



Institut Català
de Nanociència
i Nanotecnologia



GRAPHENE FLAGSHIP



RED ESPAÑOLA DE
SUPERCOMPUTACIÓN

Charge and spin Hall Kubo conductivity by $O(N)$ real-space methods

(Proposal ID: 2015133194)

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Catalan Institute of Nanoscience and Nanotechnology (ICN2)

11th RES Users' Meeting & 6th HPC Advisory Council Conference



Barcelona Institute of
Science and Technology



Generalitat
de Catalunya

The team

Catalan Institute of Nanoscience
and Nanotechnology



Stephan Roche
P.I.



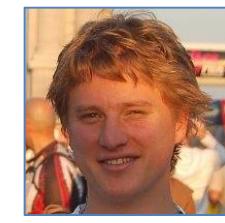
Jose H. Garcia



Aron Cummings



Jeil jung



Nicolas Leconte

University of Seoul

Current collaborators

- **Allan H. MacDonald**, The University of Texas at Austin, USA
- **Mikkel Settnes**, Technical University of Denmark, Denmark.
- **Branislav K. Nikolic**, University of Delaware, USA.
- **Alessandro Cresti**, Université Grenoble Alpes, IMEP-LAHC and CNRS, IMEP-LAHC, France.

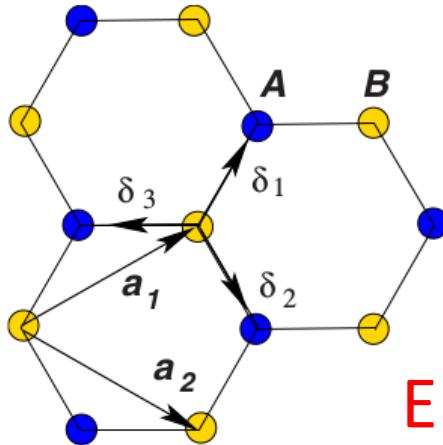
The goal

Understand the physics of Hall effects
in graphene and graphene-based
materials.

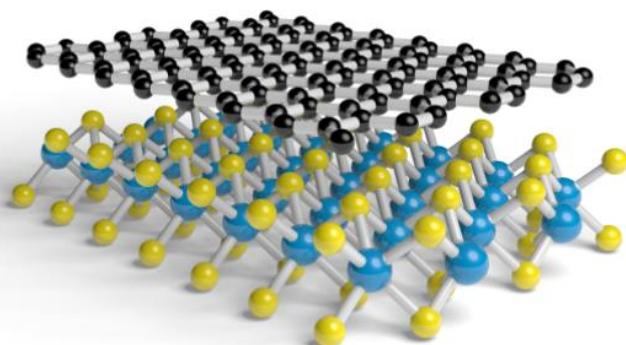
OUTLINE

- Graphene
- Hall effects
- Spintronics
- Quantum transport
- Numerical method
- Highlighted results
- Next steps

Graphene and graphene-based heterostructures

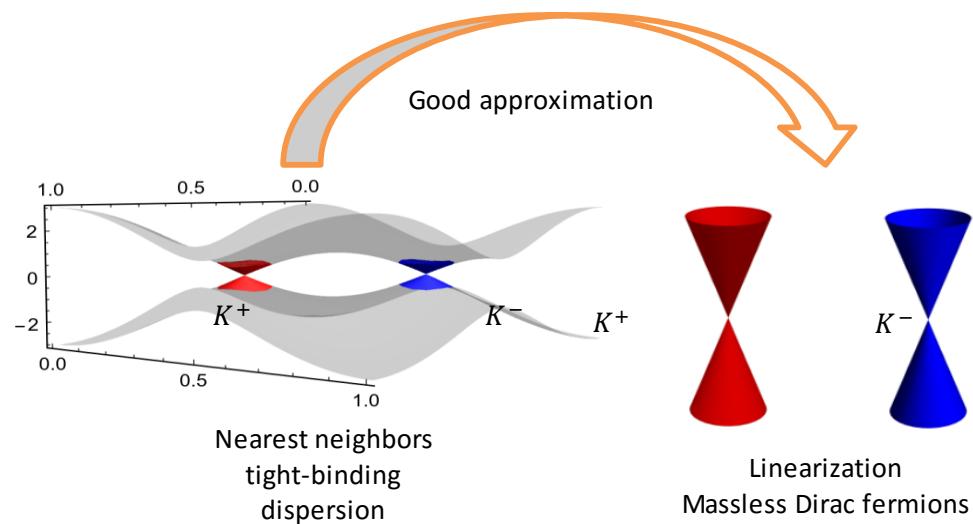


Electronic properties

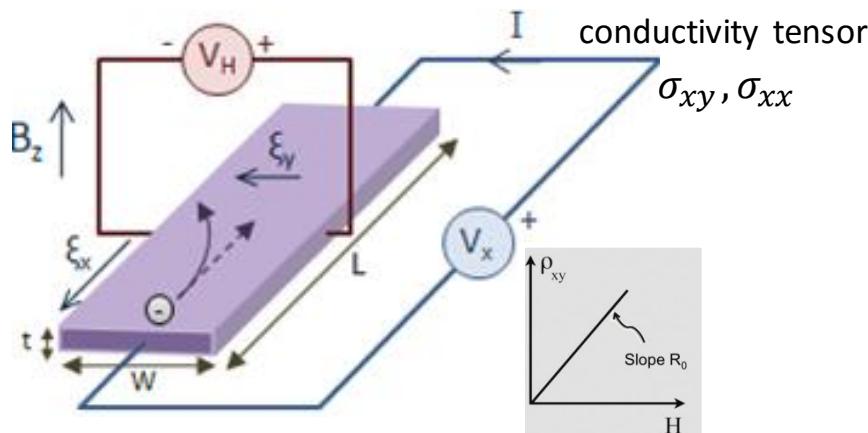


Why graphene?

