

INFN Research project (Iniziativa Specifica) Gruppo IV

TIME2QUEST

Advanced Theoretical methods for emerging 2D materials
in Quantum Information Technology Studies

Aim:

- Investigate the electronic, spin and optical properties of **two-dimensional materials** that may impact on **quantum technology and quantum information processing** —> **novel qubits**
- Exploit, and further develop, **theoretical tools relying on ab-initio approach and QI methods** (density functional theory, many-body perturbation theory and open quantum system theory).

The challenge:

Identify **new systems and technologies** overcoming the limits of current strategies, to achieve:

- Scalable solid-state qubits
- High (ambient) operating temperature
- Long decoherence time

Define **protocols to manipulate and control two level systems** in 2D solid state qubits

Synergy of many INFN Units:

- INFN Section: LNF-Gruppo Collegato di Cosenza (LNF-CS):

- Staff members**

- Prof. Antonello Sindona (100%, PA) **Responsabile Nazionale nuova IS**
 - Prof. Francesco Plastina (50%, PA)
 - Dott. Stefano Bellucci (70%)
 - Dott. Nicolino Logullo (100%, RTDB)

- Other participants (Post-docs, Ph.D students,...)**

- Dott. Michele Pisarra (50%, POST DOC)
 - Dott. Cristian Vacacela Gomez (100%, POST DOC)
 - Dott. Jacopo Settino (50%, RTDA)
 - Dott. Antonio Palamara (100%, PhD Student)
 - Dott.ssa Francesca Mazzei (100%, PhD Student)

- INFN Section: Roma 2 (RM2) :

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 - Prof. ssa Olivia Pulci (100%, PO)
 - Prof. ssa Maurizia Palummo (100%, PA)

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 - Dr. Vasil Saroka (Post-doc) (50%)
 - Dr. Igor Kupchak (Post-doc) (50%)

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Solid State Physics Theory Group

Pure and Applied
Quantum Mechanics Group

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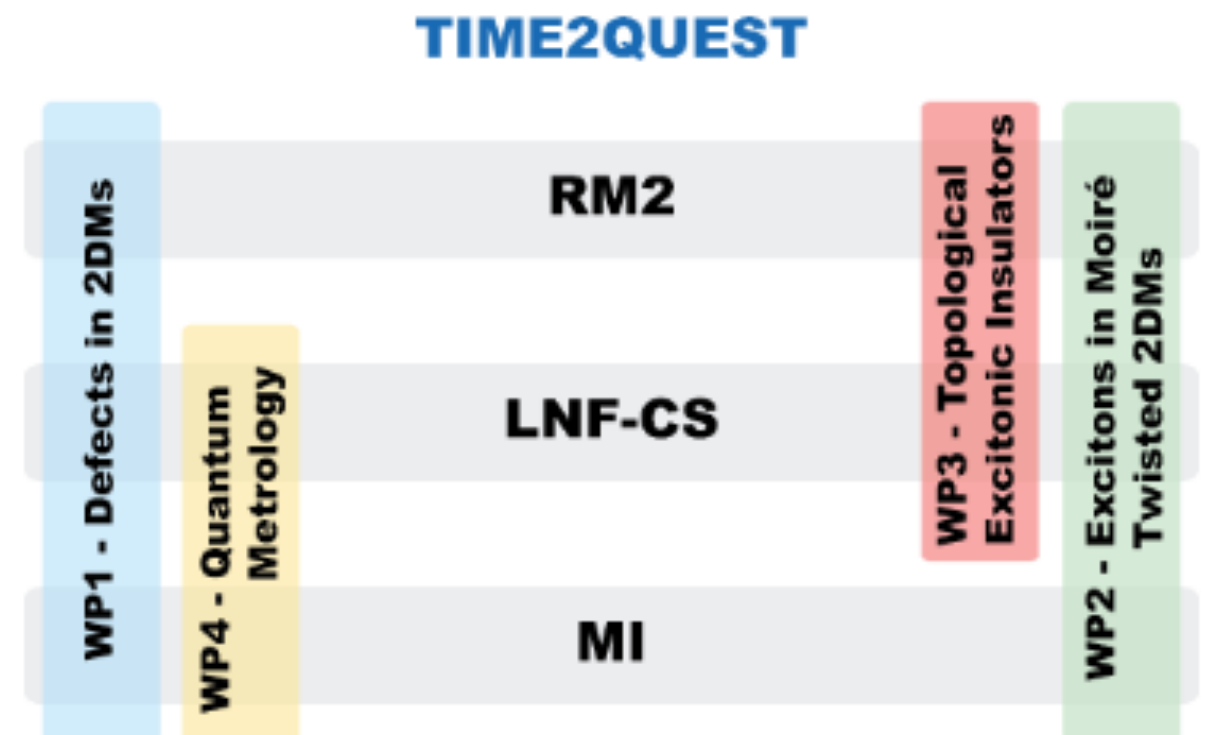
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Focus on 2D materials

