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



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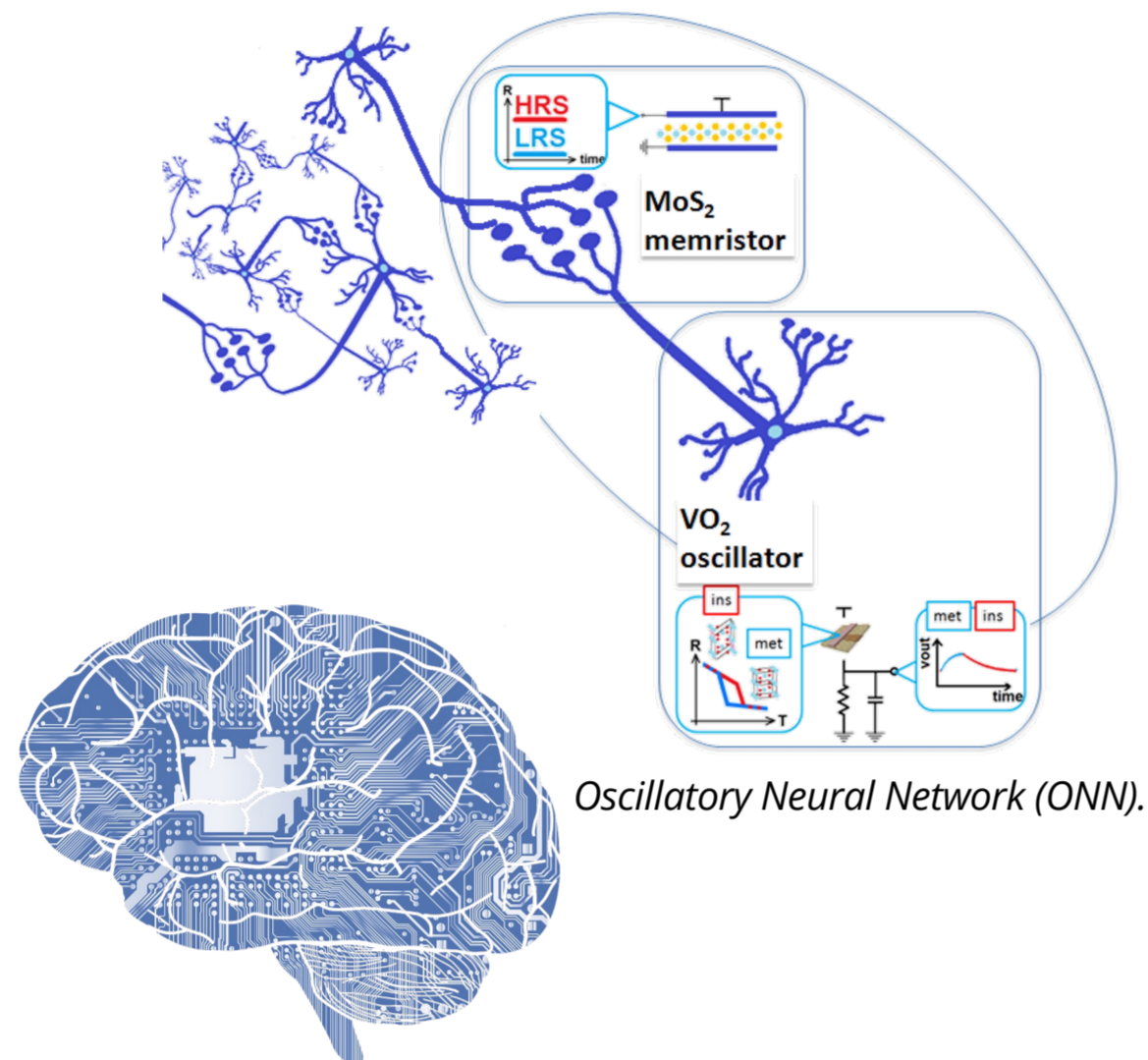
Brain-Inspired Computing

Advances in AI require powerful computing systems.