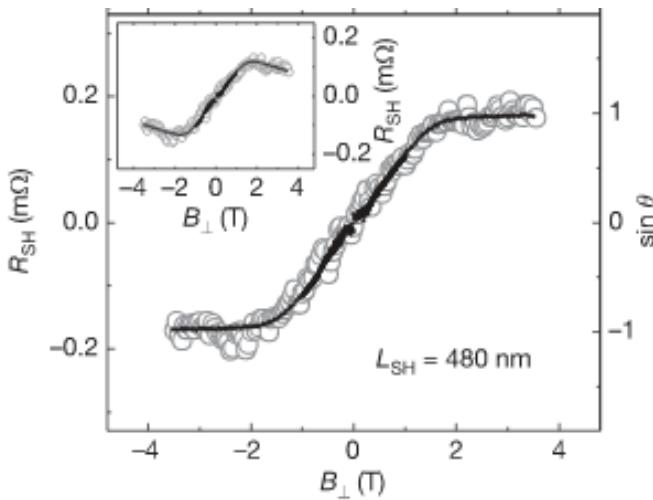
- Stronger and lighter than steel
- Transparent and flexible
- Better conductor than gold
- Ultrahigh mobility
- Tunable properties
- Among others



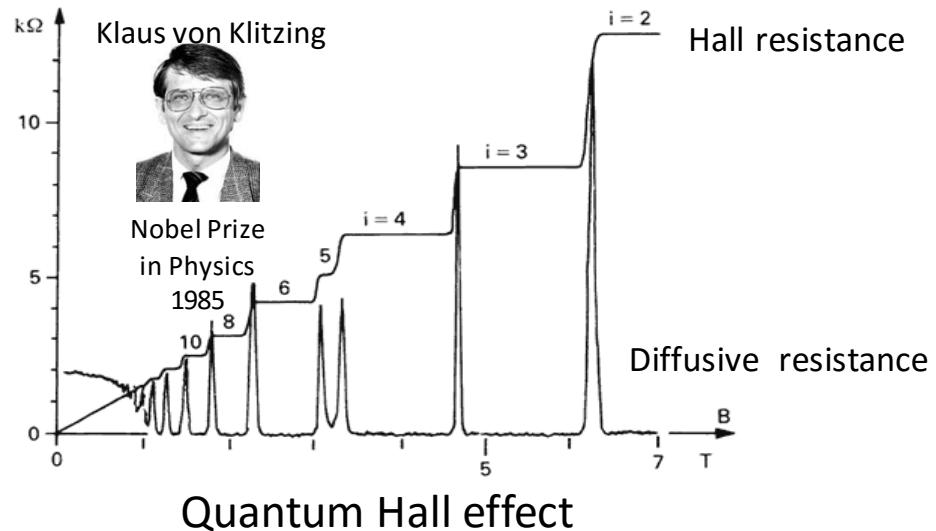
Hall effects



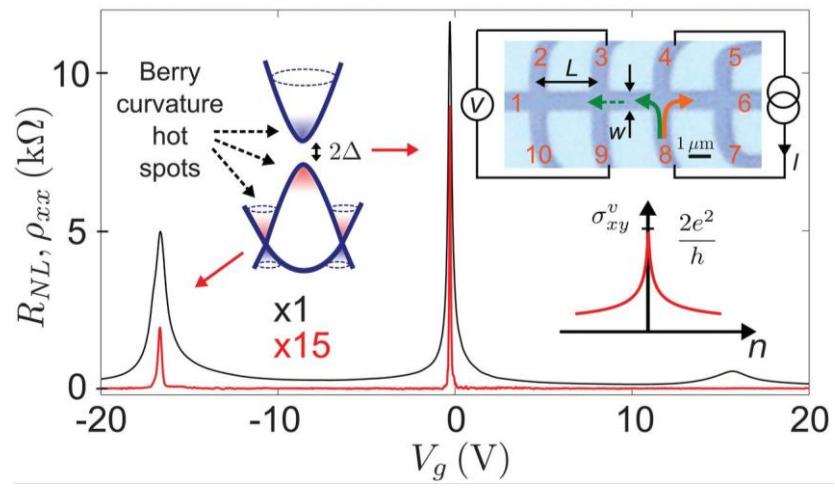
Classical Hall effect



Spin Hall effect

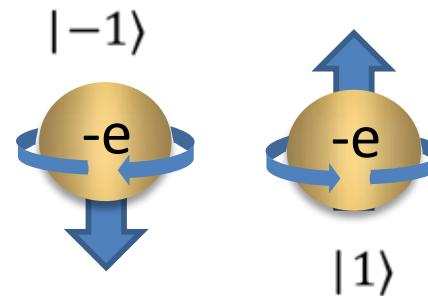
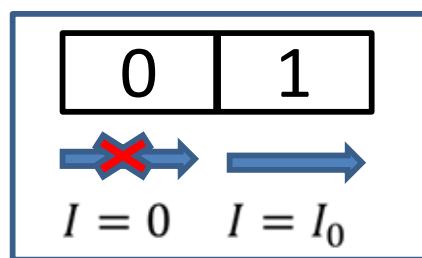


