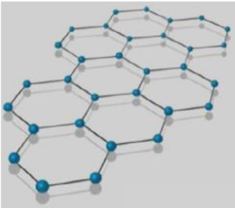
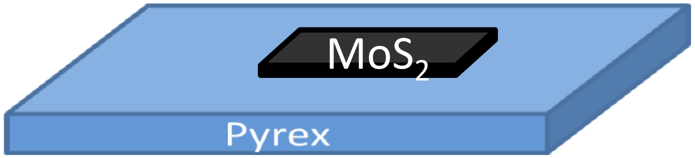
Graphene and beyond: Other 2D Materials

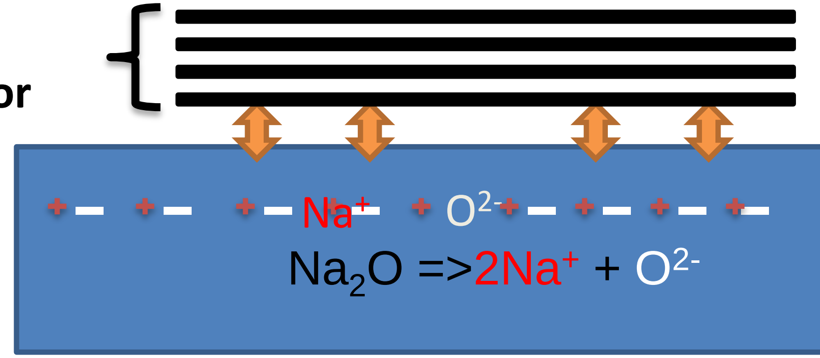
Abhay SHUKLA et al.(IMPMC, UPMC-P6)
Massimiliano MARANGOLO et al. (INSP, UPMC-P6)
Sébastien LEBESGUE et al. (CRM2, Nancy)

