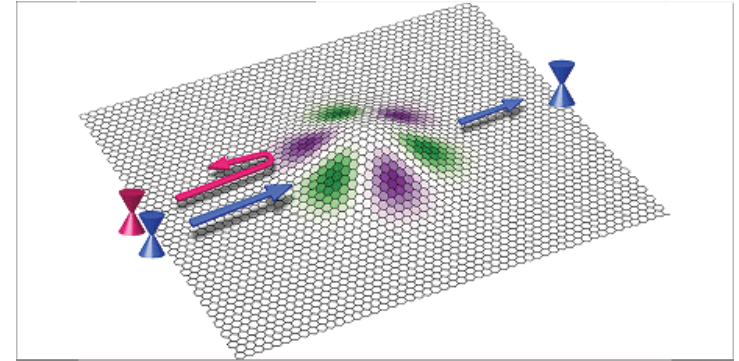
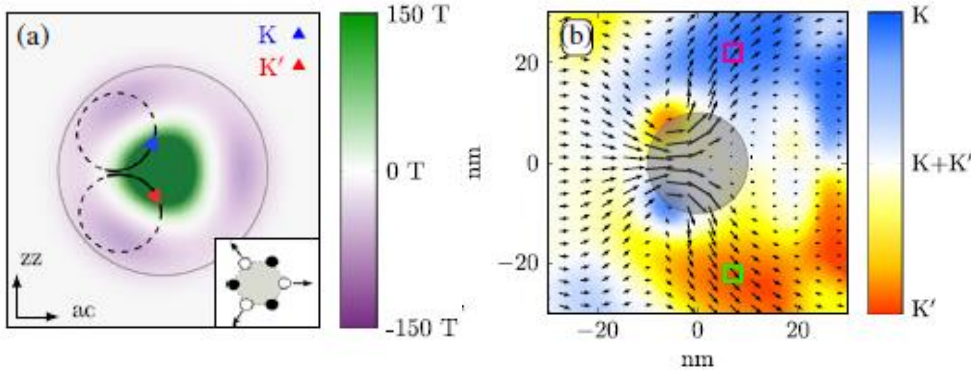
Strain of 10%  
 $B_{field} = 40$  Tesla



# Lattice deformation strain & pseudomagnetic fields

M. Settnes et al. *Phys. Rev. Lett.* **117**, 276801 (2016)

Graphene nanobubble



**$B_{\text{field}} = 1000 \text{ Tesla}$**

Signature of the pseudomagnetic field is a local sublattice symmetry breaking observable as a redistribution of the local density of states

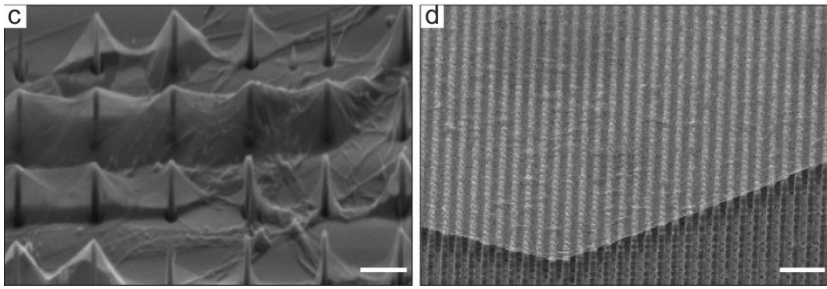
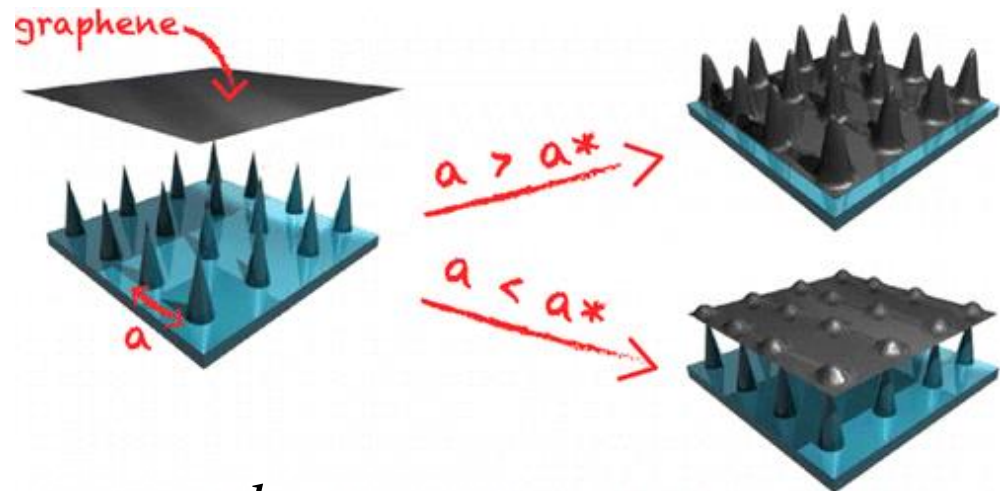
A. Georgi et al *Nano Lett.* **17** (4), pp 2240–2245 (2017)