Quantum Hall effect

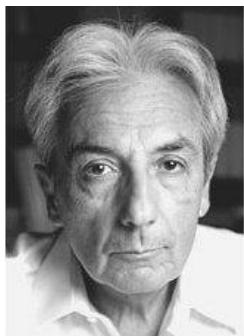


Valley Hall effect

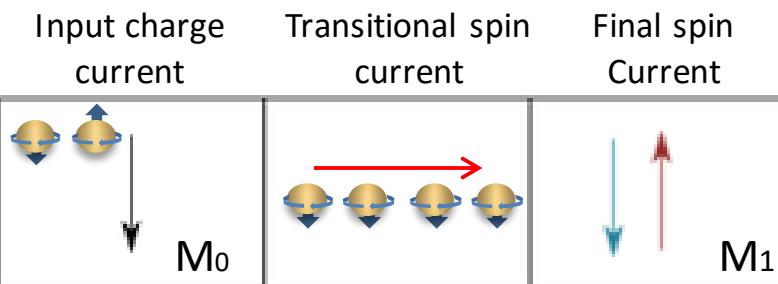
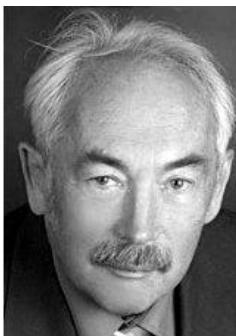
From electronic to spintronic



Albert Fert



Peter Grünberg

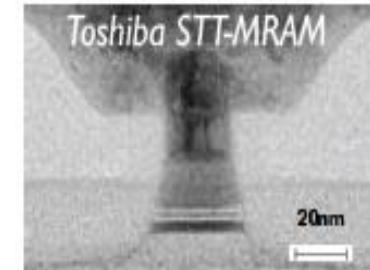
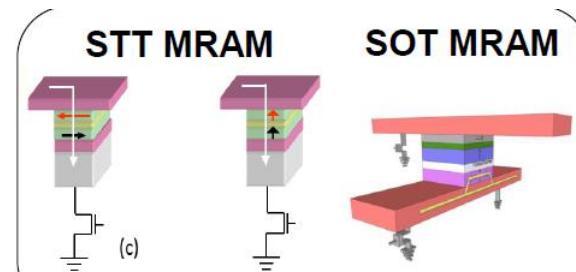


Giant magnetoresistance

2007 Physics Nobel Laureates



Spin-based information processing technologies



Spintronic and graphene



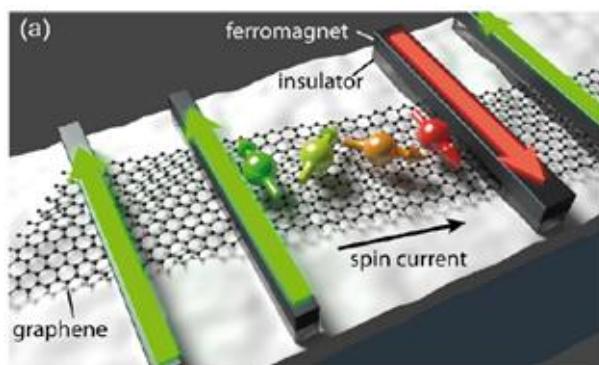
Challenges

1. Long spin lifetimes ✗
2. Electrical manipulation ✓
3. Large spin currents ✓

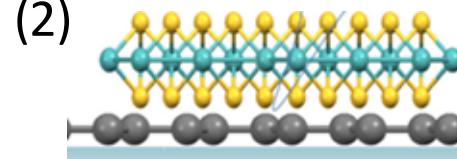
SPIN-ORBIT COUPLING!!

$$\lambda_{SOC} \vec{L}(\vec{p}) \cdot \vec{S}$$

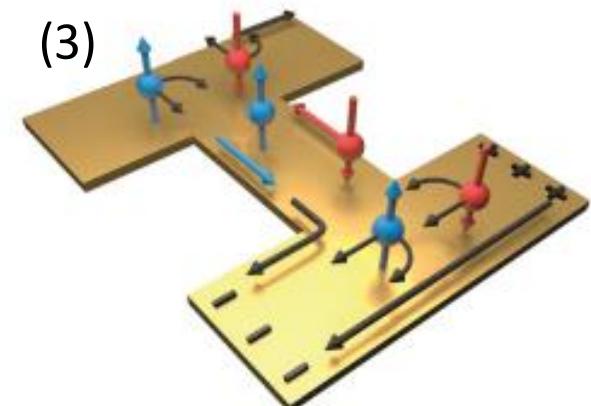
(1) Small λ_{SOC}



Spin-orbit
enhancement

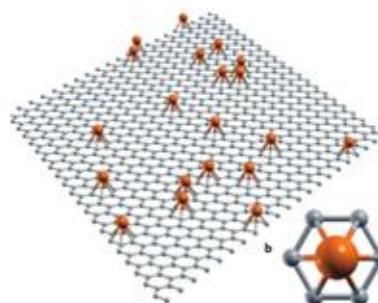


Spin Hall effect



Spin conductivity tensor

$$\sigma_{\alpha\beta}^z$$





GRAPHENE FLAGSHIP

Spintronics consortium/WP

Experimental partners

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



university of
groningen

 ICN2^R

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

MANCHESTER
1824
The University of Manchester

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

RWTHAACHEN
UNIVERSITY


UNI
BASEL

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

THALES Nanosc

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


cnrs

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

Catalan Inst. Nanoscience & Nanotech [ICN2]: **Sergio Valenzuela**

NanOSC AB : **Johan Åkerman**



Theoretical partners:

Catalan Inst. Nanoscience & Nanotech [ICN2]: **Stephan Roche**



imec

embracing a better life

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


UCL
Université
catholique
de Louvain

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



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



IMDEA : **Paco Guinea**

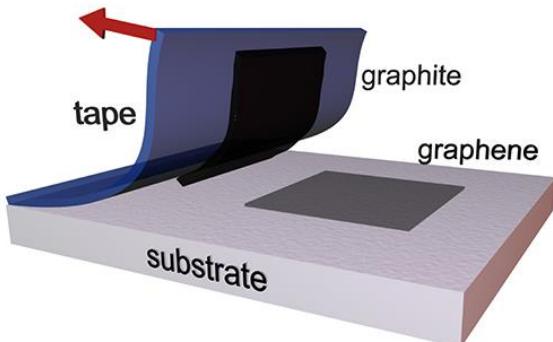

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Universität Regensburg

Quantum transport

The Kubo formula

$$\sigma_{\alpha,\beta}(\mu, T) = \int_{-\infty}^{\infty} d\varepsilon f(\mu, \varepsilon, T) \text{Tr} \left[\frac{dG^+(H, \varepsilon)}{d\varepsilon} j_\alpha \text{Im}[G^+(H, \varepsilon)] j_\beta - \text{Im}[G^-(H, \varepsilon)] j_\alpha \frac{dG^-(H, \varepsilon)}{d\varepsilon} j_\beta \right]$$