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

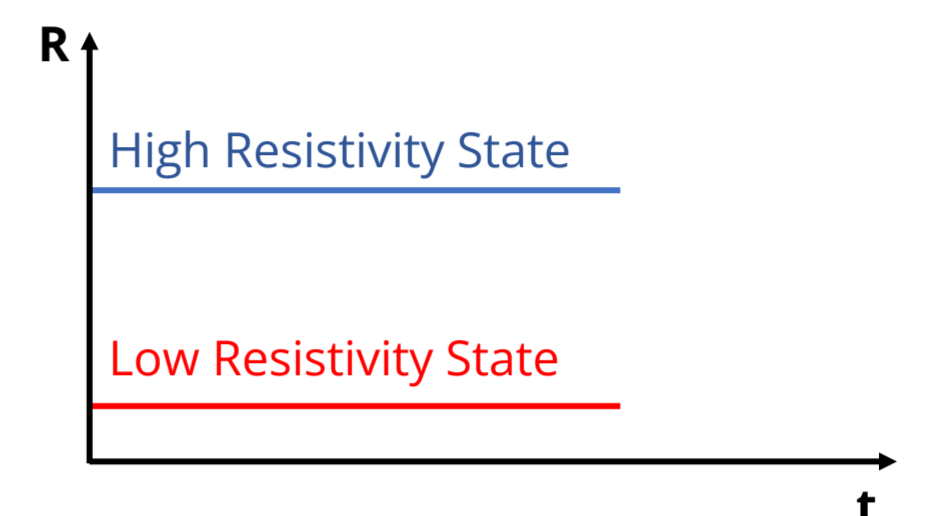
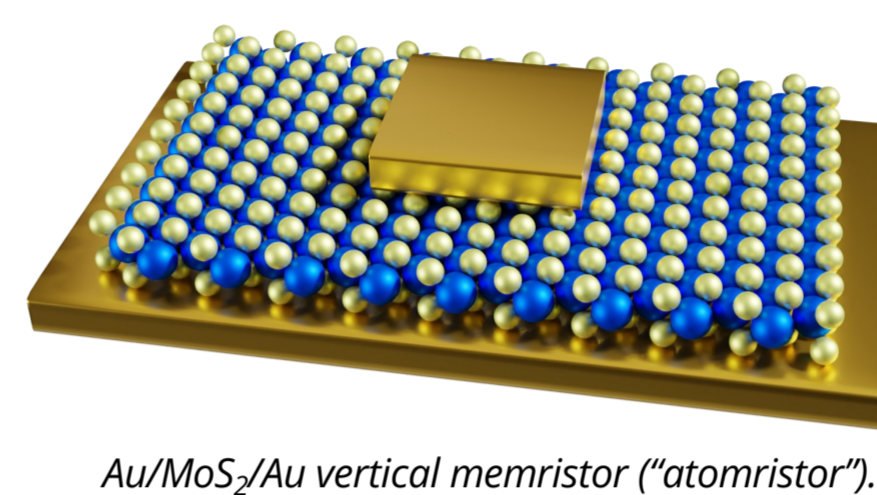
The reduced size of nanoscale devices leads to prohibitively high energy requirements!

Neuromorphic computing: novel energy-efficient paradigm.



The Synapse: MoS₂ Memristor

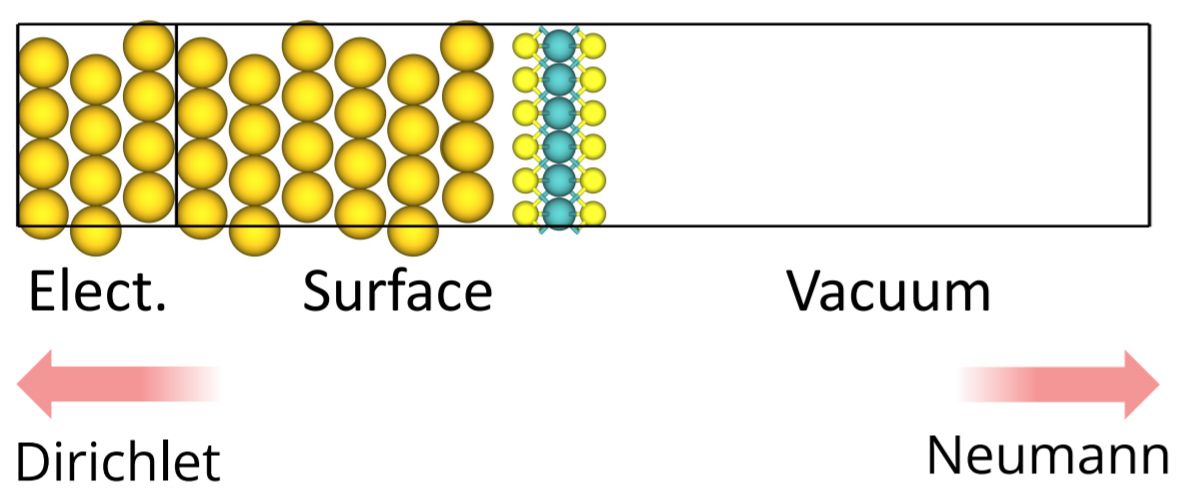
- A memristor is an electrical component that **limits/regulates the flow of electrical current in the circuit**.
- Memristors **"remember" the amount of charge** that has previously flown through.
- Memristors are **non-volatile**: they retain memory without power.