# Engineering strain fields in graphene



*Strain Superlattices in graphene induced by corrugated substrates*

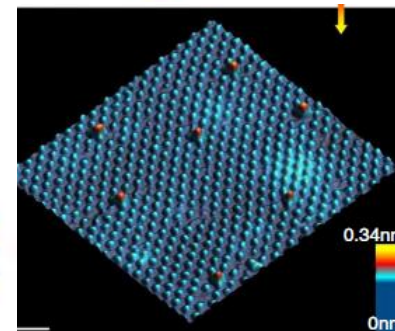
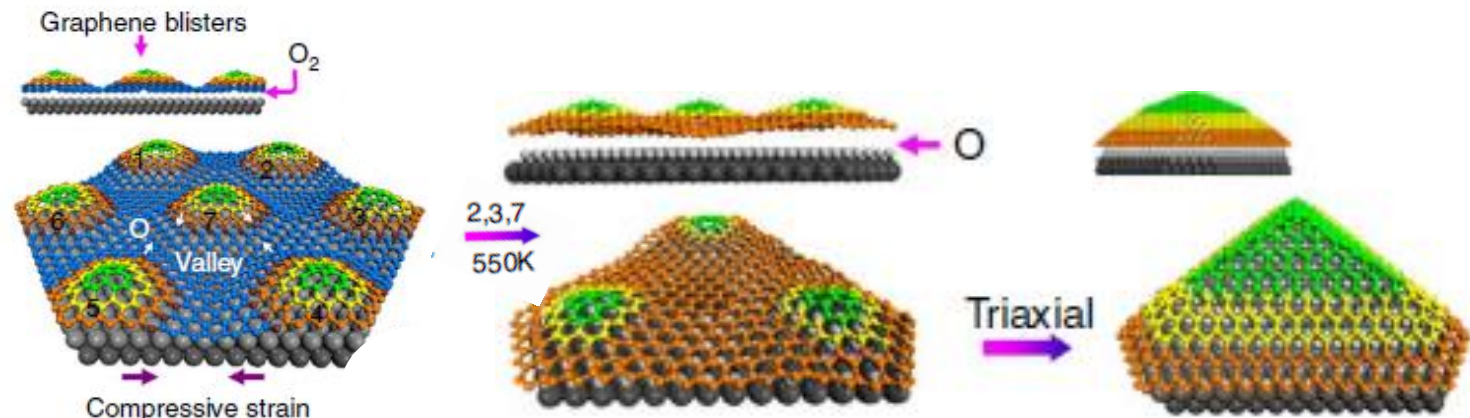
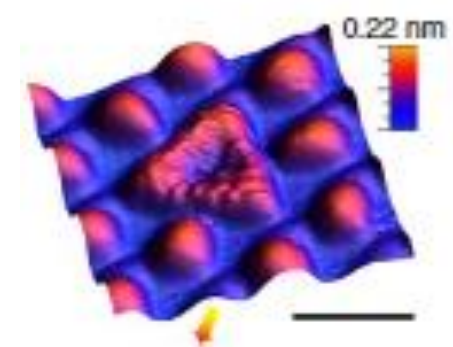
A. Reserbat-Plantey et al,  
**Nano Lett. 14 (9), 5044 (2014)**



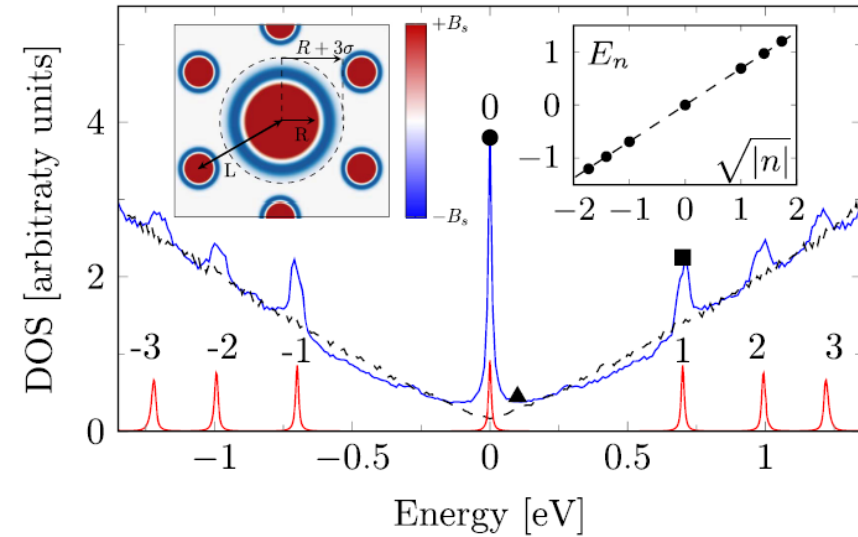
*Evolution of graphene Moiré blisters towards geometrically well-defined graphene nanobubbles*