- Exotic and peculiar electronic, magnetic, optical, and structural properties
- Functionalization and combination (heterostructure)
- Controllable 2 level systems ($|0\rangle$, $|1\rangle$ and their superposition) $\rightarrow$ qubits
- Stable at room temperature, long coherence time, scalable
- Electronic and photonics degree of freedom
- Additional spin-valley degree of freedom

Focus on 2D materials

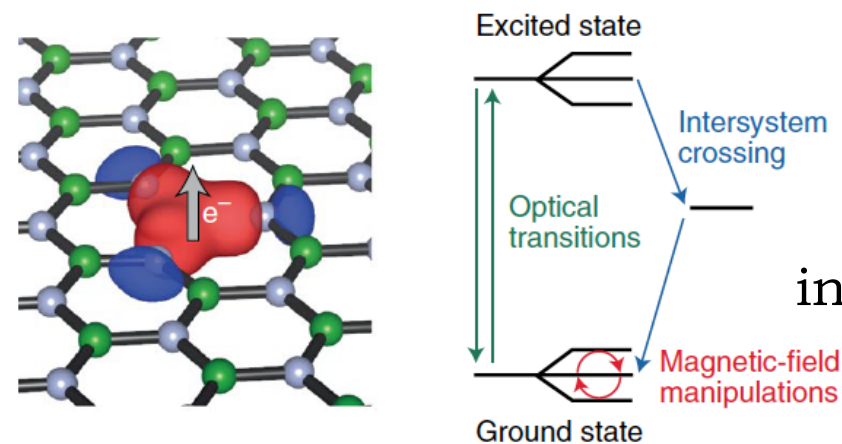
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Atomic defects / Impurity functionalization

Spin degree of freedom

Excitons in semiconducting 2D (hBN, TMD)

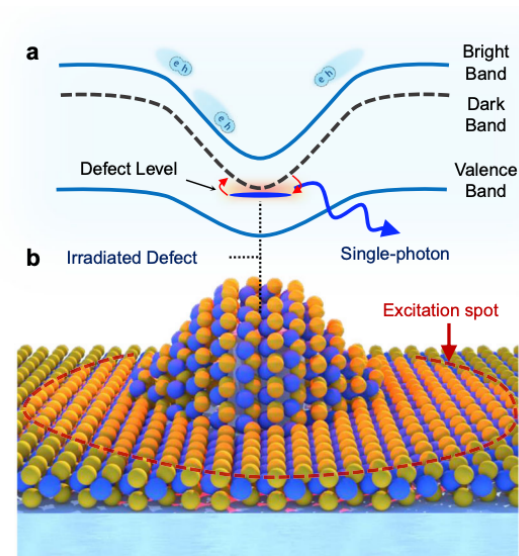
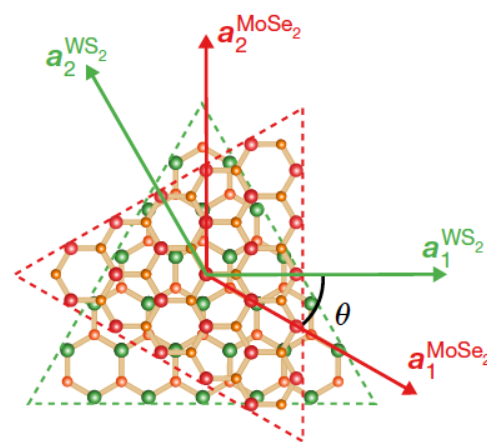
Superlattices of single photon emitters