- j_α, j_β current matrix
- H Hamiltonian matrix
- $G^\pm(H, \varepsilon)$ Green's functions



$N = 10^6 - 10^9$ atoms

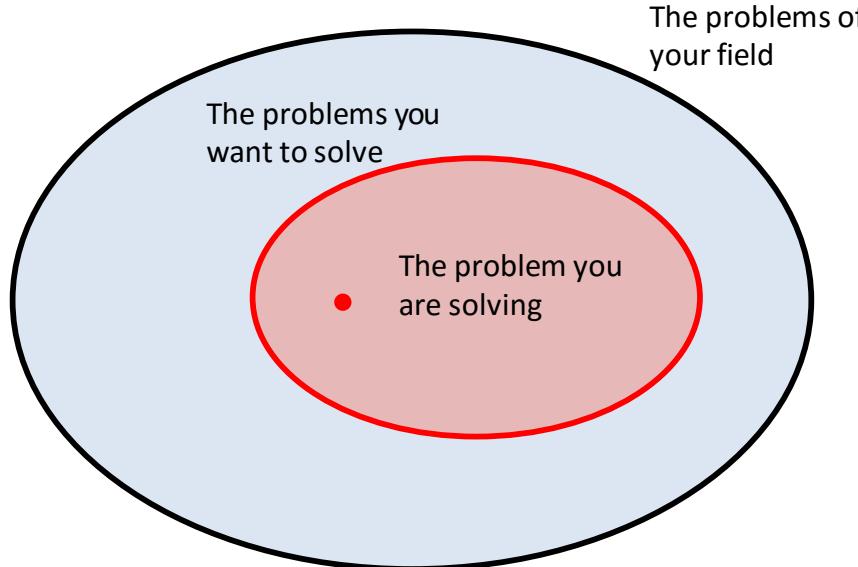
matrices with dimension
N=number of atoms

$O(N)$ real-space algorithms

- S. Roche, *Phys. Rev. B* **59**, 2284 (1999)
- F. Ortmann, N. Leconte, and S. Roche *Physical Review B* **91**, 16511 (2015)
- Jose H. Garcia, Lucian Covaci, Tatiana G. Rappoport, *Phys. Rev. Lett.* **114**, 116602 (2015)

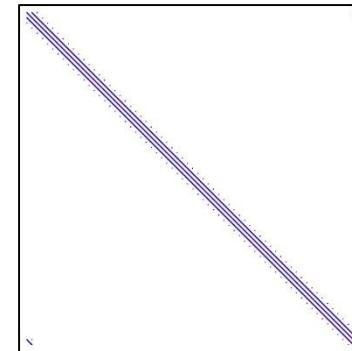
$O(N^3)$ → $O(N)$
1 billion years → 1 month

The importance of the algorithm



What kind of methods provide a better balance?

$$G^\pm(H, \epsilon) = \lim_{\eta \rightarrow 0} \frac{1}{\epsilon - H \mp i\eta}$$



Iterative methods!

Flexibility



Iterative methods

Matrix inversion

$$G^\pm(H, \epsilon) = \lim_{\eta \rightarrow 0} \frac{1}{\epsilon - H \mp i\eta} \quad \xrightarrow{\text{red arrow}} \quad G^\pm(H, \epsilon) = \sum_{m=0}^M a_m(\epsilon) P_m(H)$$

Matrix-vector product

$$P_m(H) = \alpha_1 P_{m-1}(H) + \alpha_2 P_{m-2}(H)$$

Depends on the polynomial basis

→ *Chebyshev Polynomials*
→ *Lanczos algorithm*

$$\sigma_{\alpha,\beta}(\mu, T) = \sum_{m=0}^M \sum_{n=0}^M \Gamma_{m,n}(\epsilon) \text{Tr} [P_m(H) j_\alpha P_n(H) j_\beta]$$