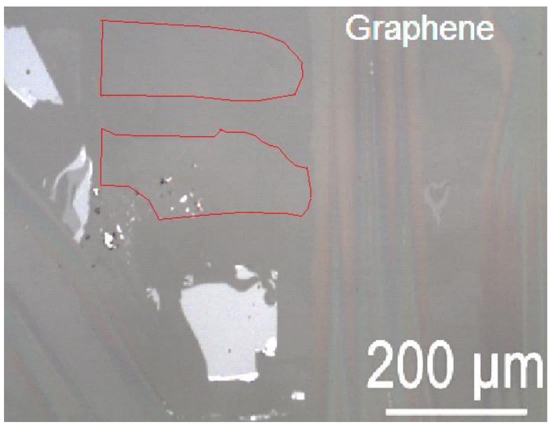


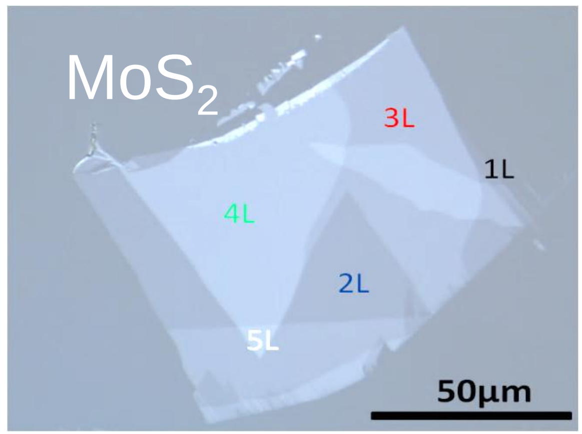
2D materials (by anodic bonding) IMPMC

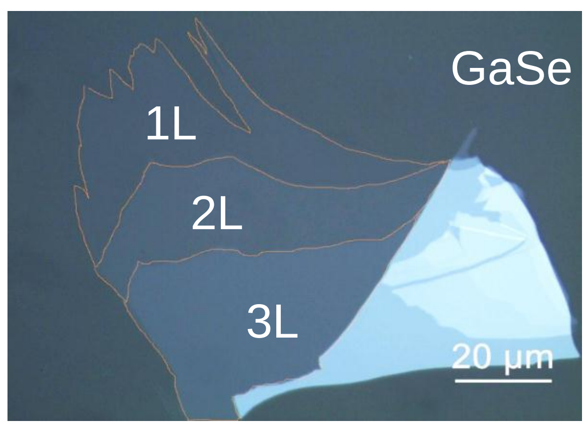


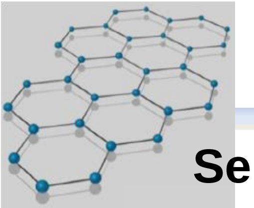
Layered precursor





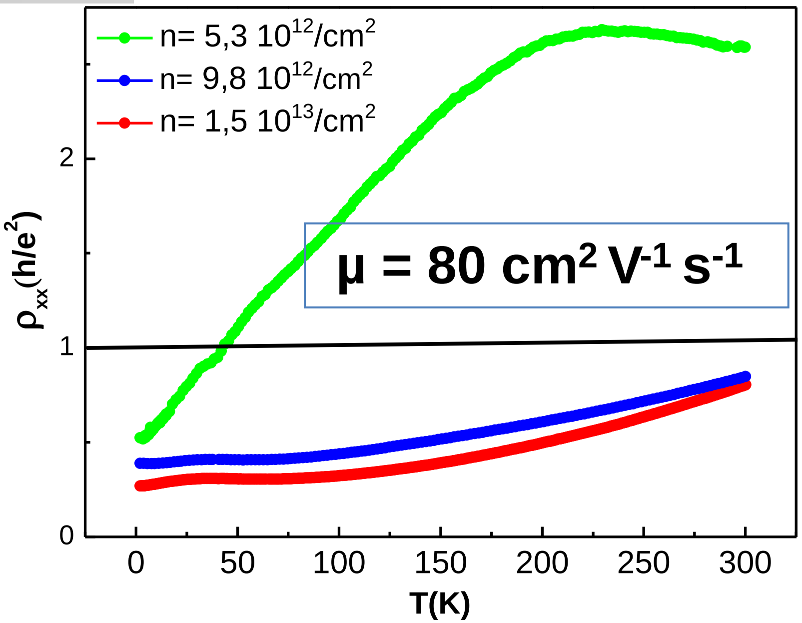