Optical
initialization and readout

Combination/deformation

Excitons with tunable properties
(depend on the registry/strain)



New “exotic” phases

Non-equilibrium excitonic-insulators $\rightarrow$ superfluid with qubit state given by 1 or 2 exciton above the condensate

Majorana fermions

Theoretical methods:

- **Density functional theory** —> ground state properties
- **Many body approaches** (GW+BSE) —> excited-state properties
(optical properties, spin non-conserving transitions, excitonic properties)
- **Quantum metrology and QI theory** —> identify and characterize quantum devices (coherence, quantum correlation).
Define specific protocols for applications in metrology, sensing, quantum communications

Computational projects:

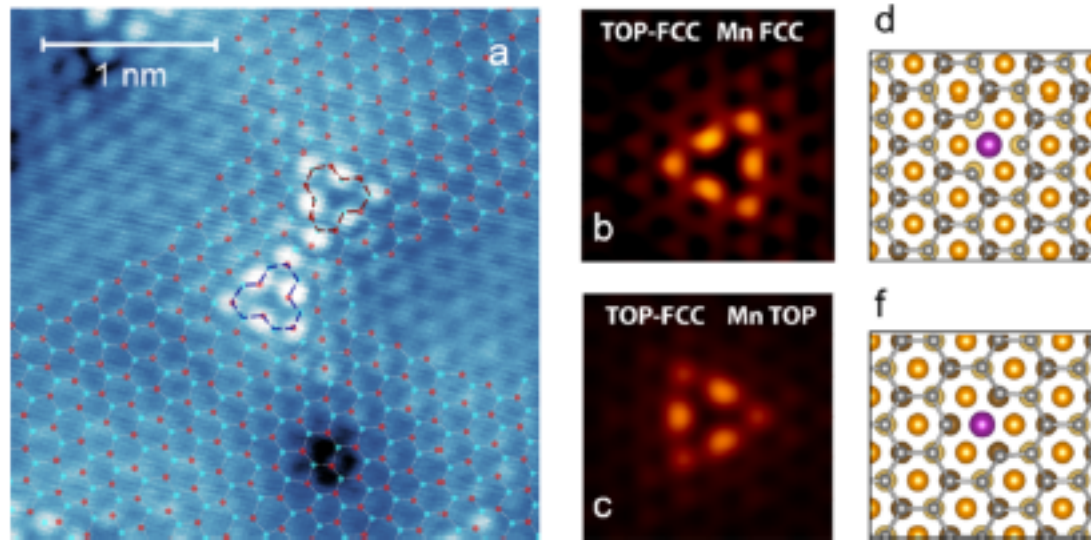
- Three approved Iskra C projects @ CINECA (size 100'000 hours on CPU, 10'000 hours on GPU)
- One submitted Iskra B projects @ CINECA (size 3'600'000 hours on CPU, 250'000 hours on GPU)

Experimental Collaborations:

- Nanoscale Foundries and Fine Analysis infrastructure
- POLIMI
- CNR-IMM

Activity (Sezione di Milano - Solid state physics theory group)

