INFN Research project (Iniziativa Specifica) Gruppo IV

TIME2QUEST

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

Aim:

- Investigate the electronic and optical properties of **two-dimensional materials** that may impact on **quantum technology and quantum information processing**

- Exploit, and further develop, **theoretical tools relying on ab-initio methods** (density functional theory, many-body perturbation theory and open quantum system theory).

The challenge:

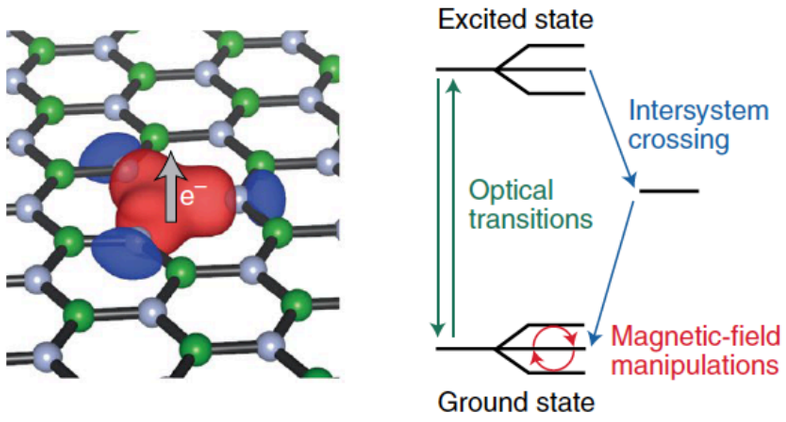
Identify **new systems and technologies** overcoming the limits of current strategies, to achieve:

- Scalability
- High (ambient) operating temperature
- Long decoherence time

Define protocols to manipulate peculiar quantum states suitable for realize solid state qubits operating at room temperature.

Why 2D materials are promising

Atomic defects / Impurity functionalization



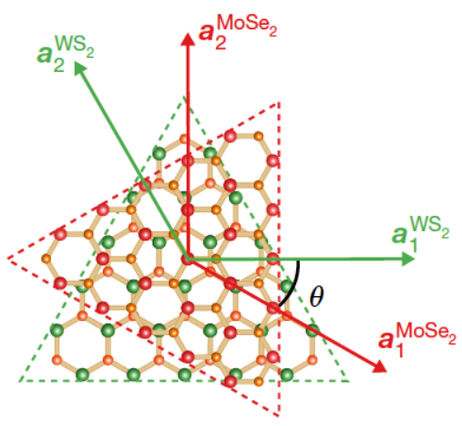
NATURE MATERIALS | VOL 19 | MAY 2020 | 481–490

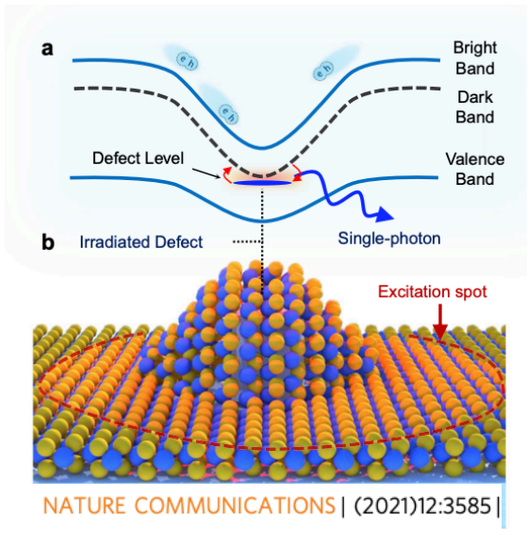
Spin states: two level system —> |0>, |1> qubit states

Optical initialization and readout

Additional spin-valley degree of freedom

Combination/deformation





NATURE COMMUNICATIONS | (2021)12:3585 |

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

Superlattices of single photon emitters

New “exotic” phases

Non-equilibrium excitonic-insulators —> superfluid with qubit state given by 1 or 2 exciton above the condensate

Majorana fermions

Specific Objectives:

- Characterize atomic defects and impurities in 2D materials (hBN, TMD)
- Investigate how Moiré patterns and strain modify the properties of excitons in 2DM
- Exploring exotic phases
- Identify system suitable for quantum devices through methods borrowed from quantum metrology and quantum information

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

Synergy of many INFN Units:

- Laboratori Nazionali di Frascati **(LNF):**
  - Staff members
    - Dott. Stefano Bellucci
    - Prof. Antonio Maffucci
    - Prof. Davide Mencarelli
    - Prof. Luca Pierantoni
  - Other participants (Post-docs, Ph.D students
    - Dott. Antonino Cataldo (Post-doc)

      Dott. Alessio Di Tinno (Post-doc)

- Sezione di Milano **(MI):**
  - Staff members
    - Prof. Giovanni Onida
    - Prof. Matteo Paris
    - Prof. Stefano Olivares
    - Dott. Marco Genoni
    - Dott. Guido Fratesi
    - Dott.ssa Simona Achilli