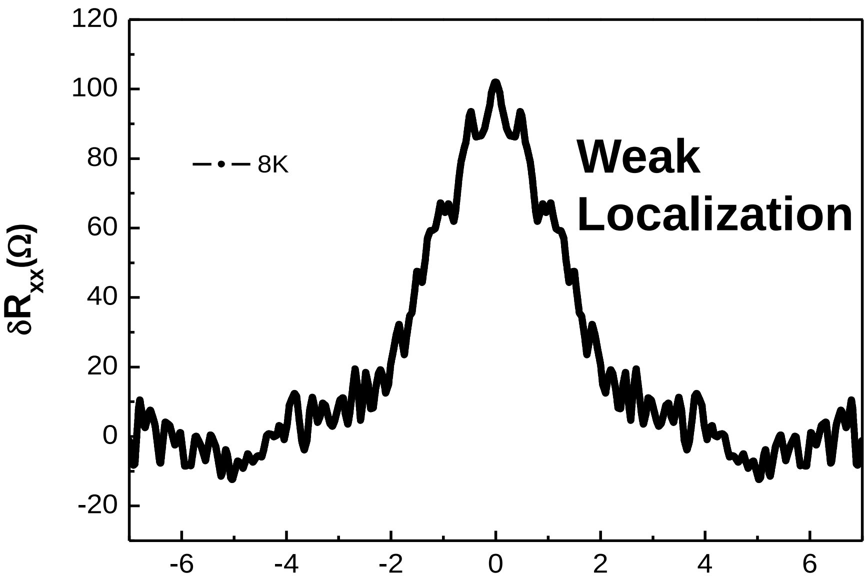




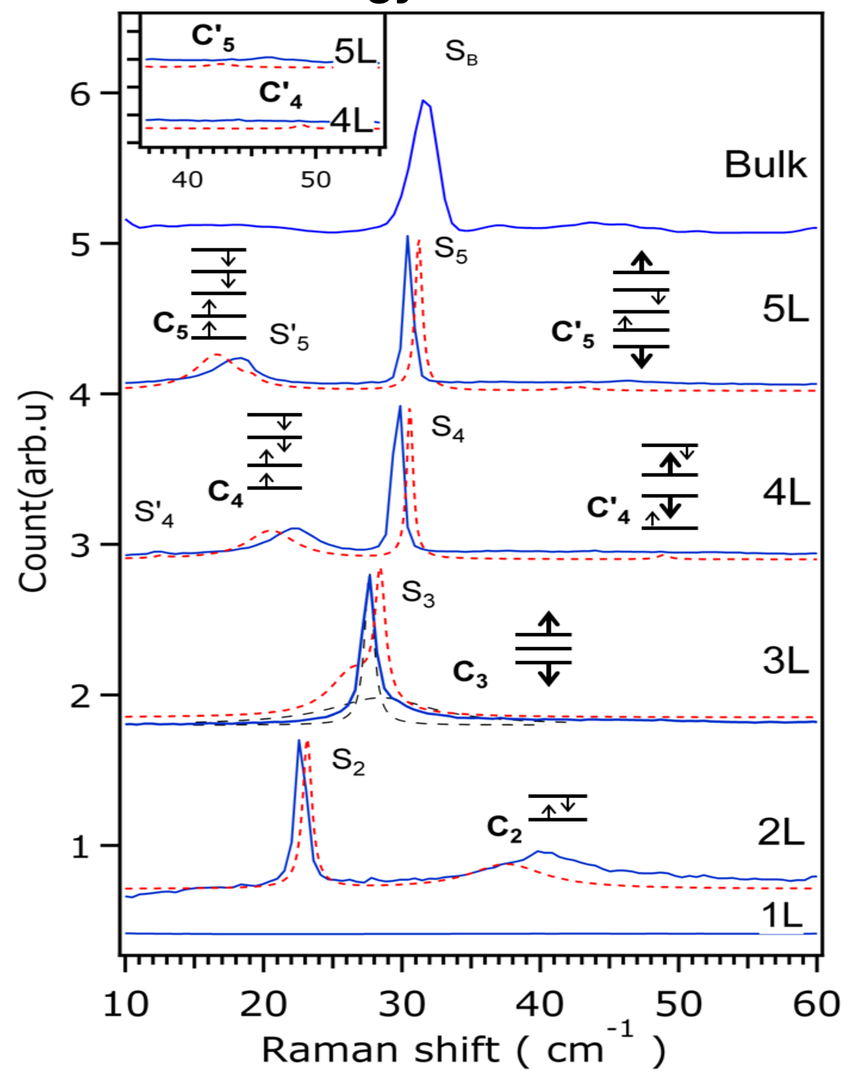
MoS_2 IMPMC

Semiconductor-metal transition

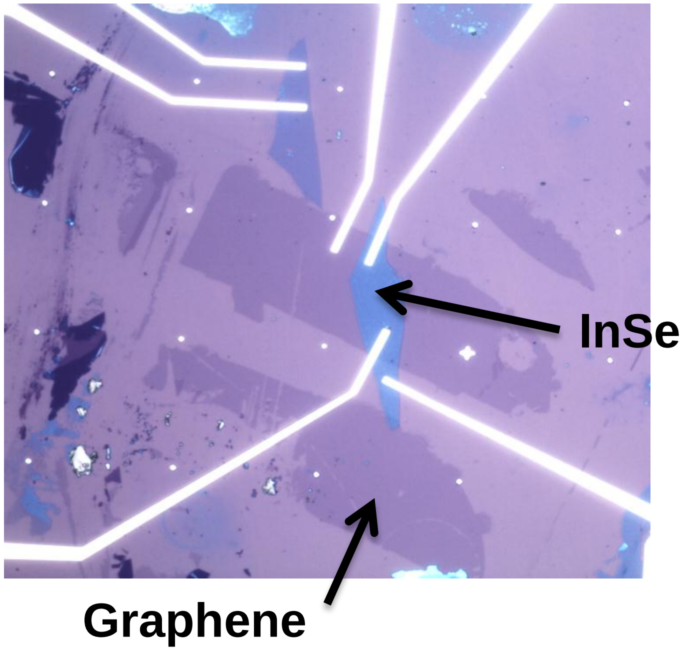


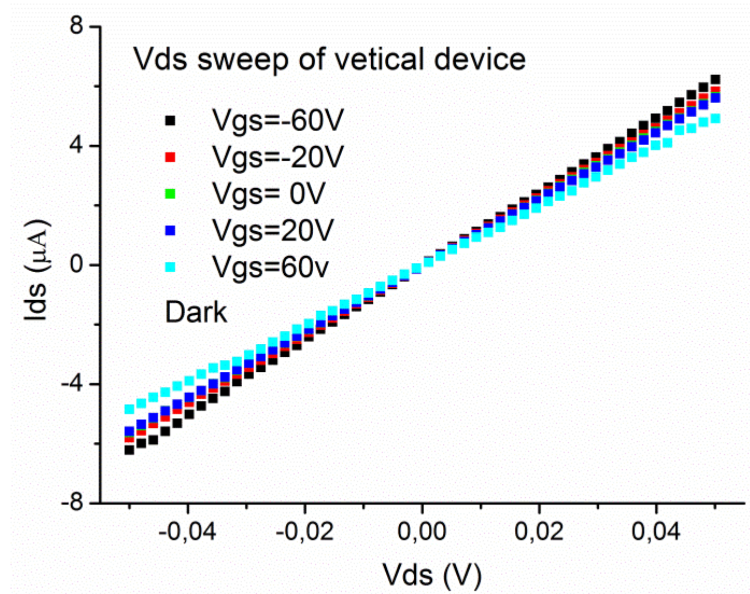


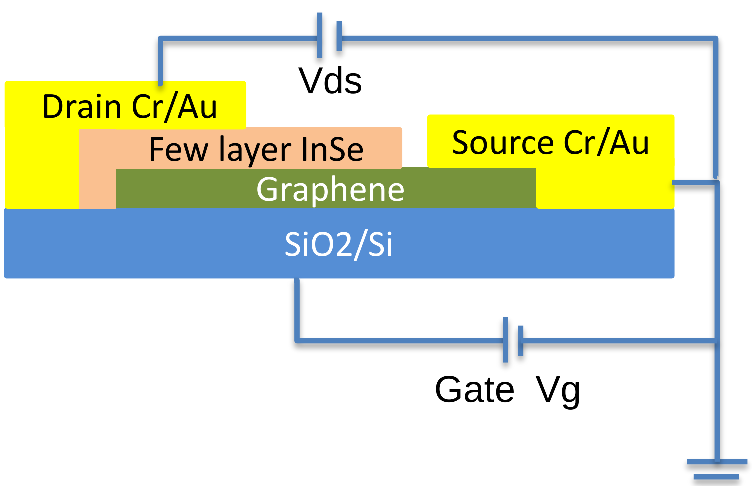
Compression-shear modes: ultra low energy

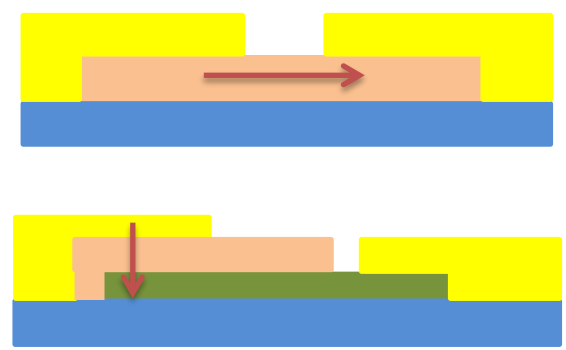


Devices, Heterostructures IMPMC









Historique d’activité

Shukla et al. IMPMC
Graphène, dichalcogenures, semiconducteurs II-VI
Fabrication, Raman,
(magneto)transport, dispositifs simples