Jiong Lu, A.H. Castro Neto & Kian Ping Loh

**Nature Communications 3, 823 (2012)**



# Pseudomagnetic fields for an array of nanobubbles



DoS of a strain array (blue) with local  $B_s=450$  Tesla  
(dashed : unstrained)  
(red: inner part of the strained region)

$$E_n = \hbar\omega^{Dirac} \text{sgn}(n) \sqrt{|n|}$$

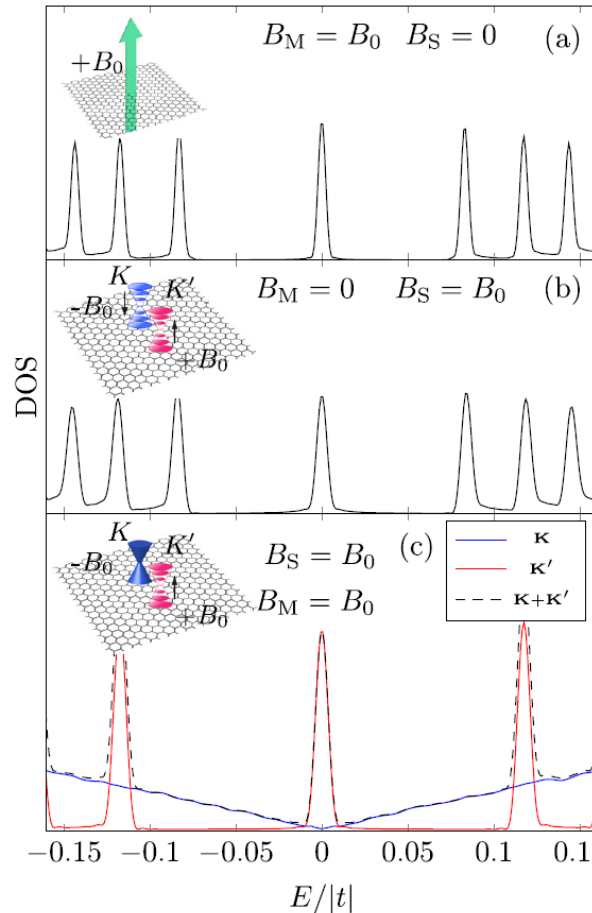
$$\omega^{Dirac} = v_F \sqrt{\frac{2eB}{\hbar c}}$$

M. Settnes, J.H. Garcia, S. Roche  
**2D Mater.** 4, 031006 (2017)

$\pm \vec{A}_S$  Valley-dependent strain-induced gauge

$\vec{A}_S \propto (\epsilon_{xx} - \epsilon_{yy}, -2\epsilon_{xy})$  strain tensor  
- triaxial deformation-