Expansion moments $\mu_{m,n}$

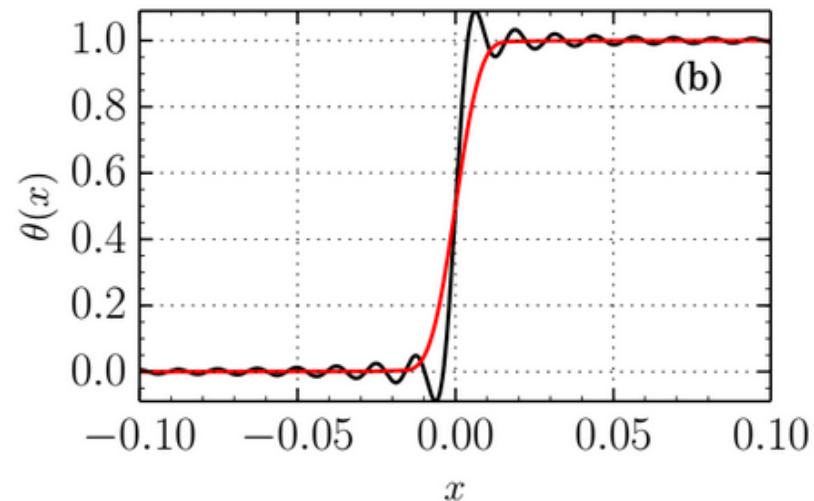
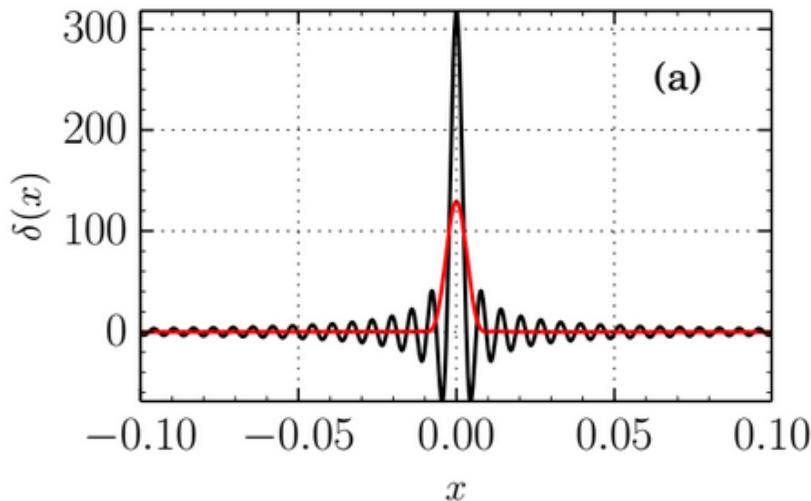
The Chebyshev Polynomials

Recursive relation:

$$T_m(H) = 2 H T_{m-1}(H) - T_{m-2}(H)$$

Chebyshev kernel:

$$\sigma_{\alpha,\beta}(\mu, T) = \sum_{m=0}^M \sum_{n=0}^M \Gamma_{m,n}(\varepsilon) g_m^M g_n^M \mu_{m,n}$$



Stochastic trace approximation

$$\mu_{m,n} = \text{Tr} [T_m(H) j_\alpha T_n(H) j_\beta]$$

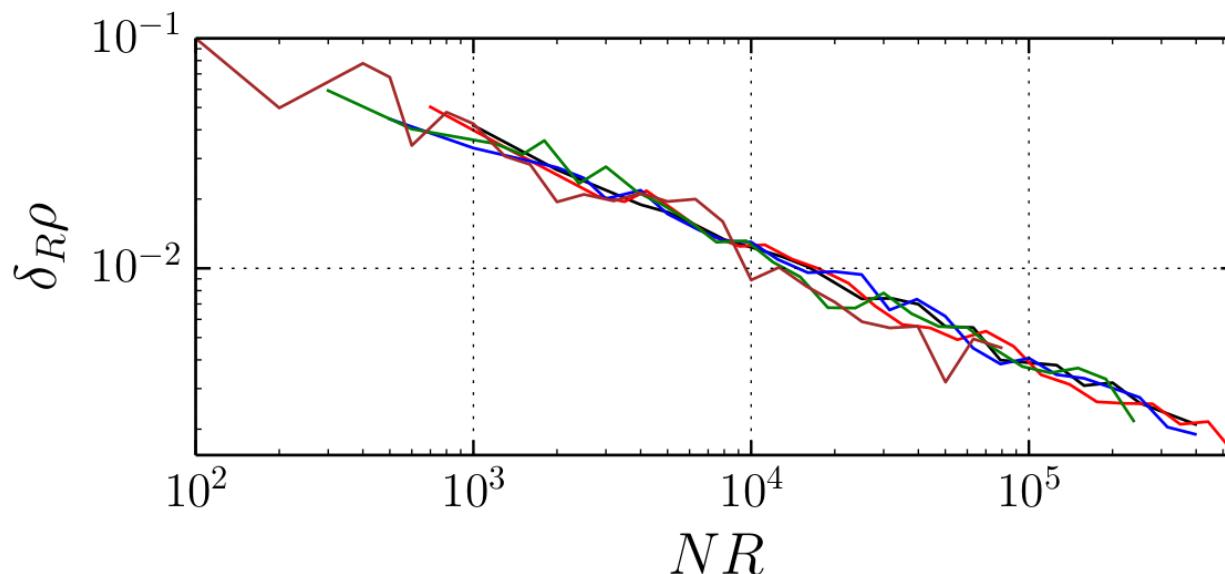
$10^4 - 10^6$ N-dimensional traces

Special random vectors

$$|r\rangle = \sum_{i=0}^N \xi_i^r |i\rangle \quad \left\{ \begin{array}{l} \langle\langle \xi_i^r \rangle\rangle = 0 \\ \langle\langle \xi_i^r \xi_j^s \rangle\rangle = \delta_{ij} \delta_{rs} \end{array} \right.$$

Trace as average of mean values

$$\text{Tr} [A] \approx \frac{1}{R} \sum_{r=1}^{R \ll N} \langle r | A | r \rangle, \quad \text{Err}(\text{Tr}[A]) \propto \frac{1}{\sqrt{NR}}$$



