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

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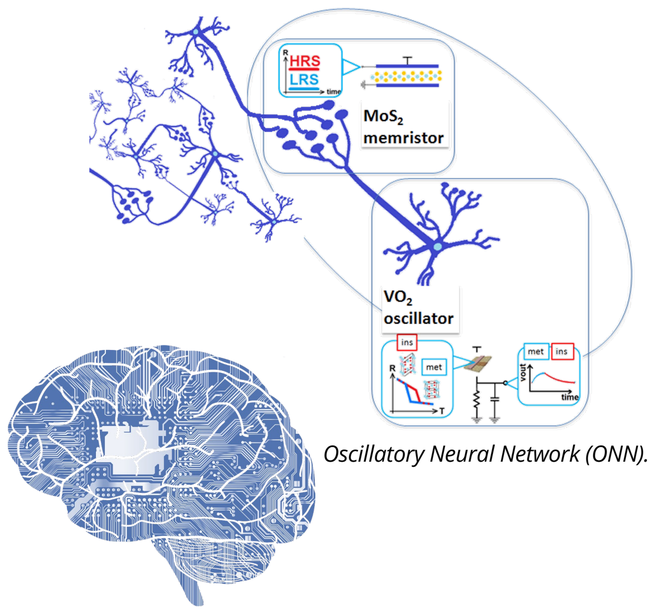
Brain-Inspired Computing

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!

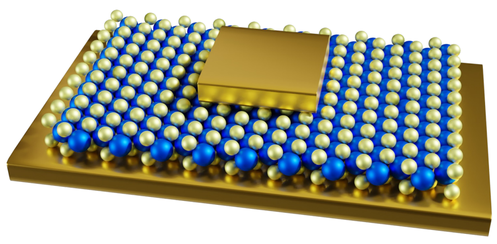
Neuromorphic computing: novel energy-efficient paradigm.



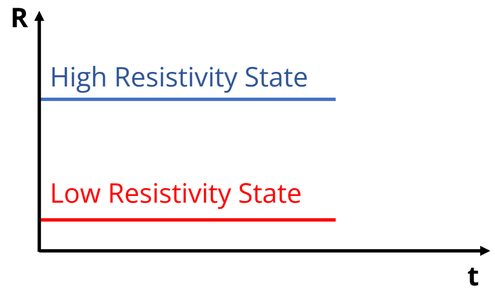
Oscillatory Neural Network (ONN).

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.



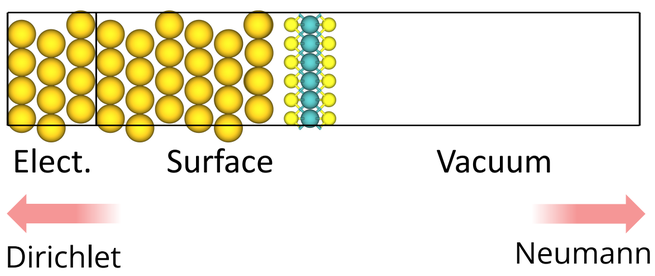
Au/MoS_2/Au vertical memristor ("atomristor").



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.

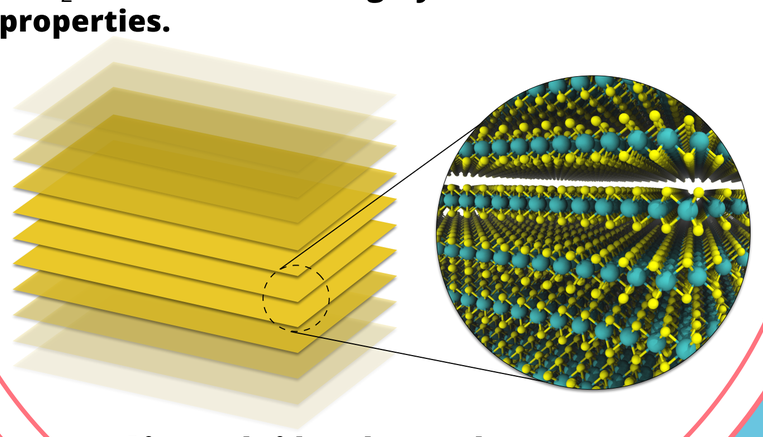


Simulation Details

- *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

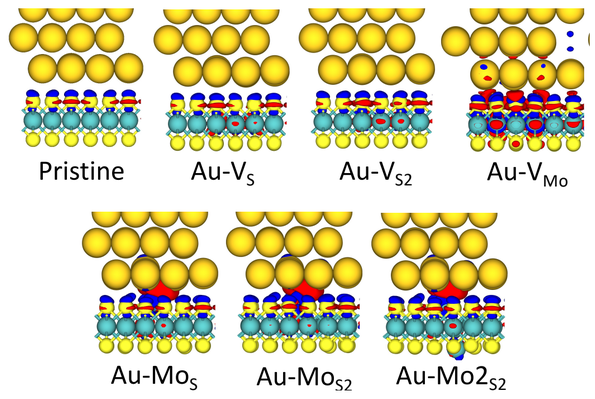
- 2D materials could enable compact and low-power devices, **beyond CMOS technology.**
- MoS_2 has desirable and **highly tuneable electronic properties.**



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

Charge Redistribution at the Interface

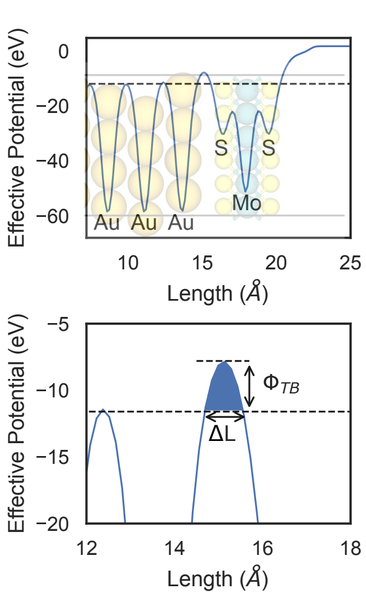
- We computed **electron density difference maps** of each defective interface to qualitatively assess the strength of the Au/MoS_2 interaction.
  - Relaxed geometries provide hints of **different reactivities** between defective MoS_2 and Au.



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

Electron Injection Rates

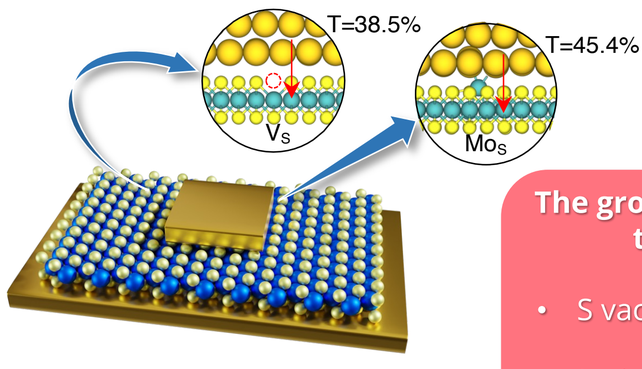
- We computed **defect-mediated electron injection rates** by looking at the effective potential at the materials' interface.



	Interface	T (%)	
Vacancies	Pristine	39.7	*Decrease*
	Au-V_S	38.5	
	Au-V_{S2}	39.0	
	Au-V_{Mo}	64.3	
Antisite	Au-Mo_S	45.4	*Increase*
	Au-Mo_{S2}	43.8	
	Au-$Mo2_{S2}$	46.9	

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

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