GDR Groupement de recherche
HOWDI Low dimensional van der Waals heterostructures

Axis 2: Electronic transport in van der Waals heterostructures and relationship to other fields

Organization team

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Axis 2: Electronic transport in van der Waals heterostructures and relationship to other fields

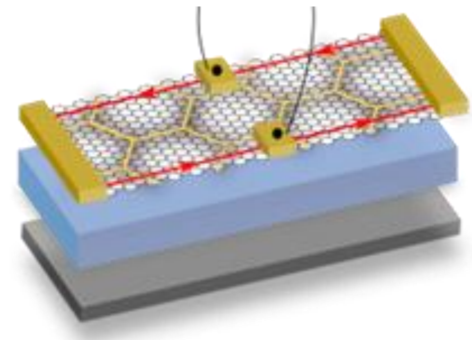
Synergies with axis 1, axis 3 and axis 4

Objectives:

- Electronic transport for exploring:
  - new vdW heterostructures
  - their manipulation/engineering with new degrees of freedom (stacking angle between 2D layers, pressure, …)

- Electronic transport combined with other experimental techniques to tackle :
  - phenomena beyond simple electron transport (→ transport of excitons, phonons, heat…)
  - coupling between properties, electrical – magnetic - optical – thermal…

→ New materials, new physics, new phenomena, new devices, new applications



Transport at RT, FET, RF transport, magnetotransport, LT quantum transport, STM, noise measurements, etc...

From fundamental aspects to applications with support of theory & simulation

Identification of the research topics:

Collection of interests in the community (June 2020)
46 people contacted / ~23 teams responding

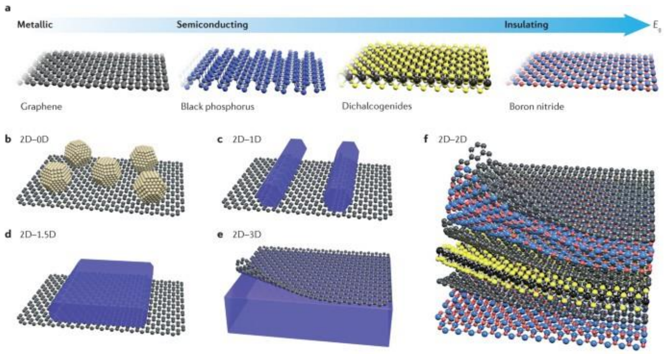
The following topic lists stay fully open!

Teams: IPCMS (Strasbourg), LPS (Orsay), TRT (Palaiseau), CEA Grenoble / IRIG, LNCMI (Toulouse), LSI/QCMX (Palaiseau), LNE (Trappes), LPENS (Paris), L2C (Montpellier), I. Néel (Grenoble), C2N (Palaiseau), CEA Saclay / SPEC, IM2NP (Marseille), IMEP-LAHC (Grenoble),…

+ Suggestions of liaison with international teams (22 in EU + 9 extra-EU)

Axis 2: Transport – Fundamental aspects

– Mixed-dimensional vdW heterostructures (2D-1D, 2D-0D, 2D-molecules,…), 2D COF-MOF,…

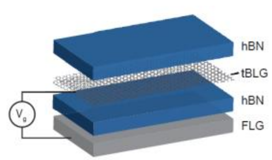


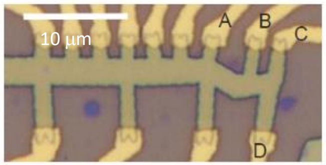
Nat Rev Mater 1, 16042 (2016)

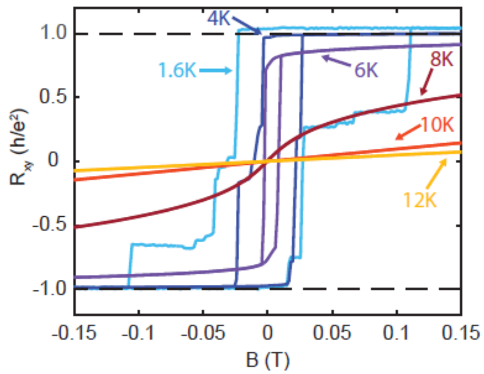
(see Jean-François Dayen's talk in a few minutes)