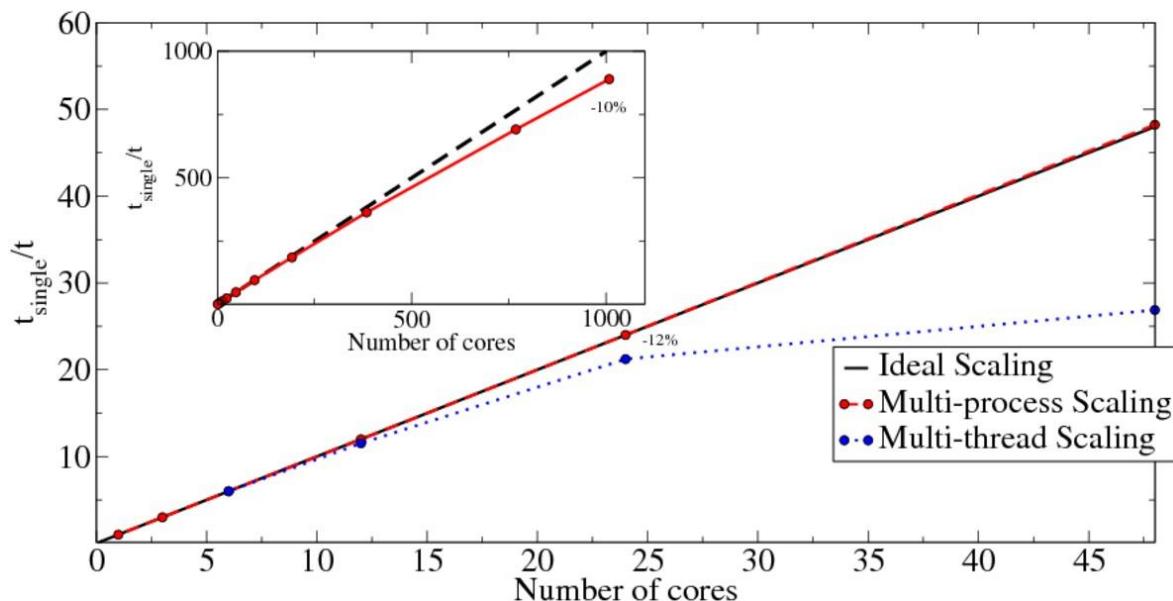
Parallelizability

$$\mu_{m,n} = \text{Tr} [T_m(H) j_\alpha T_n(H) j_\beta]$$

Multi-threaded
sparse matrix-vector
multiplication

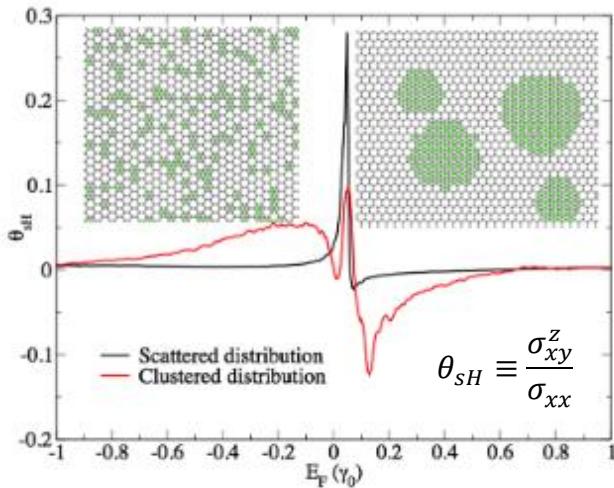
μ_{00}	$\mu_{0,1}$	$\mu_{0,2}$...	$\mu_{0,M-1}$	$\mu_{0,M}$	Process #1
$\mu_{1,0}$	$\mu_{1,1}$	$\mu_{1,2}$...	$\mu_{1,M-1}$	$\mu_{1,M}$	Process #2
$\mu_{2,0}$	$\mu_{2,1}$	$\mu_{2,2}$...	$\mu_{2,M-1}$	$\mu_{2,M}$	Process #3
:	:	:	:	:	:	⋮
$\mu_{M-1,0}$	$\mu_{M-1,1}$	$\mu_{M-1,2}$...	$\mu_{M-1,M-1}$	$\mu_{M-1,M}$	Process #N-1
$\mu_{M,0}$	$\mu_{M,1}$	$\mu_{M,2}$...	$\mu_{M,M-1}$	$\mu_{M,M}$	Process #N

Multi-process
stripes
distributions

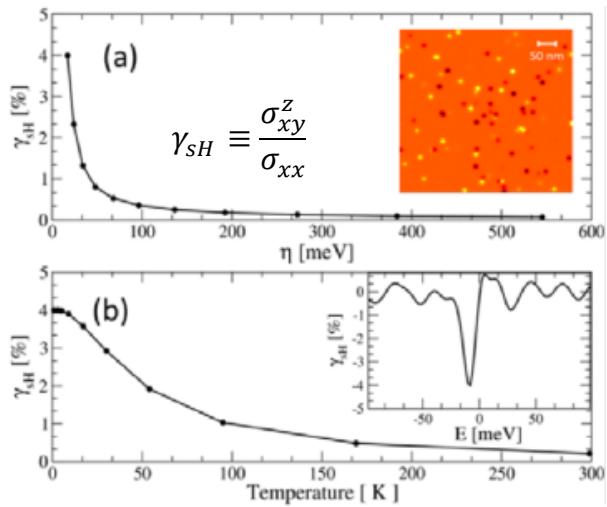


Our results

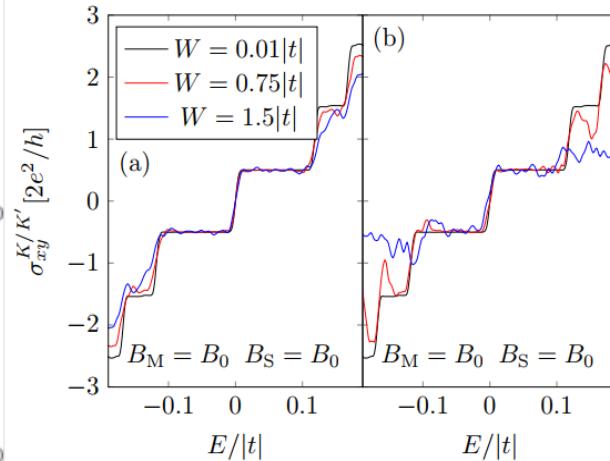
10⁷ atoms, samples of 400 nm



Physical Review Letters
117, 176602 (2016)