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

Au/MoS₂ Interface Model

- We use **DFT coupled with Green's function surface simulations** with QuantumATK to model realistic Au/MoS₂ contacts with small and extended defects.

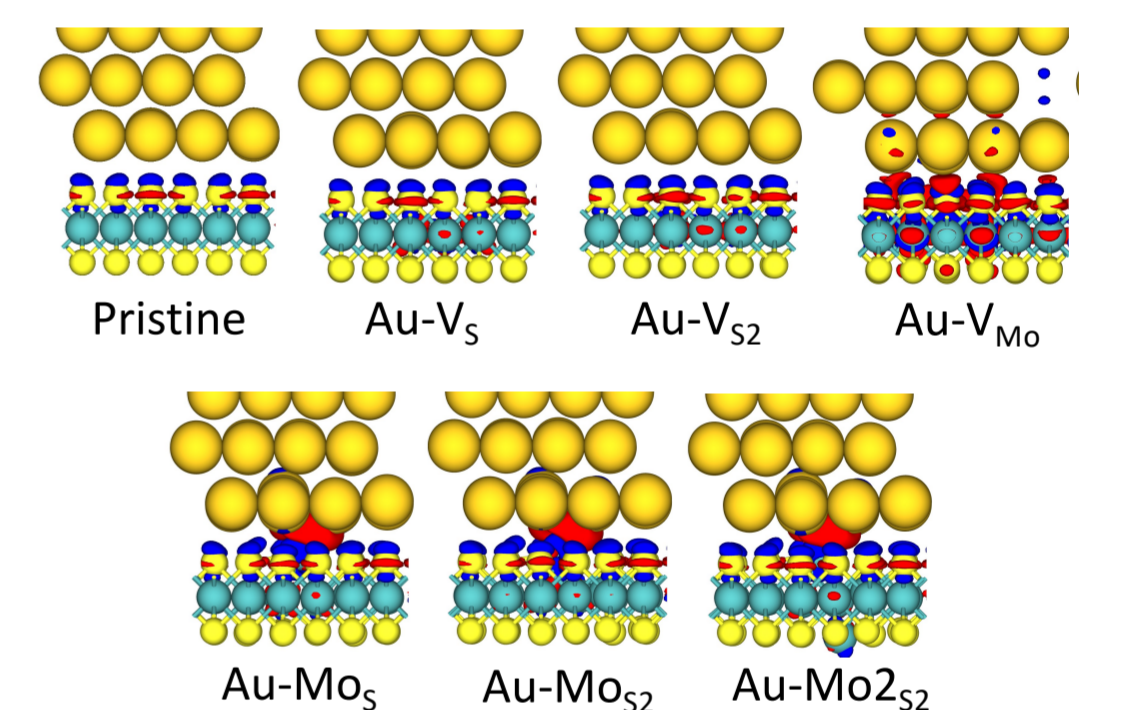


Simulation Details

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

Charge Redistribution at the Interface

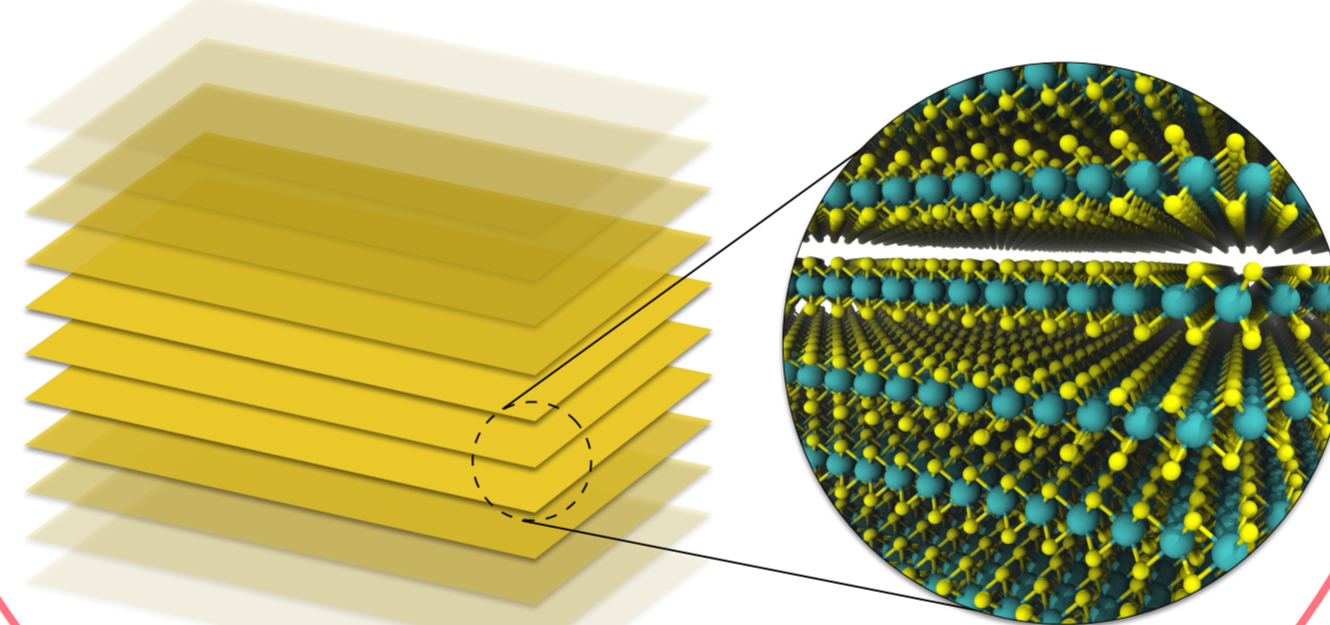