M. Settnes et al. **2D Mater.** 3, 034005 (2016)



Real magnetic field

$$\mathbf{B}_M = \nabla \times \mathbf{A}$$

Pseudomagnetic field

$$\mathbf{B}_S = \nabla \times \mathbf{A}_S$$

**Valley K'**

Total effective field  
 $= 2B_0$

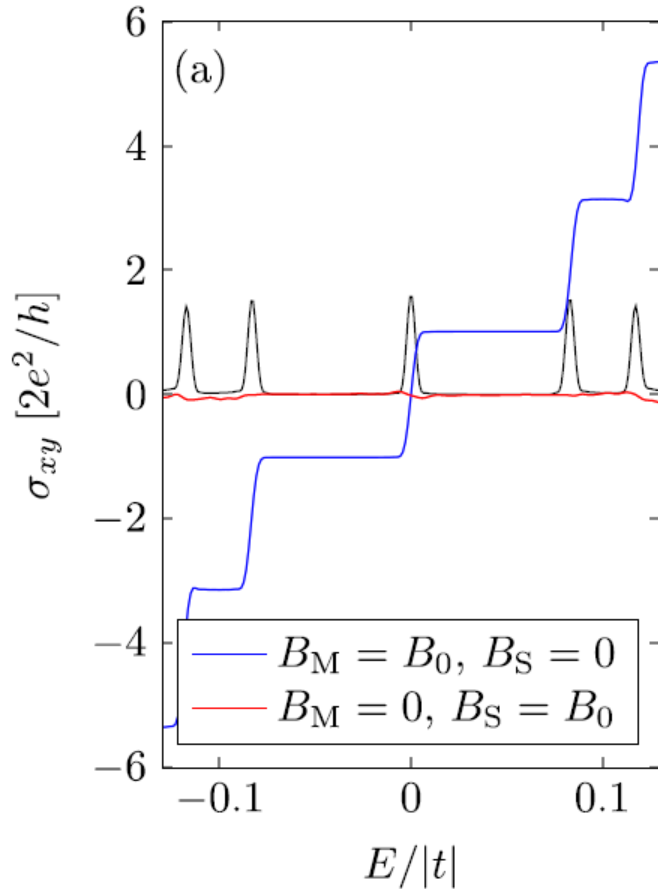
**Valley K**

Total effective field  
 $= 0$

# Charge and valley Hall Kubo conductivity

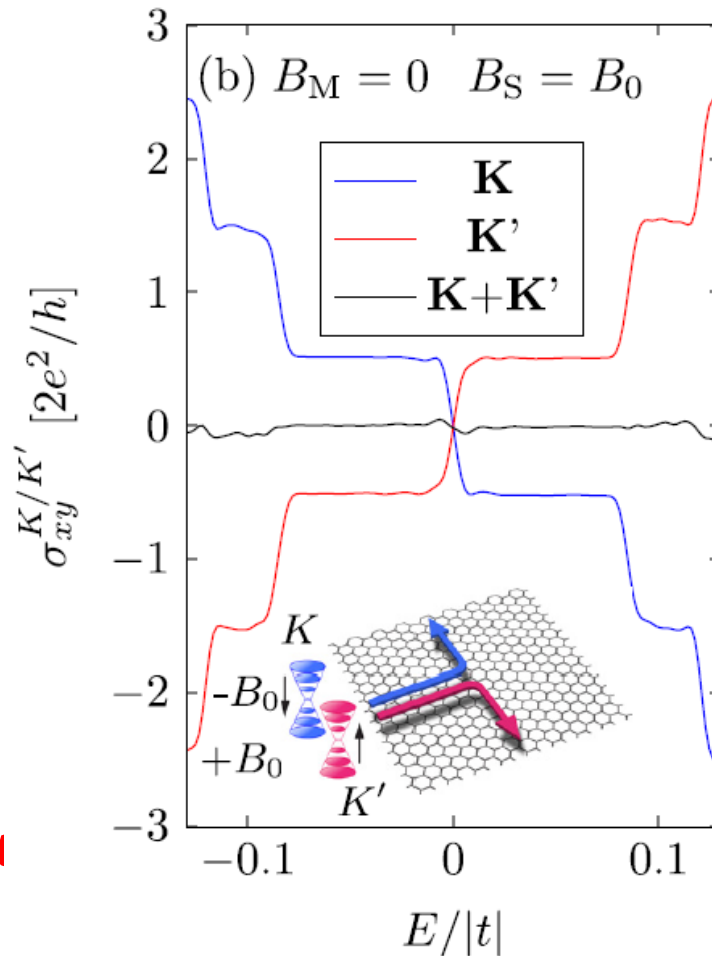
$$\sigma_{\alpha\beta} = \frac{ie^2\hbar}{\Omega} \int_{-\infty}^{\infty} d\epsilon f(\epsilon) \text{Tr} \left[ v_{\alpha} \delta(\epsilon - H) v_{\beta} \frac{dG^r(\epsilon)}{d\epsilon} - v_{\alpha} \frac{dG^a(\epsilon)}{d\epsilon} v_{\beta} \delta(\epsilon - H) \right], \quad v_{\beta}^v \equiv P_{\vec{K}} v_{\beta} P_{\vec{K}} - P_{\vec{K}'} v_{\beta} P_{\vec{K}'},$$

