Ab Initio Quantum Mechanical Simulations of Defective MoS2 and Au Interfaces in 2D nanodevices

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Gabriele Boschetto[1], Stefania Carapezzi[1], and Aida Todri-Sanial[1,2]

[1]Microelectronics Department, University of Montpellier, CNRS, Montpellier 34095, France

[2]Department of Electrical Engineering, Eindhoven University of Technology, 5612 AZ Eindhoven, Netherlands

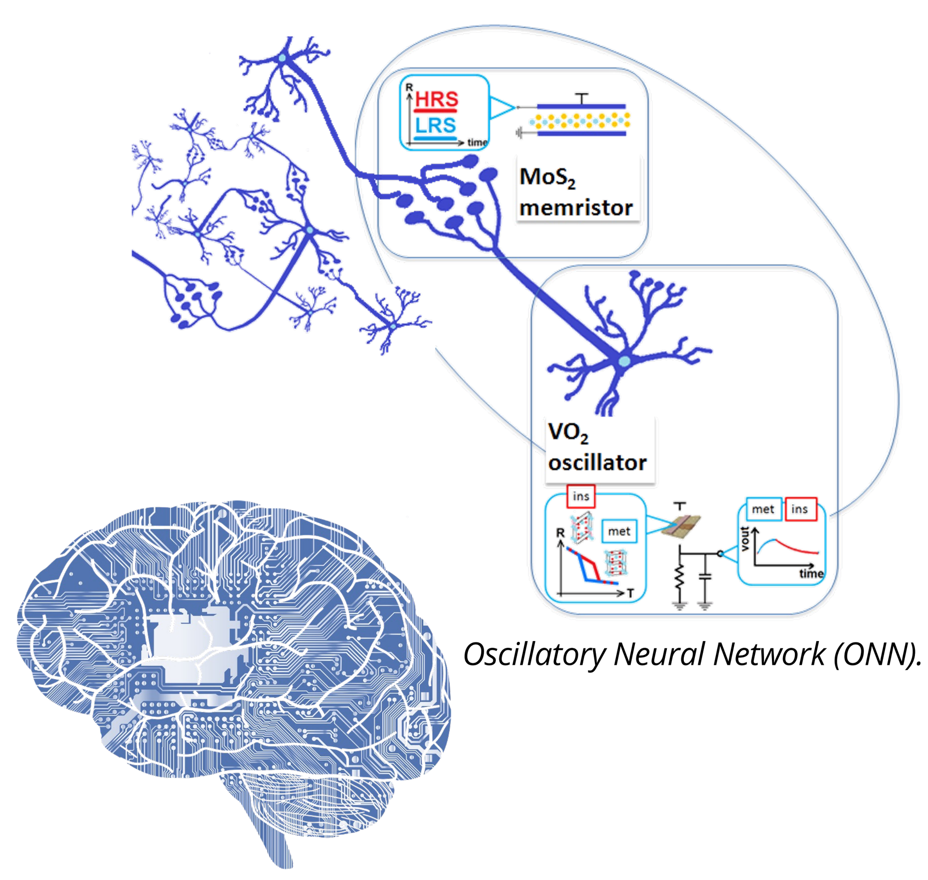
Brain-Inspired Computing

Advances in AI require powerful computing systems.

SOLUTION: increase the amount of transistors per processor. But…

The reduced size of nanoscale devices leads to prohibitively high energy requirements!

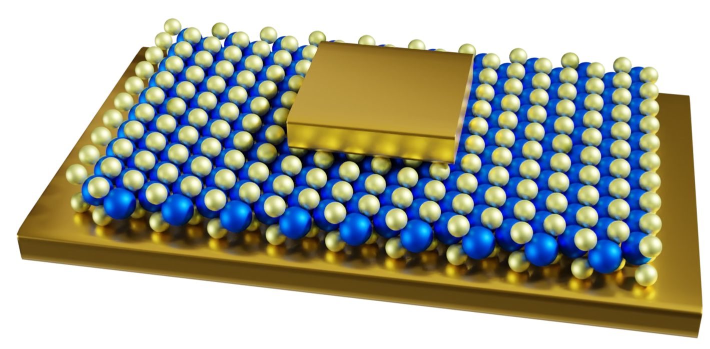
Neuromorphic computing: novel energy-efficient paradigm.