- We computed **electron density difference maps** of each defective interface to qualitatively assess the strength of the Au/MoS₂ interaction.
- Relaxed geometries provide hints of **different reactivities** between defective MoS₂ and Au.



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

Beyond Graphene: MoS₂

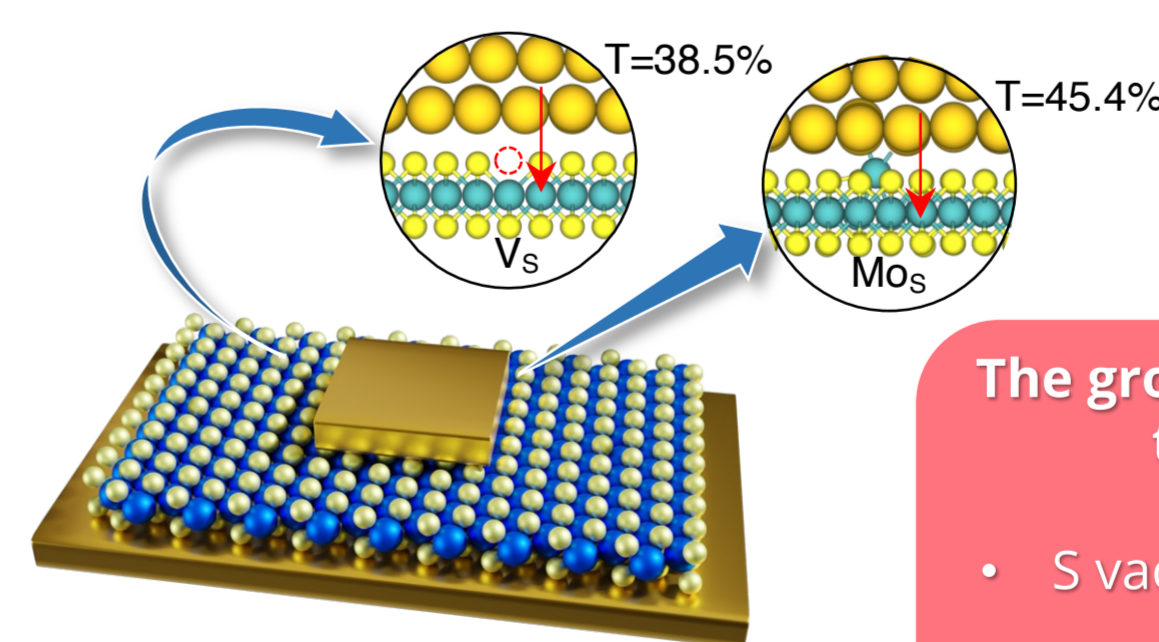
- 2D materials could enable compact and low-power devices, **beyond CMOS technology**.
- MoS₂ has desirable and **highly tuneable electronic properties**.