– 2D magnets, 2D multiferroics, 2D superconductors, …
– Twisted vdW heterostructures (twistronics), Moiré effect, and new electronic phases at magic angle : QAH, superconductivity, Josephson effect,…

Twisted bilayer graphene encaplusated in h-BN







"Intrinsic quantized anomalous Hall effect in a moiré heterostructure"
M. Serlin *et al.* Science. **367**, 900 (2020)

– Effect of pressure on vdW heterostructures (magnetism, …)
– Other new exotic states emerging from interactions between layers, correlations, confinement…
– …

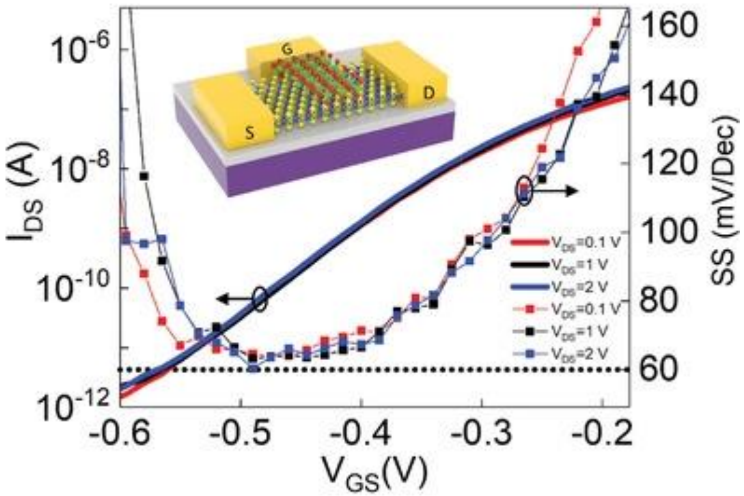
Axis 2: Transport – Applications

In microelectronics, RF-electronics, opto-electronics, nanoelectronics, quantum electrial metrology, biosensors, and other sensors, …

Common challenges on materials (defects,…) and devices (contacts, reproducibility, scaling, …)

<u>Examples of applications with vdW heterostructures:</u>

- Towards low-power electronics with tunnel-FET and cold-source FET with 2DM
- Towards high-performance thermoelectric properties (ZT > 2 @RT) with independent control of thermal and electrical transport in graphene/MoS_2
- Towards on-chip quantum electrical standards under relaxed experimental conditions in twisted graphene-hBN heterostructures
- Optoelectronics applications : photodetectors, photovoltaics, photocatalysis…
- Towards micowave bolometers based on JJ
- Electronic noise thermometry
- …