Magnetic defects in 2D materials



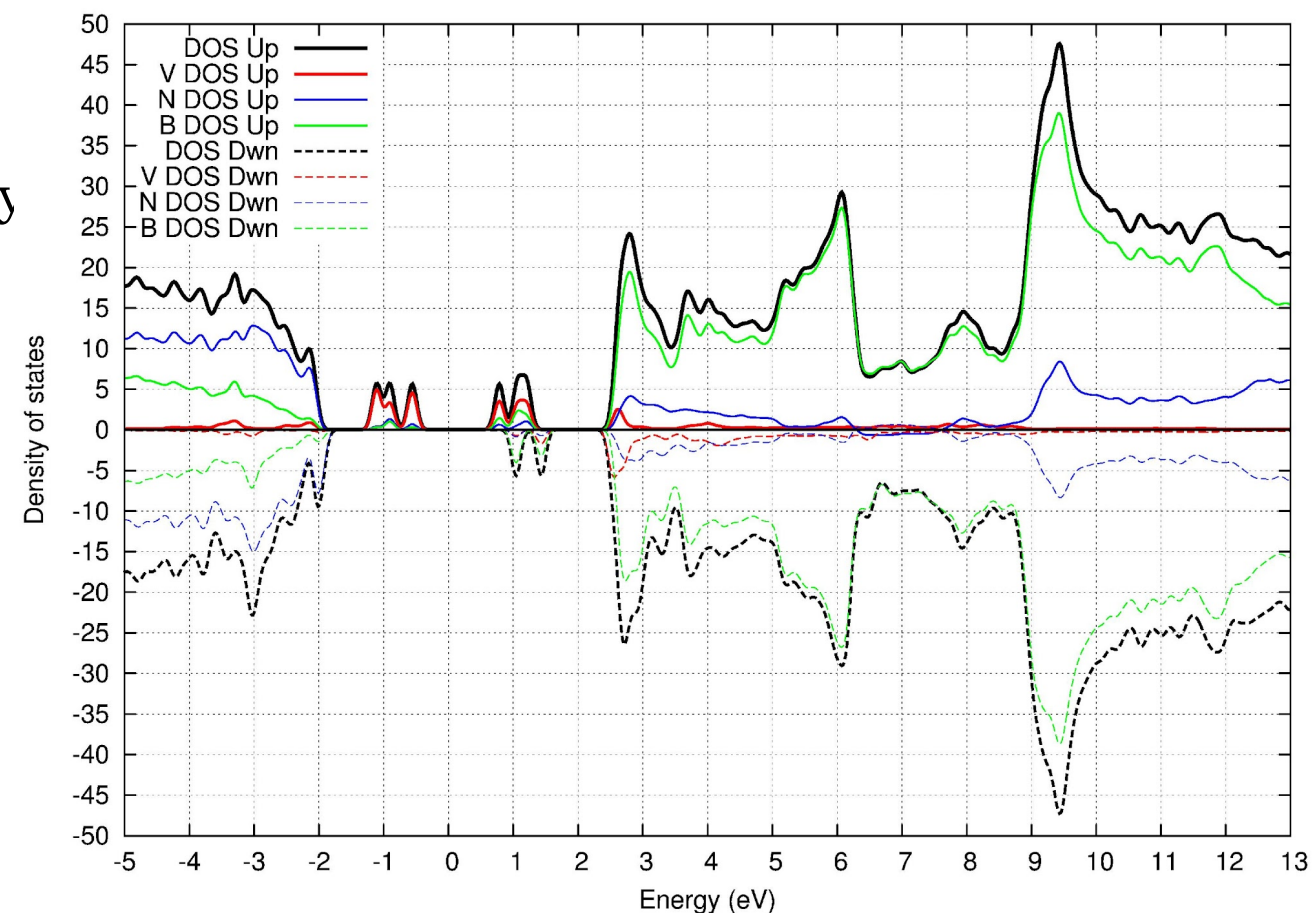
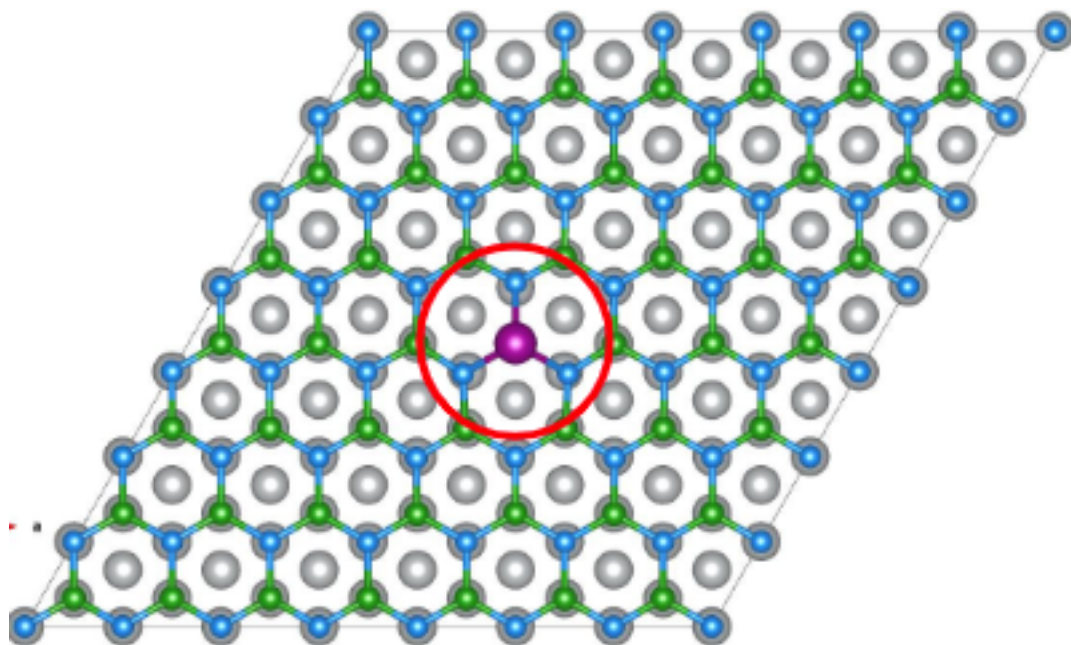
ACS Nano 15, 5449 (2021)