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    - Prof.ssa Olivia Pulci
    - Prof.ssa Maurizia Palummo
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Collaborations

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Solid State Physics Theory Group

Pure and Applied Quantum Mechanics Group

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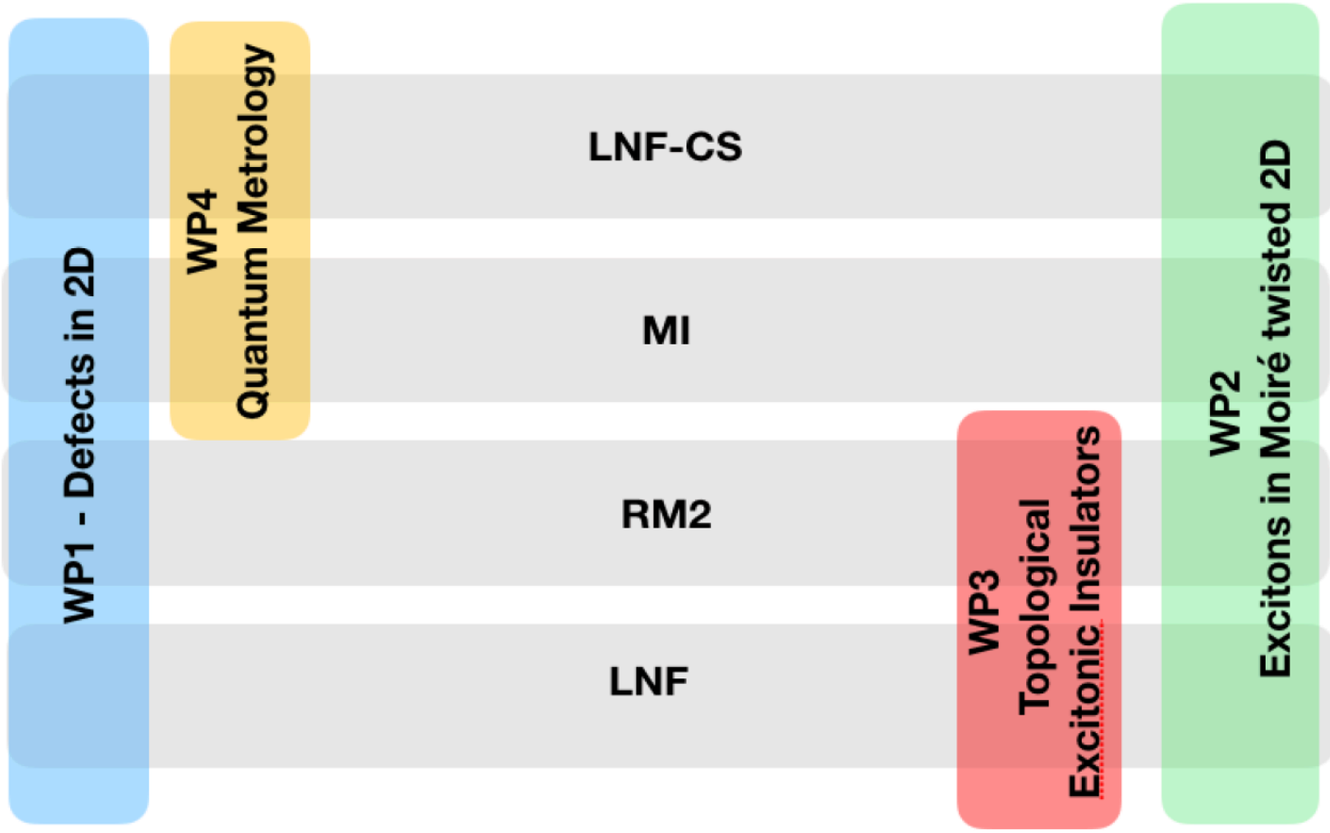
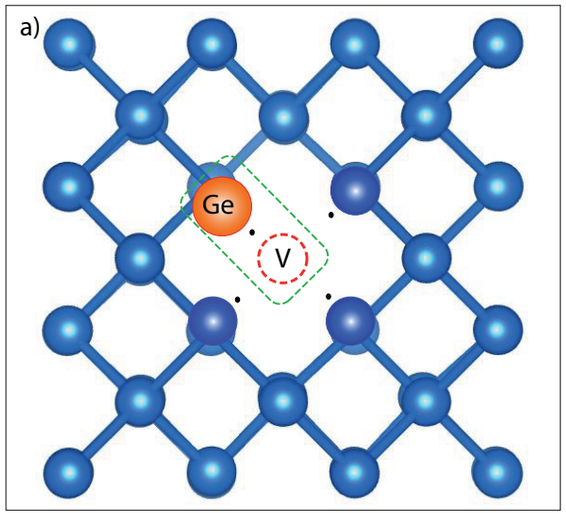


Preliminary results (Sezione di Milano)