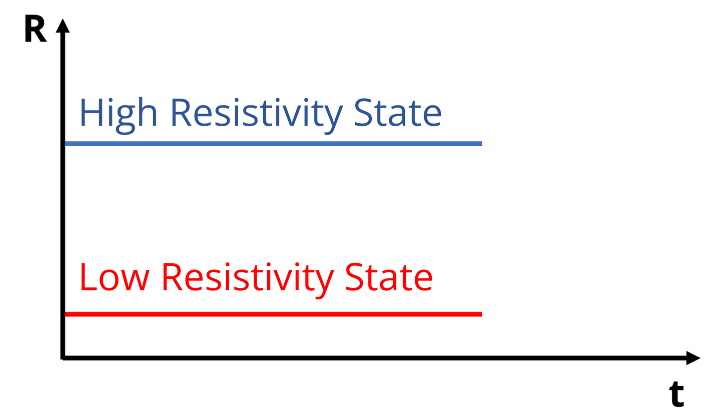
Oscillatory Neural Network (ONN).

The Synapse: MoS_2 Memristor

- A memristor is an electrical component that **limits/regulates the flow of electrical current in the circuit**.
- Memristors **"remember" the amount of charge** that has previously flown through.
- Memristors are **non-volatile**: they retain memory without power.



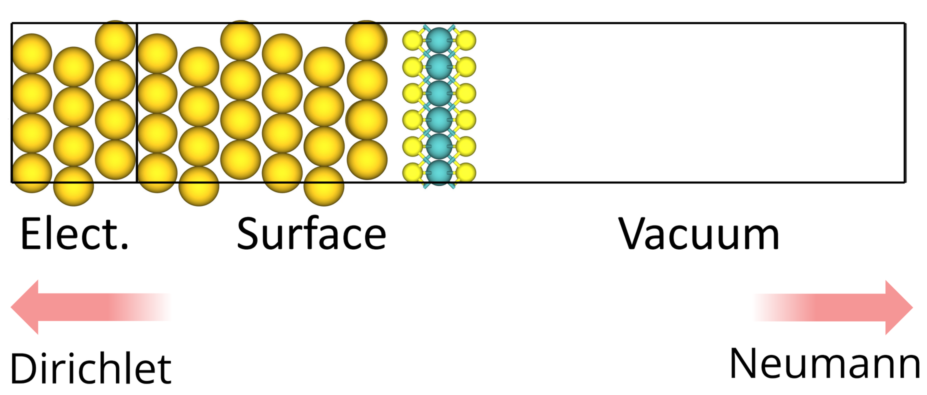
Au/MoS_2/Au vertical memristor ("atomristor").



1. What is the **physical mechanism** of the resistive switch?
2. Do **defects in the material** play any role?

Au/MoS_2 Interface Model

- We use **DFT coupled with Green's function surface simulations** with QuantumATK to model realistic Au/MoS_2 contacts with small and extended defects.