$P_{\vec{K}} (P_{\vec{K}'})$  is the valley projection operator



Total charge Hall current

$$\sigma_{xy} = \sigma_{xy}^K + \sigma_{xy}^{K'} = 0$$



**K-valley Hall conductivity**

$$\sigma_{xy}^K$$

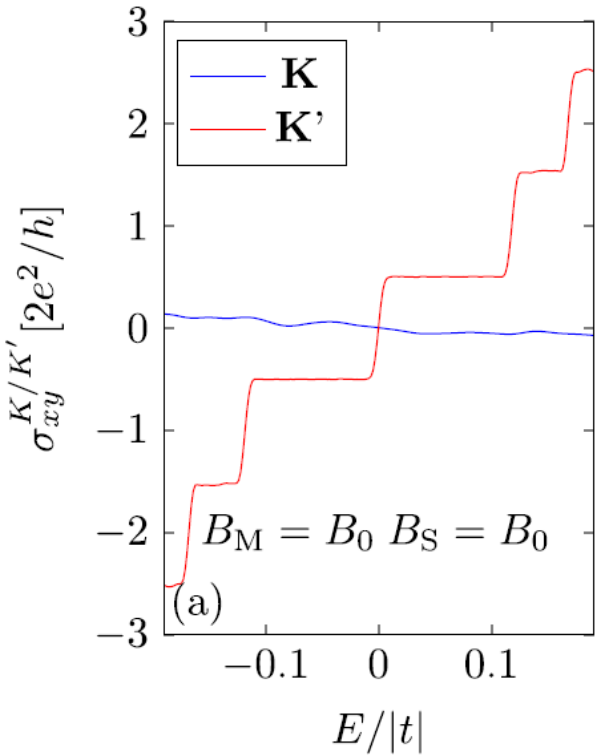
**K'-valley Hall conductivity**

$$\sigma_{xy}^{K'}$$

Valley Hall effect but valley Hall conductivities

**Are NOT observables**

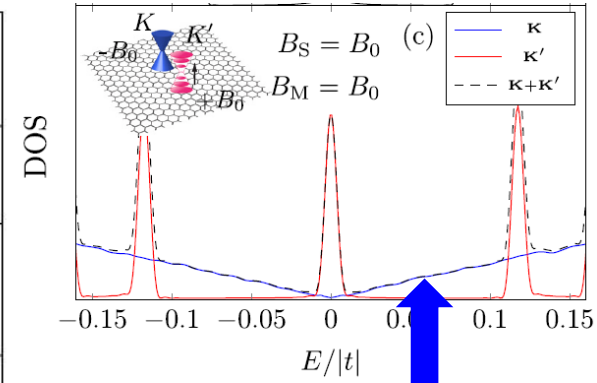
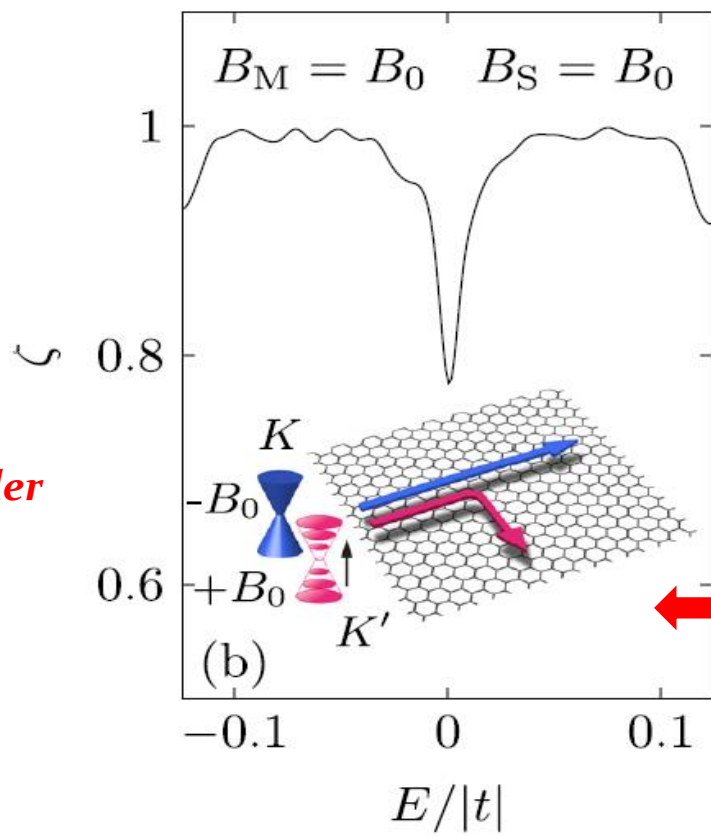
# Charge and valley Hall Kubo conductivity



Total charge Hall current

$$\sigma_{xy} = \sigma_{xy}^{K'} \neq 0$$

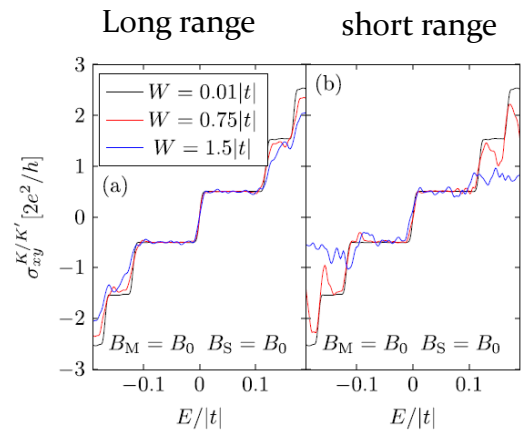
Valley polarization  $\zeta = (\sigma_{xx}^K - \sigma_{xx}^{K'}) / (\sigma_{xx}^K + \sigma_{xx}^{K'}) \approx 1$