Mauri et al. IMPMC
Théorie ab-intio
M. Calandra, ce matin

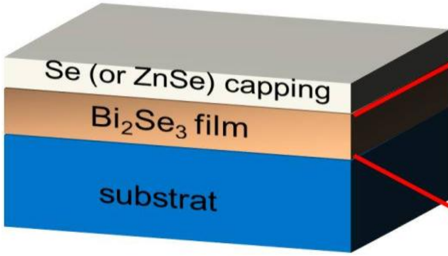
ANR en cours,
collaborations,
publications

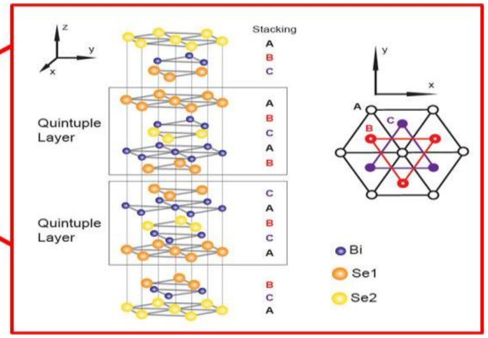
Ouerghi et al. LPN
SiC Graphène, fonctionnalisation
Spectroscopie synchrotron

Marangolo et al. INSP
Isolants topologiques (MBE)
Spectroscopies synchrotron

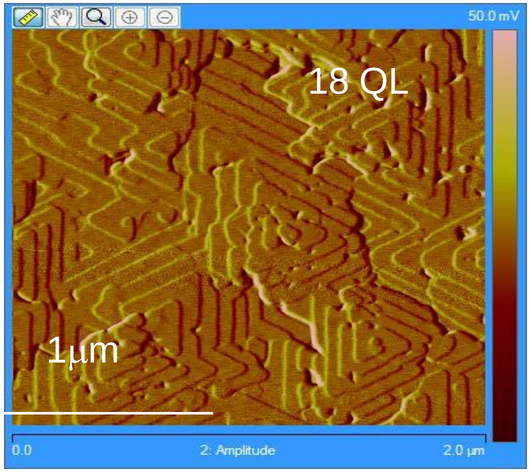
Boutchich et al. LGEP
Dispositifs, Photovoltaique