Mn atoms implanted in graphene

- Characterization of structural, electronic and magnetic properties
- Support to the experiments

Mn and V atoms implanted in hBN (ongoing)

- Large unit cells - different possible stoichiometry
- Gap states

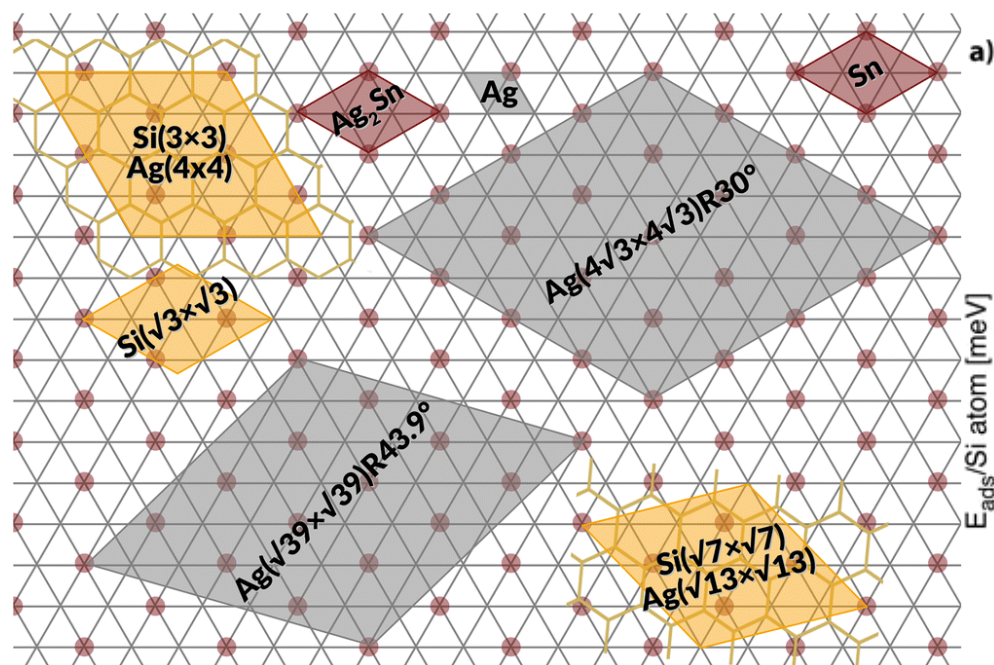
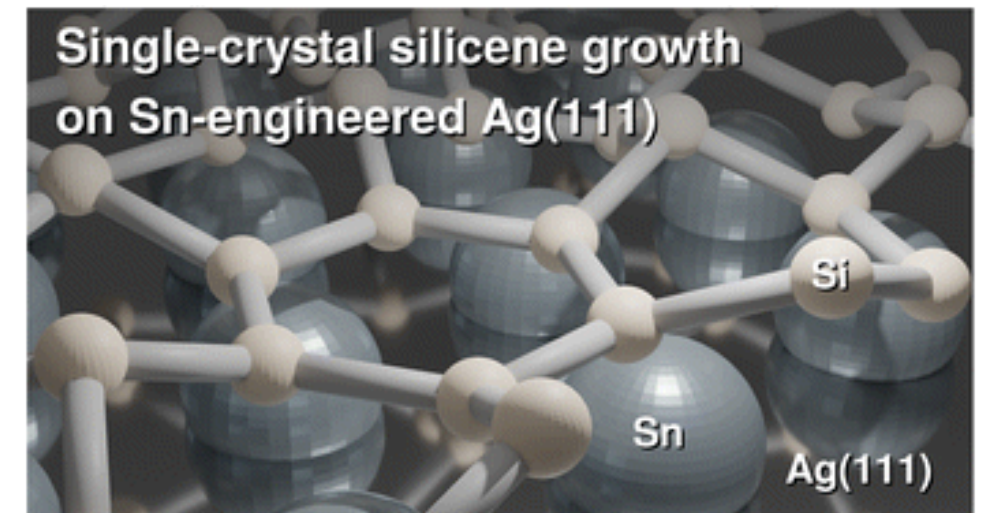