K-Valley polarized  
dissipative conductivity

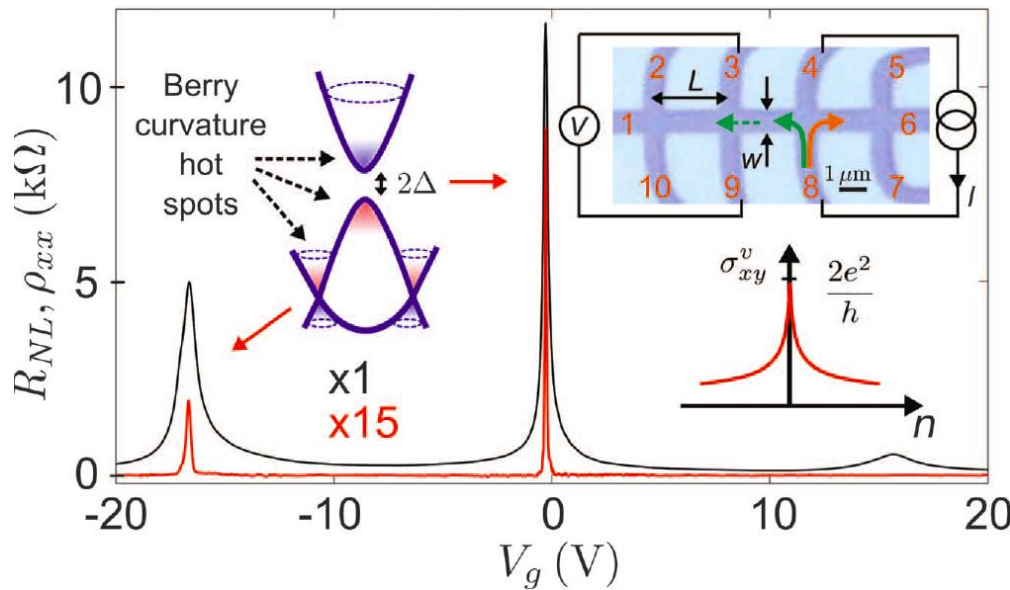
K'-Valley polarized  
Hall Conductivity

Robust with respect to disorder

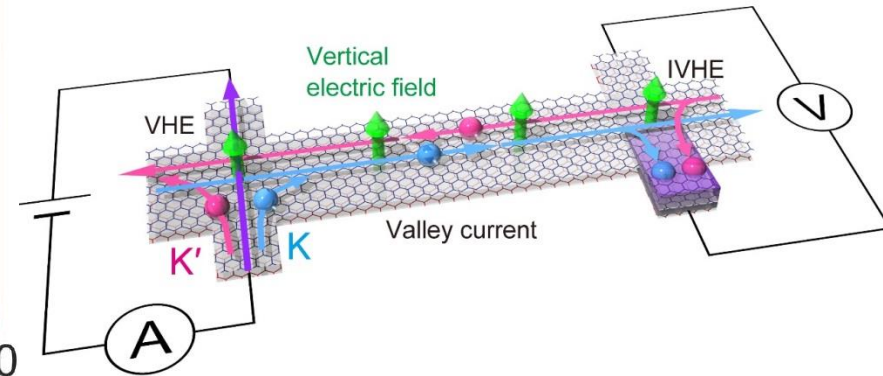


# Valleytronics and Valley currents

Recent claims of VHE measurements in Graphene/hBN  
in non-local transport geometries  
*(large non-local resistance at the Dirac point)*