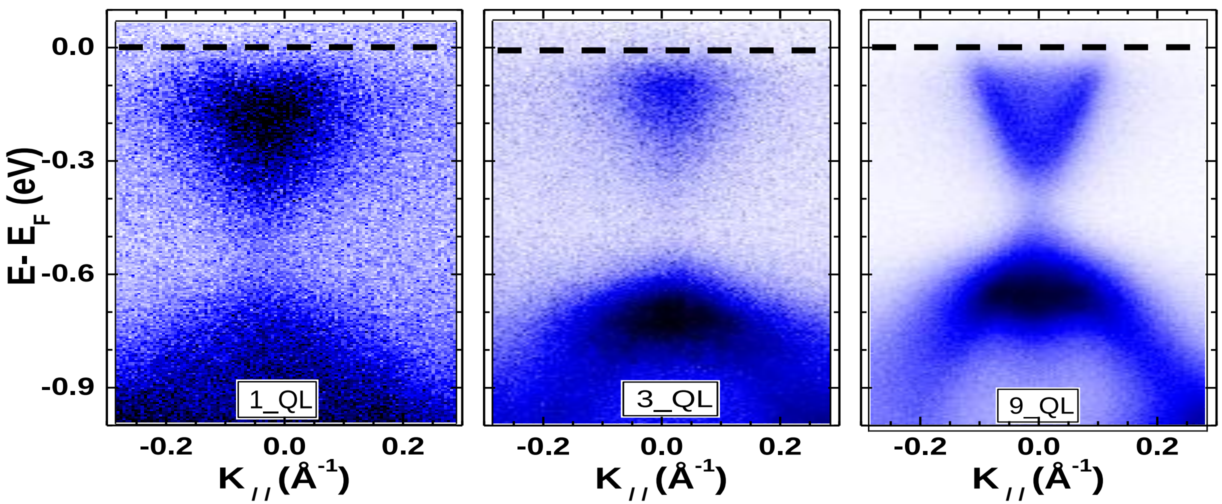
Topological insulators INSP





1-QL
3-QL
6-QL
9-QL
60-QL

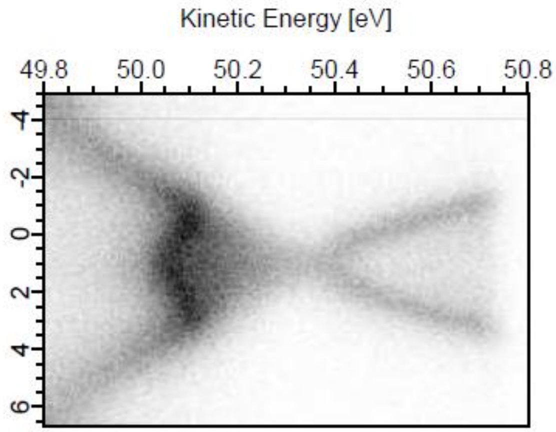


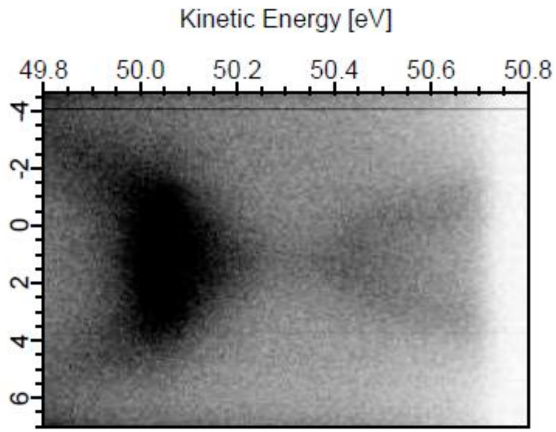


MBE grown state-of the art Bi2Se3

Thickness dependent gap

Topological insulators INSP





Fe doping: dilute
Dirac cones stable with Fe doping

Probable dilution in thin films

Collab. THALES, ELETTRA, LPEM, LPS

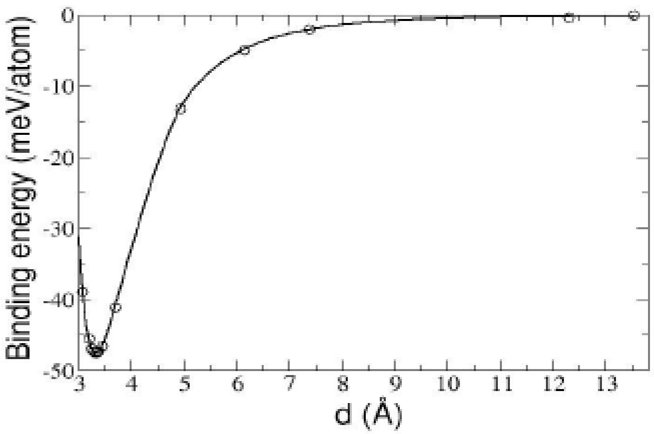
Graphene and other materials: C2RM Nancy

Van der Waals forces are crucial to describe the interaction between 2D systems

Not correctly described by standard approximation of DFT

Calculation of the binding energy of Graphite using the Random Phase Approximation (RPA):

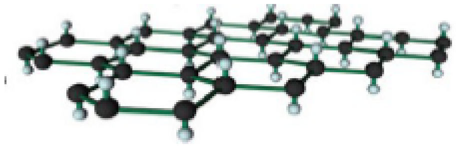
Ref: S. Lebègue et al. Phys. Rev. Lett. 105, 196401 (2010)

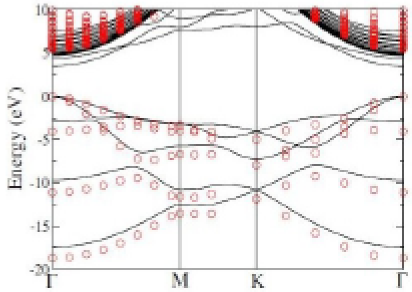


Prediction/calculation of the band-gap of 2D systems:

Band gap problem of DFT; use of the GW approximation.