(collaboration with Dr. Lino Pereira (Leuven))

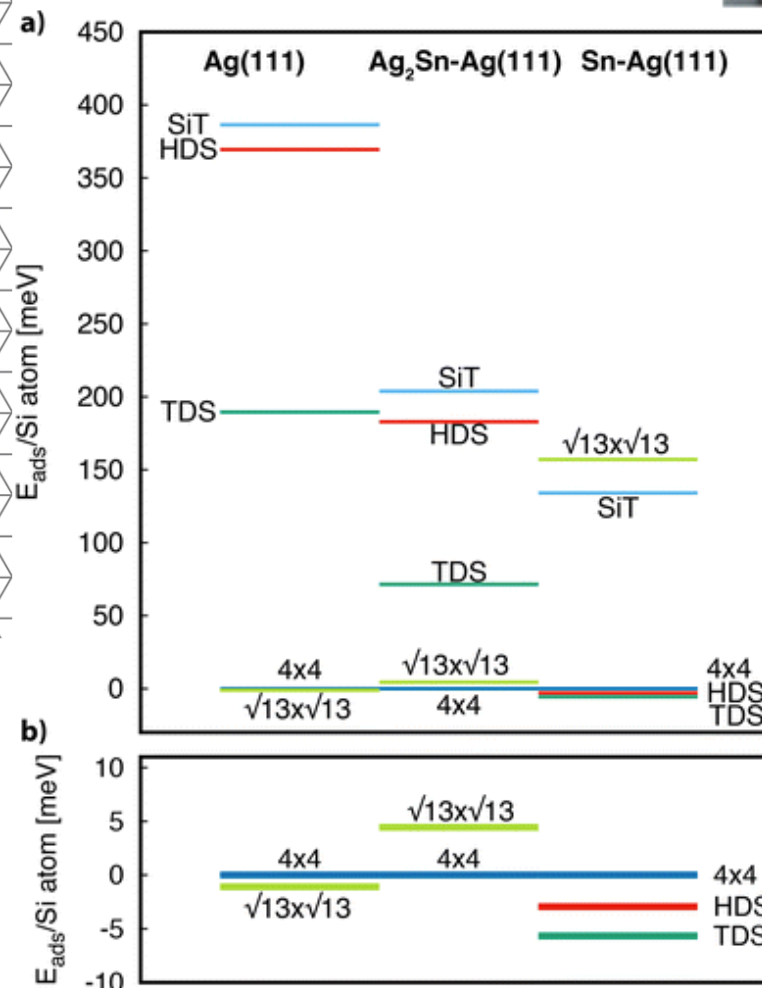
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2D Xenes

- Stabilize a particular phase of silicene among the ones usually observed on Ag(111), via substrate surface decoration with Sn atoms forming a thin alloy film.
- Nanoengineering of 2D Xenes vertical heterostructures.