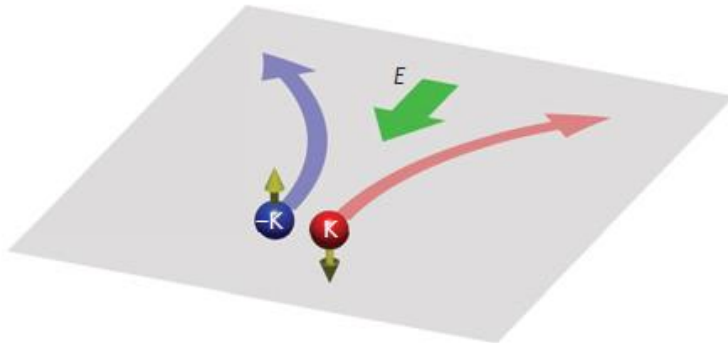


Gorbachev et al.  
**Science 346, 448 (2014)**

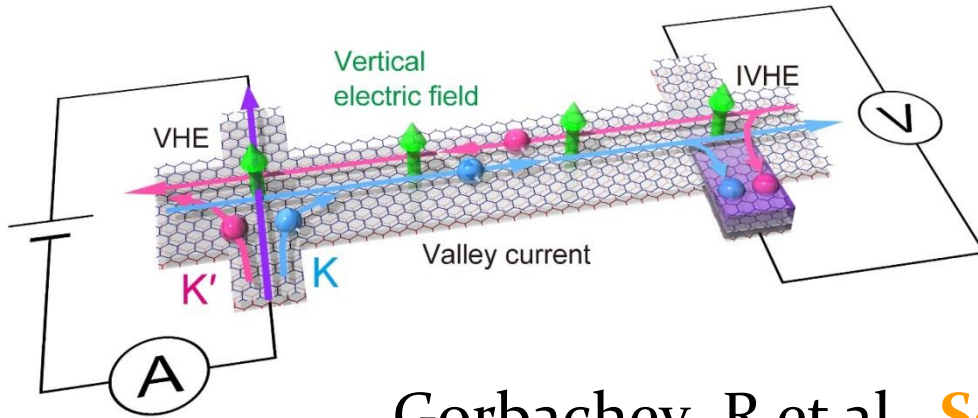


Gapped Dirac fermions+ electric field  
An anomalous perpendicular velocity is generated by the “**Berry curvature**”  
Valley Hall effect

$$\mathbf{v} = \frac{1}{\hbar} \frac{\partial \epsilon_{nk}}{\partial \mathbf{k}} - \partial_t \mathbf{k} \times \boldsymbol{\Omega}_{nk}$$



# Valleytronics and Valley currents ?



## Problems !!

Semiclassical argument of gap-induced Berry's curvature is not enough  
For generating topologically protected edge states

Gorbachev R et al. **Science** 346, 448 (2014)

Sui M. et al. **Nature Phys.** 11, 1027–1031 (2015)

Shimazaki, Y. et al. **Nature Phys.** 11, 1032–1036 (2015)

## Exact calculations

of bulk transport coefficients (Kubo)