Example of graphane:





Conformation	Transition	GGA value (eV)	GW value (eV)
Chair	$\Gamma_v \to \Gamma_c$	3.5	5.4
	$M_v \to M_c$	10.8	13.7
	$K_v \to K_c$	12.2	15.9
Boat	$\Gamma_v \to \Gamma_c$	3.3	5.1
	$X_v \to X_c$	7.0	9.0
	$S_v \to S_c$	10.7	13.9
	$Y_v \to Y_c$	9.4	12.6
Chair+OH	$\Gamma_v \to \Gamma_c$	3.3	5.0
Chair+H vacancy	$\Gamma_v \to \Gamma_c$	3.7	5.4

Ref: S. Lebègue et al. Phys. Rev. B 79, 245117 (2009)

Graphene and other materials: C2RM Nancy

Current work:

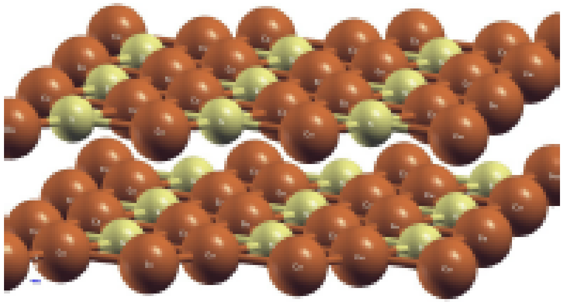
- Development of simplified models to describe the interaction of 2D systems: T. Gould, J. F. Dobson, and S. Lebègue PRB, 87, 165422 (2013).
- Electronic structure of MoX2 bilayers: L. Debbichi (postdoc).
- Datamining in crystallographic database to find new 2D materials.

  Example:

  Crystal structure of bulk Cu2S is referenced in the ICS database (ICSD number 166578)

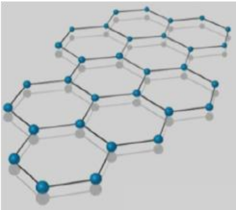
  Cu2S is a layered material: possibility to obtain single layers ?

  Many more to be discovered when doing a systematic search !



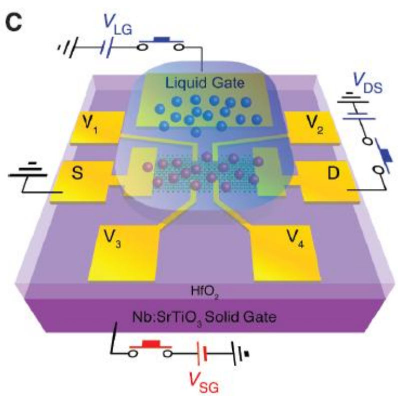
Collaborations:

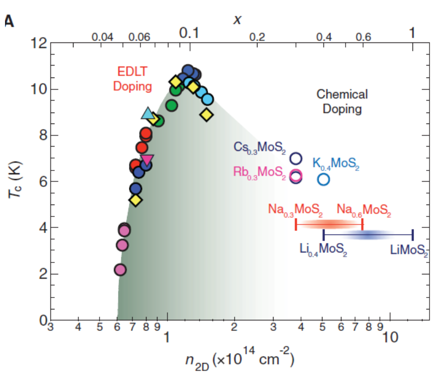
- Group of O. Eriksson (Uppsala, Sweden)
- Group of M. Kastnelson (Nijmegen, Netherlands)
- Group of J. Dobson (Brisbane, Australia)