Nanoscale, 2023, Advance Article

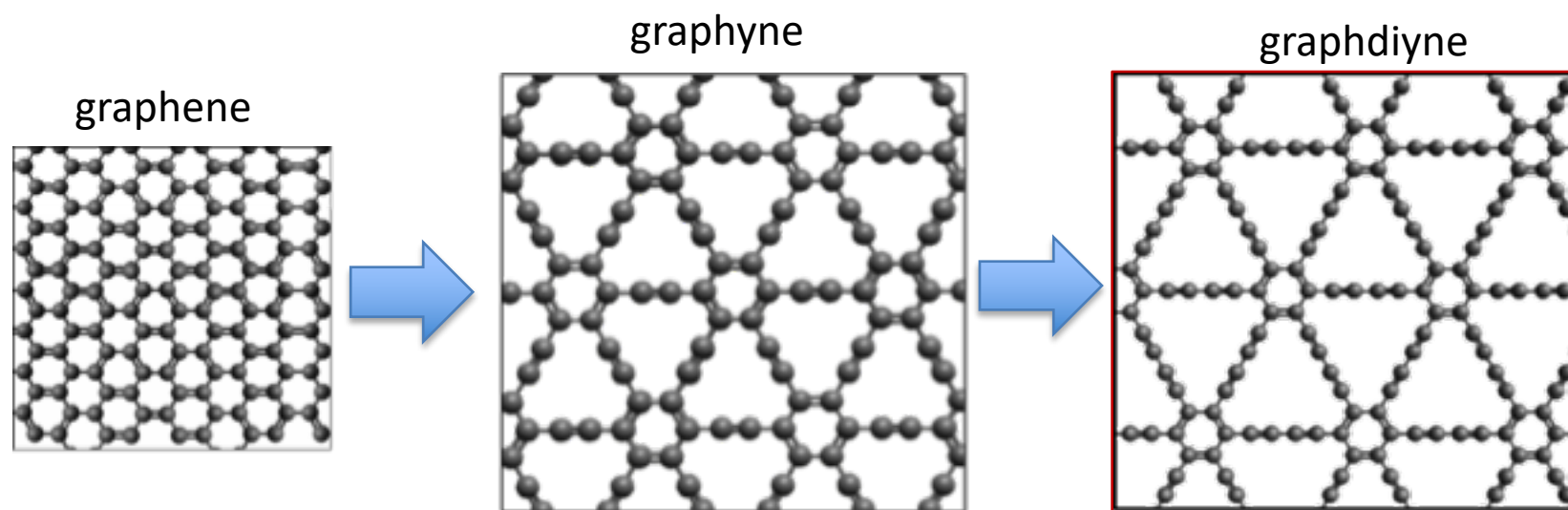


(collaboration with Dr. A. Molle (CNR-IMM))

Activity (Sezione di Milano - Solid state physics theory group)