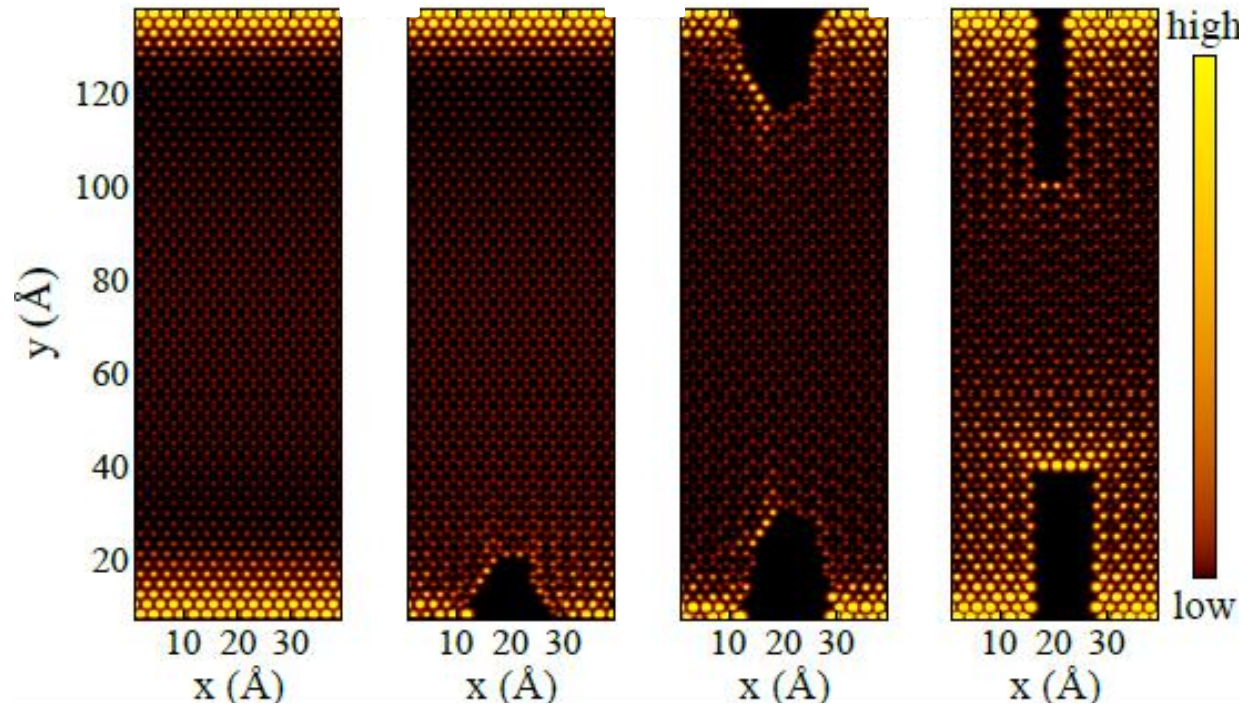
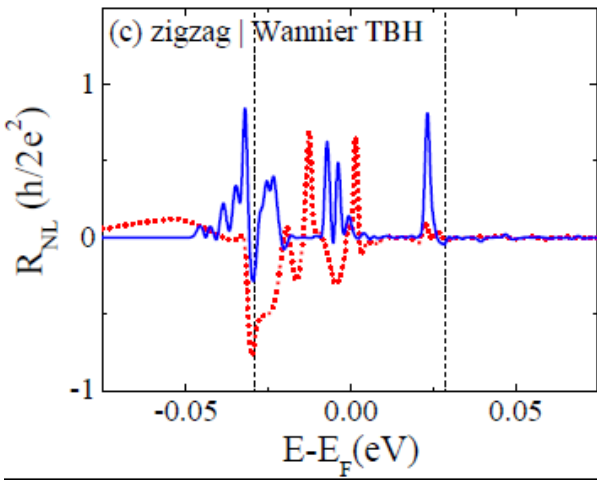
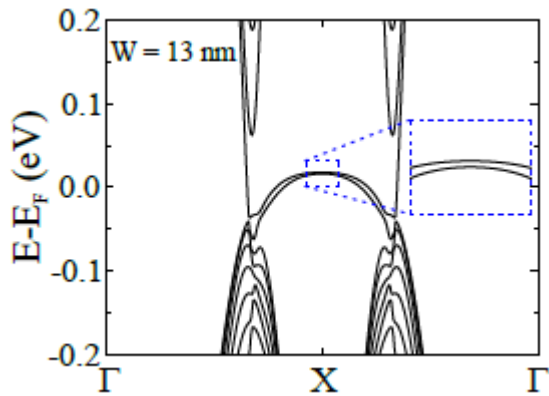
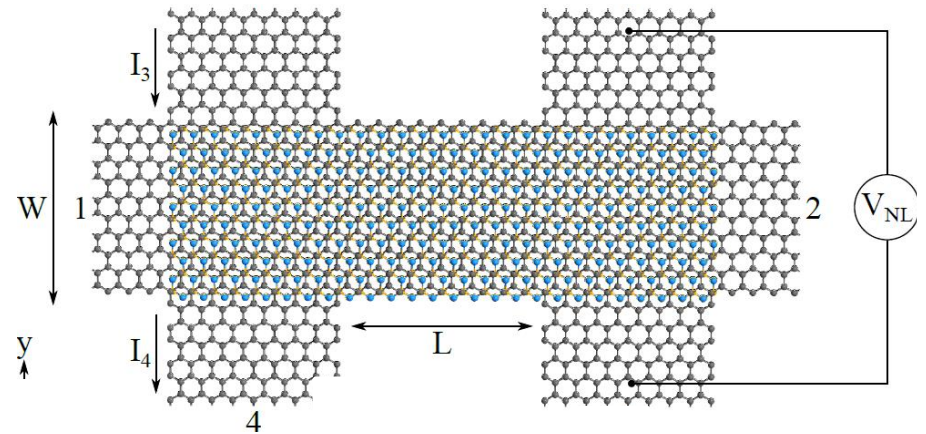
of non-local resistance (multiterminal Landauer-Büttiker)

$$R_{NL} \propto (\sigma_{xy}^v)^2 \rho_{xx}^3$$

**Gapped G/hBN leads to quantized valley Hall conductivity, and zero  $R_{NL}$  + disorder broadening invalidates the formula**

# Origin of nonlocal resistance in multiterminal G/hBN heterostructures

J. M. Marmolejo-Tejada et al  
(PRL, arXiv:1706.09361)





# Acknowledgements: Theoretical & Computational Nanoscience



$$\frac{\text{Tr}[[N, \hat{U}(t)]^\dagger \delta(E - \mathcal{H})[N, \hat{U}(t)]]}{\text{Tr}[\delta(E - \mathcal{H})]}$$

## Members

- ICREA Prof. Stephan Roche
- Aron W. Cummings (staff researcher)
- José Garcia (Pdoc)
- Kenan Song (SO PhD student)
- Stephen Power (P-sphere postdoc)
- Marc Vila (PhD la Caixa – 10/2016)
- Bruna Gabrielly (PhD 09/2017)



*And now dancing with the stars...  
In Memoriam*