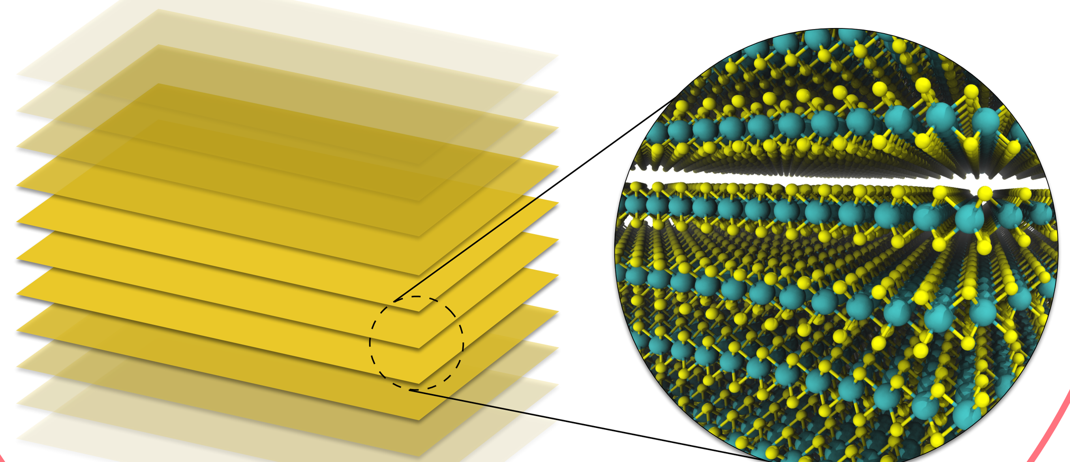


Simulation Details

- *XC functional: PBE-D2*
- *LCAO Medium basis set*
- *Density cut-off: 150 Ry*
- *K-point mesh: 3 x 2 x 138 MP grid*

Beyond Graphene: MoS_2

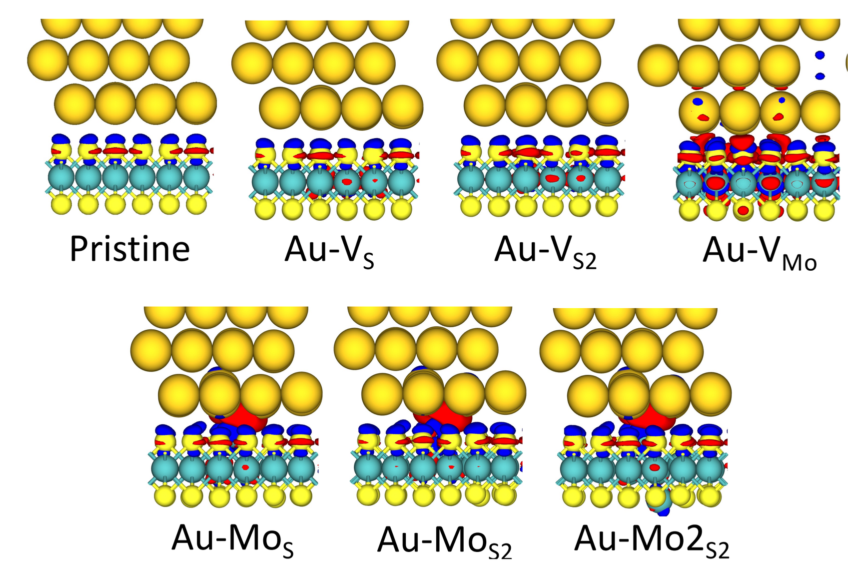
- 2D materials could enable compact and low-power devices, **beyond CMOS technology.**
- MoS_2 has desirable and **highly tuneable electronic properties.**



Aim: to bridge the gap between materials' properties and device physics.

Charge Redistribution at the Interface

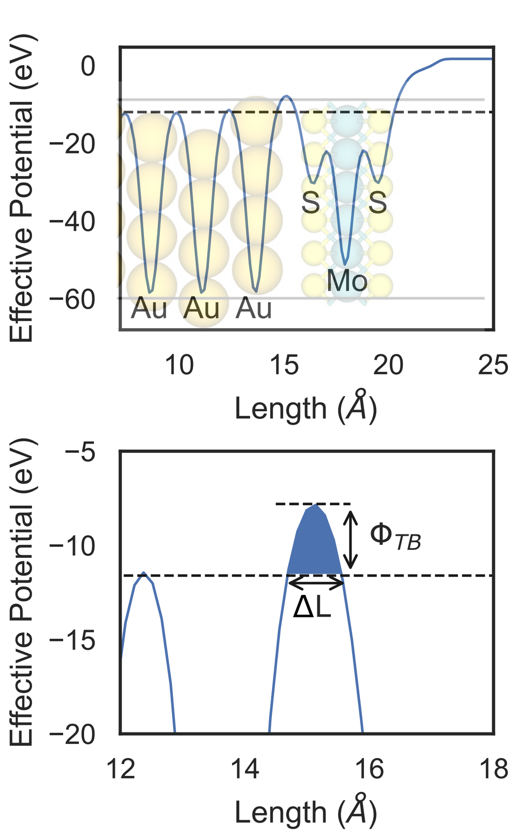
- We computed **electron density difference maps** of each defective interface to qualitatively assess the strength of the Au/MoS_2 interaction.
  - Relaxed geometries provide hints of **different reactivities** between defective MoS_2 and Au.