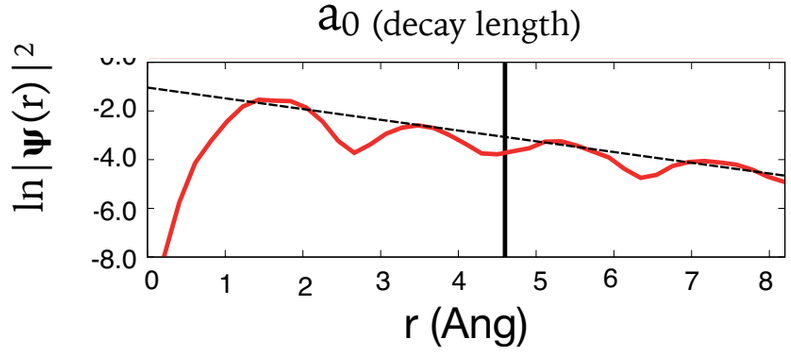
Collaboration with
E. Prati, IFN
T. Tanii, Waseda Univ.
T. Shinada, Tohoku Univ.

Sci. Rep. 8, 18054 (2018)
Adv. Funct. Mater. 31, 2011175 (2021)

Ge*V* in silicon



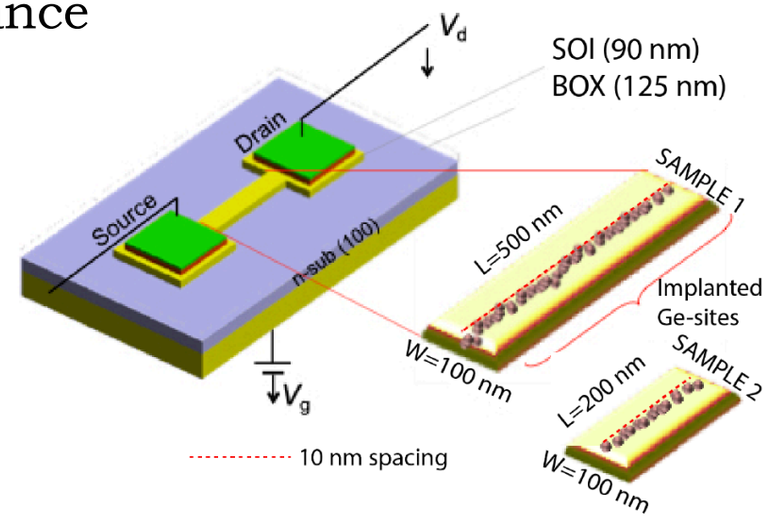
Deep states in the gap:
excited states preserved at high temperature



Strongly confined and correlated electrons

Theoretical model combining ab-initio methods and parametrized model

explains the observed temperature activation of the conductance

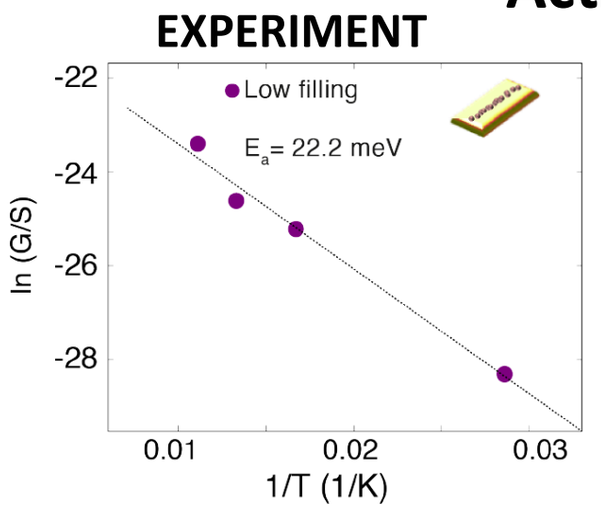


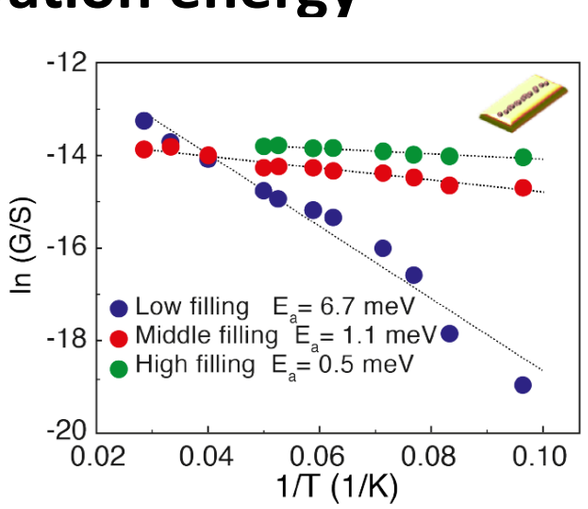
Define a protocol for the generation/activation of the defects

Employment as Hubbard simulator

Activation energy

EXPERIMENT





THEORY