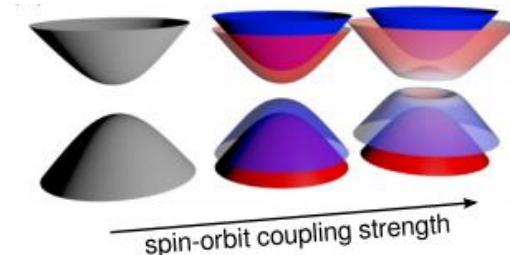
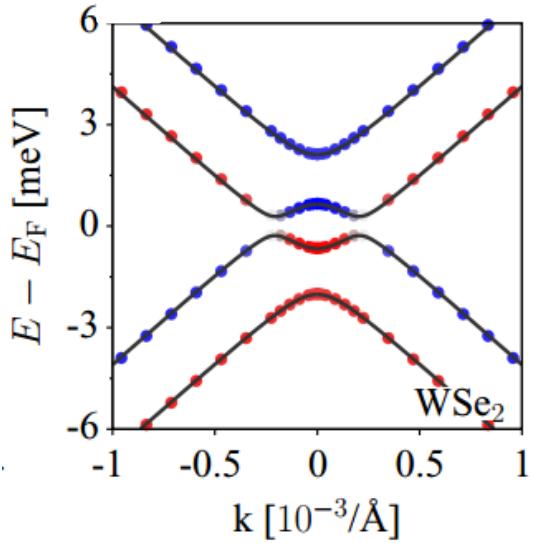
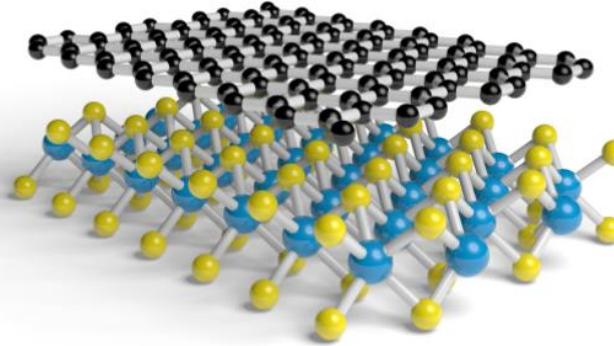
Nano Letters
17 (08), 5078-5083(2017)



2D Materials
4 (03), 031006 (2017)

- Spin Hall effect and Weak Antilocalization in Graphene/Transition Metal Dichalcogenide Heterostructures, J.H. Garcia et al, **Nano Letters** **17** (8), 5078-5083 (2017).
- Valley-Polarized Quantum Transport Generated by Gauge Fields in Graphene, M. Settnes et al. **2D Materials** **4** (3) (2017)
- Spin Hall Effect and Origins of Nonlocal Resistance in Adatom-Decorated Graphene. D Van Tuan et al. **Phys. Rev. Lett.** **117** (17), 176602 (2016).
- (OPEN ACCESS) Charge, spin and valley Hall effects in disordered graphene, A. Cresti, et al. **Rivista del Nuovo Cimento** **39**, N. 12, pp.586-664 (2016).
- Spin lifetime anisotropy in graphene/TMDC heterostructures.A.W. Cummings et al, submitted to **Phys. Rev. Lett.**
- Theory of quantum magneto-transport in graphene on hexagonal boron nitride, N. Leconte et al, to be submitted to **Phys. Rev. B**
- Extension of the levitation scenario for interaction of states coming from primary and secondary Landau levels in a superlattice system, N. Leconte et al, **ongoing calculations**.

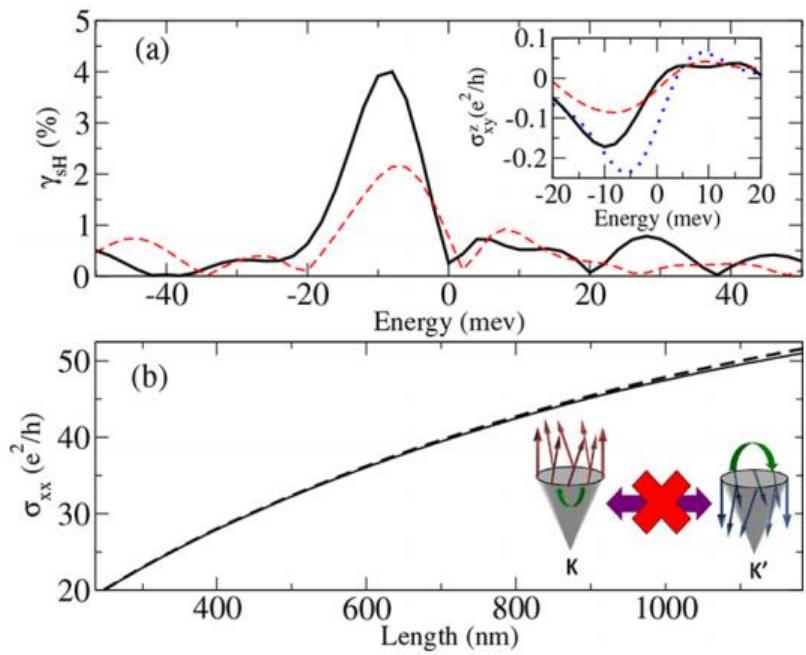
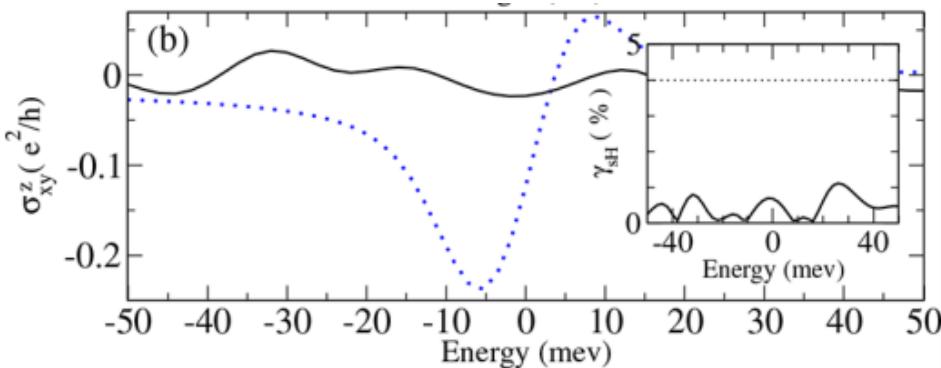
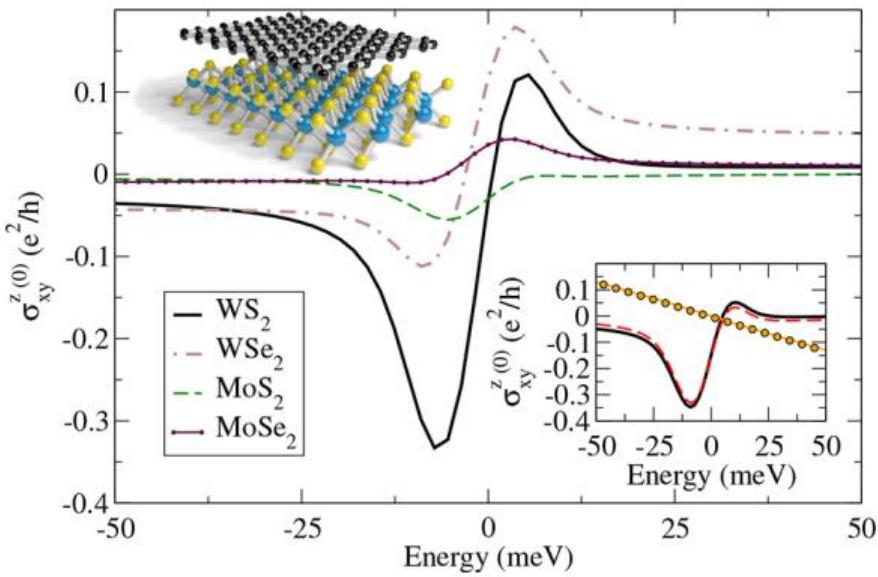
Graphene/TMDC heterostructure