EDD maps of selected defective interfaces. Red isosurface: electron enrichment; blue isosurface: electron depletion. Isovalue: 0.002 eV/Å

Electron Injection Rates

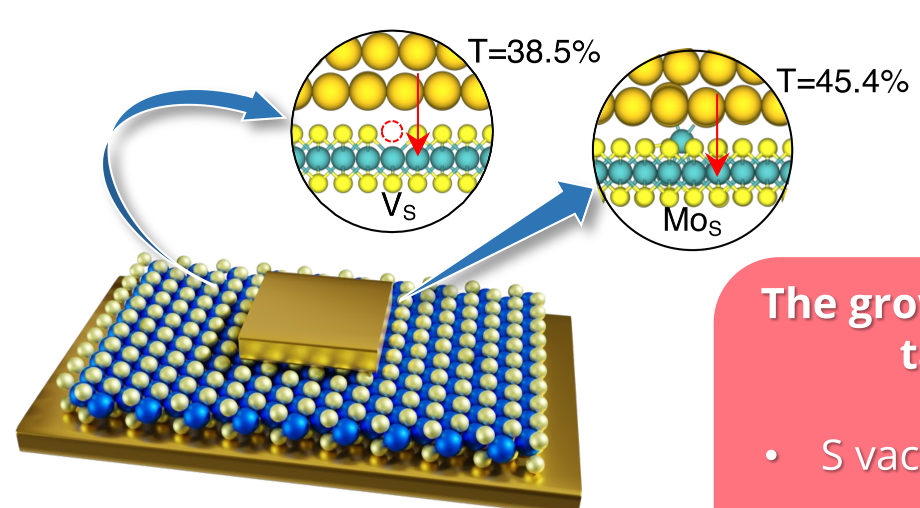
- We computed **defect-mediated electron injection rates** by looking at the effective potential at the materials' interface.



	Interface	T (%)	
	Pristine	39.7	
Vacancies	Au-V$_S$	38.5	*Decrease*
Vacancies	Au-V$_{S2}$	39.0	*Decrease*
Vacancies	Au-V$_{Mo}$	64.3	*Increase*
Antisite	Au-Mo$_S$	45.4	*Increase*
Antisite	Au-Mo$_{S2}$	43.8	*Increase*
Antisite	Au-Mo2$_{S2}$	46.9	*Increase*

Quality of Au/MoS_2 Contacts

- **Sulfur vacancies** appear to be **detrimental** for the quality of the contact.
- **Antisite Mo** atoms bridge MoS_2 with the Au electrode and **improve** the quality of the contact.



The growth process has to be carefully taken into consideration:

- S vacancies are mainly generated with CVD.
- Antisite Mo defects are generated with PVD.

Conclusions and Outlook

- We combined DFT with Green's function surface simulations **to predict and assess the impact of defects** on the electronic properties of MoS_2 and Au contacts.
- We obtained important insights into the **physics at the interface** between the core material and the metal electrode for two-dimensional nanodevices.
- In the near future, we aim **to extend and to increase the complexity of the interface models** by:
  - Including **adatoms** (e.g., Au) adsorbed either on the Au electrode or on MoS_2;
  - **Combining more than a single defect type** in the same simulation.

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References

[a] G. Boschetto, S. Carapezzi, C. Delacour, et al., ACS Appl. Nano Mater. (2022), 5, 10192-10202.
[b] S. Carapezzi, G. Boschetto, C. Delacour, et al., *IEEE J. Emerg. Sel. Top. Circuits Syst.* (2021), 11, 586-596.
[c] C. Delacour, S. Carapezzi, M. Abernot, et al., *IEEE ISVLSI* (2021), 326-331.
[d] S. Carapezzi, C. Delacour, G. Boschetto, et al., IEEE NEWCAS (2021), 1-5.

Contact: gabriele.boschetto@lirmm.fr