Other materials: closer look at MoS2

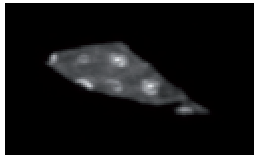
Doping, superconductivity

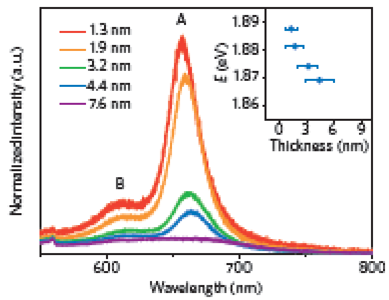




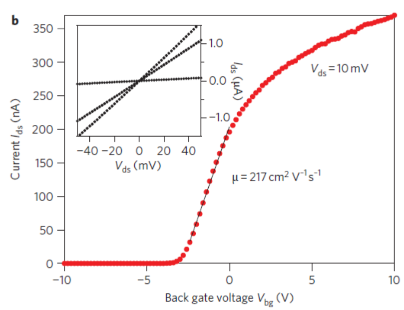
Ye et al. Science (2012)

Properties, devices



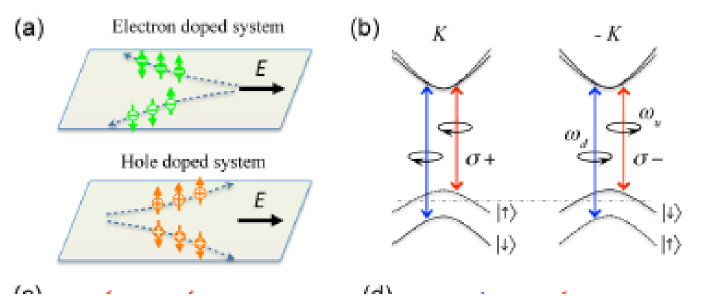


Eda et al.Nanoletters (2012)

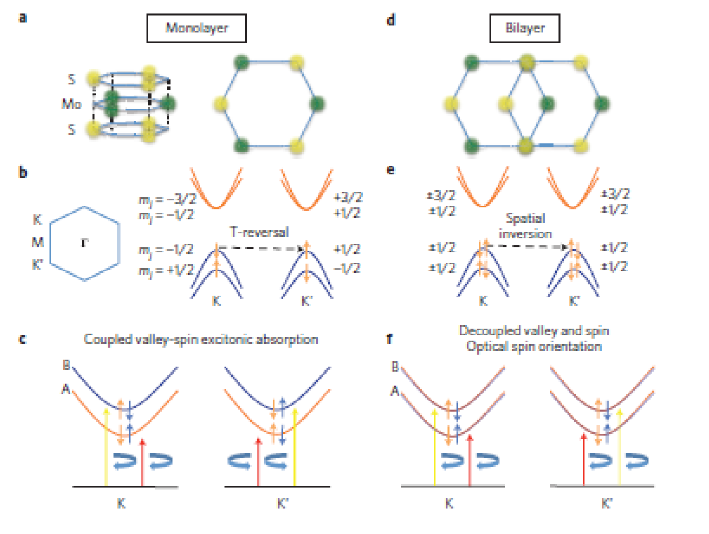


Radisavljevic et al.NatureNano (2011)

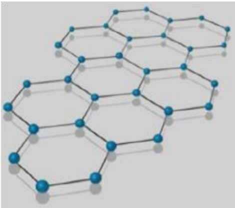
Spin Hall, Valley Hall



Xiao et al. PRL (2012)



Mak et al. Nature Nano (2012)



Why go beyond Graphene?

- **New domain of 2D materials, more difficult than graphene but much larger field**

❑ **Fundamental Physics**
- Phase transitions with electrostatic doping
- Quantum effects: Localization, Conductance fluctuations
- Topologically protected states
- New phenomena: spin-Hall, valley Hall effects;

❑ **Applied Physics**
- Use above phenomena for new devices
- Combine properties of different 2D materials for more efficient devices