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

Quality of Au/MoS₂ Contacts

- Sulfur vacancies** appear to be **detrimental** for the quality of the contact.
- Antisite Mo** atoms bridge MoS₂ with the Au electrode and **improve** the quality of the contact.

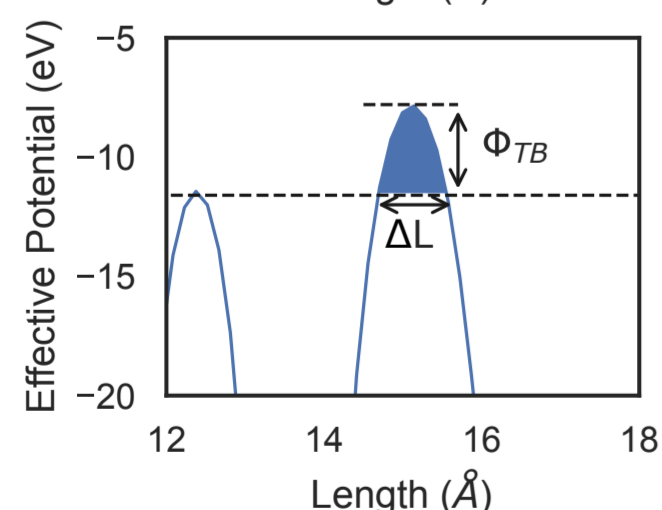
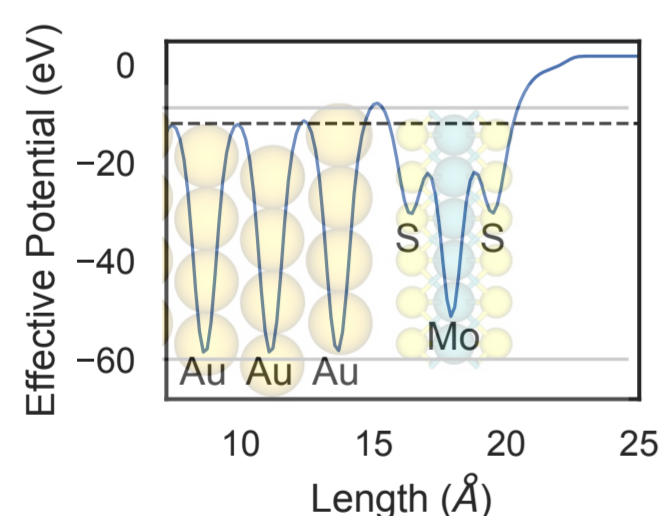


The growth process has to be carefully taken into consideration:

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

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
Au-V _s	38.5
Au-V _{s2}	39.0
Au-V _{Mo}	64.3
Au-Mo _s	45.4
Au-Mo _{s2}	43.8
Au-Mo _{2s2}	46.9

Vacancies: Decrease
Antisite: Increase

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 MoS₂ 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 MoS₂;
 - Combining more than a single defect type** in the same simulation.



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