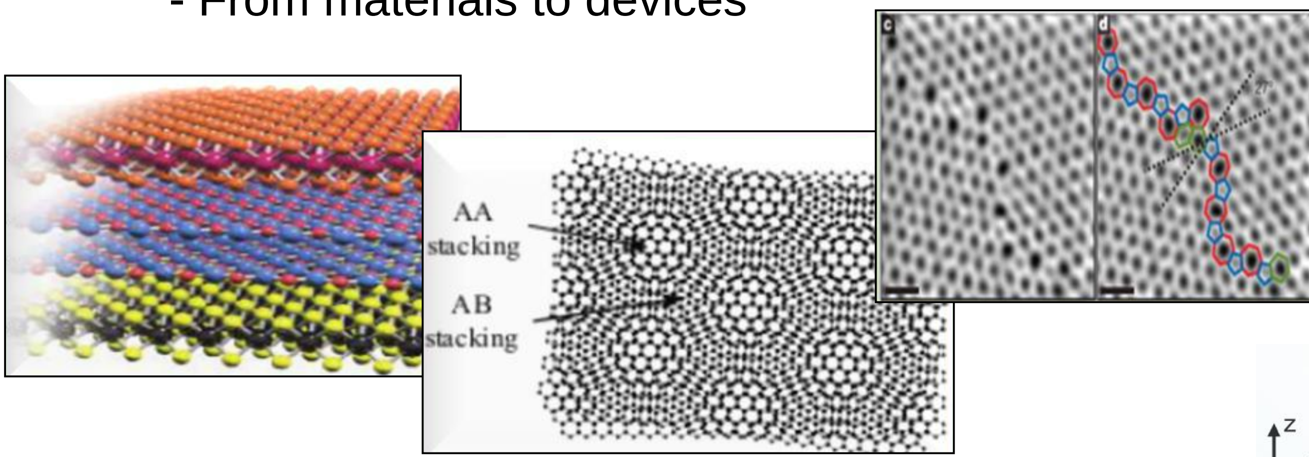


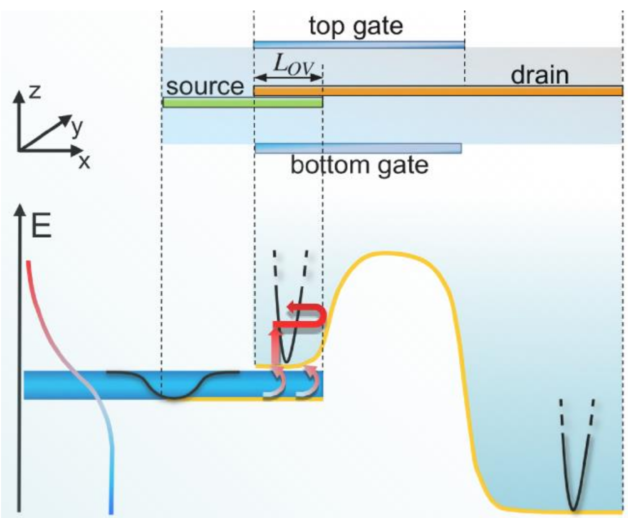
“SnSe/MoS2 van der Waals Heterostructure Junction Field-Effect Transistors with Nearly Ideal Subthreshold Slope”
Guo et al., Adv. Mater. 2019 , 31, 1902962

Axis 2: Transport – Theory/Simulation

Requirements: **Atomistic description + quantum effects**

- Able to include: - interfaces, defects,
  - coupling with phonons, photons,…
  - coupling with 1D or 0D structures, with contacts
- From materials to devices





Role:

→ Support to experimental investigations

→ Suggestions of new effects and possible applications (electronics, thermoelectrics, photodetection, sensors, metrology, exotic states,…)

→ Development of new methods

Logoteta et al., Phys. Rev. Research 2 (2020) 043286

Axis 2: Transport – Theory/Simulation

State of the art:

→ Material level: **Ab initio Hamiltonians** (reference)

- Band structure, basic properties of materials and elementary structures
- but not suitable for device simulation (with > thousands atoms)

→ Device level: **Tight-Binding Hamiltonian** + **NEGF** + **Poisson**

- Semi-empirical TB parameters to fit ab initio outputs (≠ levels of accuracy)
- Easy to include in an NEGF formalism coupled with Poisson's equation
- Suitable for device, including scattering
- but, in principle, always less accurate than what ab initio can provide

To be developed:

→ Tight-Binding Hamiltonians for a wide range of materials

→ New methods to make ab initio Hamitonians usable for device simulation (to bridge the gap between material science and device engineering)

(see Marco Pala's talk in a few minutes)

Axis 2: Transport

→ Jean-François Dayen (IPCMS)

« 0D/2D Mixed-dimensional heterostructures : a versatile platform from optoelectronics to single electron electronics »

→ Marco Pala (C2N)

« Ab-initio quantum transport simulation of 2D-materials-based electron devices »