TMDC	ΔE_v (eV)	ΔE_c (eV)	dipole (Debye)	W_{grp} (eV)	W_{TMDC} (eV)	$v_F/10^5$ (m/s)	t (eV)	Δ (meV)	λ_I^A (meV)	λ_I^B (meV)	λ_R (meV)	λ_{PIA}^A (meV)	λ_{PIA}^B (meV)
MoS ₂	1.51	0.04	0.628	4.12	4.407	8.506	2.668	0.52	-0.23	0.28	0.13	-1.22	-2.23
MoSe ₂	0.56	0.92	0.624	4.3	4.577	8.223	2.526	0.44	-0.19	0.16	0.26	2.46	3.52
WS ₂	1.13	0.30	0.675	4.12	4.432	8.463	2.657	1.31	-1.02	1.21	0.36	-0.98	-3.81
WSe ₂	0.22	1.15	0.641	4.3	4.587	8.156	2.507	0.54	-1.22	1.16	0.56	-2.69	-2.54

Spin Hall effect in Gr/TMDC

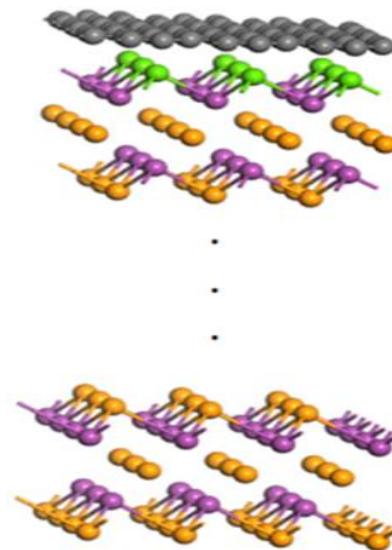
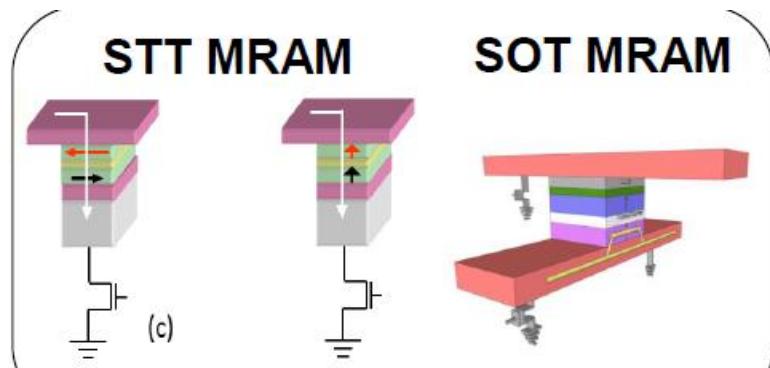
10⁷ atoms, M=4000



Suppression of spin Hall angle
 due to intervalley scattering!

The next steps

- Study spin-orbit torque in Gr/TMDC heterostructures
- Study spin Hall effect and spin-orbit torque in Gr/Topological Insulator heterostructures
- Improve the SpMV multiplication in order to achieve linear scaling up to 48 threads



Conclusions

- The Chebyshev approximation of the Kubo formula can be implemented to efficiently use more than 1000 cores using a hybrid multithread-multicores strategy.
- Using MareNostrum infrastructure we manage to simulation the transport properties of systems containing tenth of millions of atoms.
- Through numerical simulations we proved that a large spin hall angle can be achieve in graphene-based materials, showing it suitability for spintronic devices.

The End

Thank you for your attention