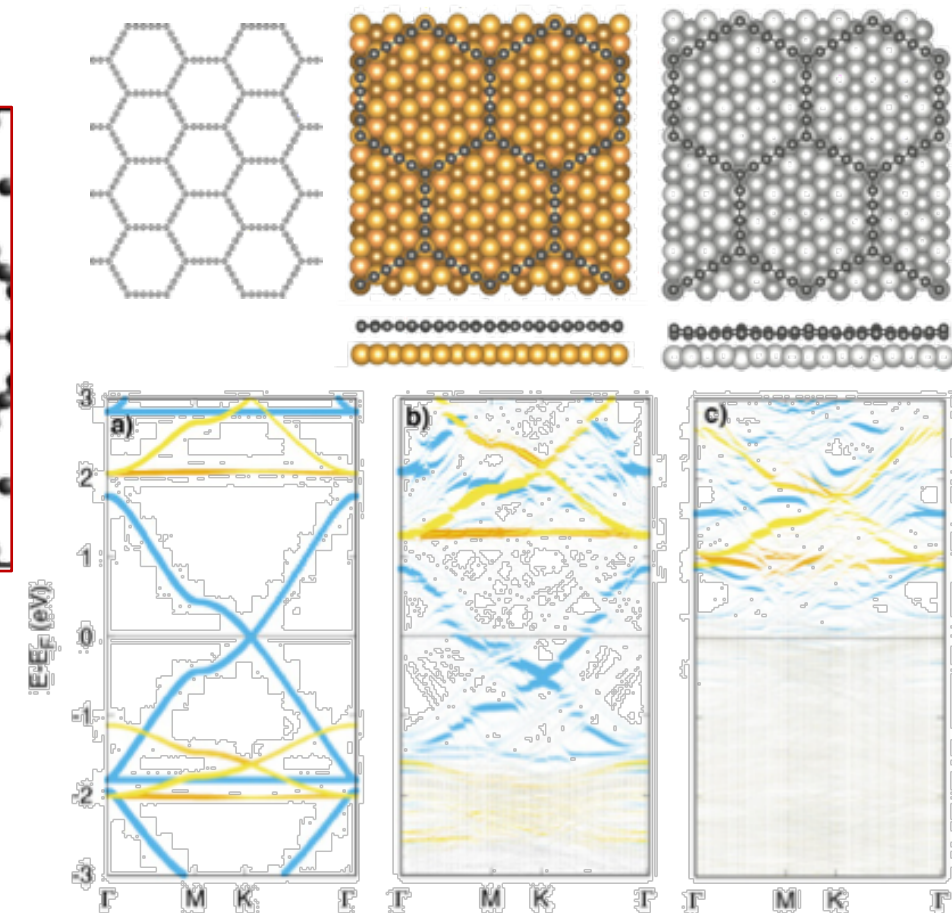
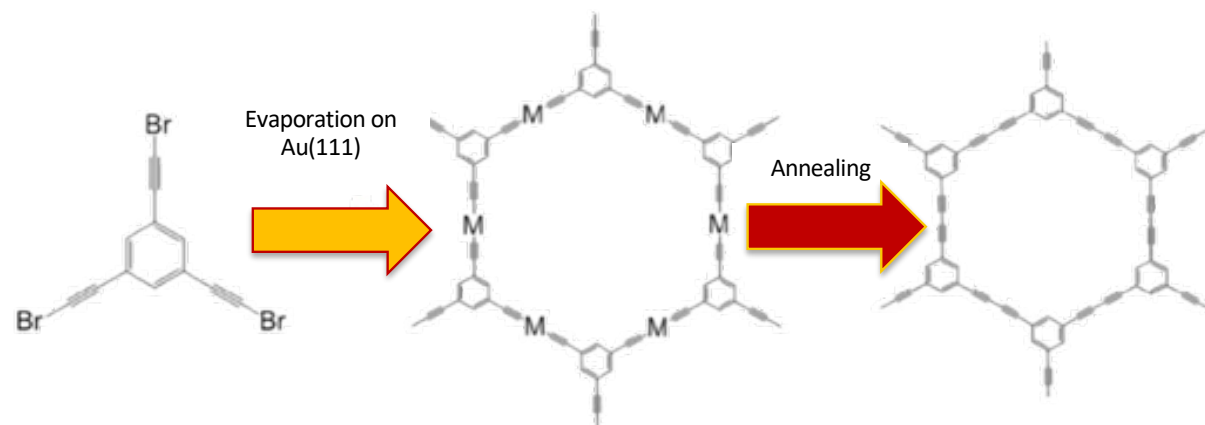
Novel 2D carbon materials (GDY)

- Tunable properties controllable through the choice of the precursors + substrate
- New structures poorly explored
- Potential topological properties
- Hybrid sp-, sp² carbon



2D Mater. (2021) 8, 044014

ACS Appl. Nano Mater. (2020) 3, 12178–12187



(collaboration with Prof. Casari (POLIMI))