Simulating Electronic Defects in 2D Materials

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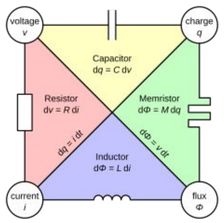
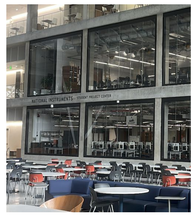
Background of Memristors

Leon Chua theorized the memristor in 1971.



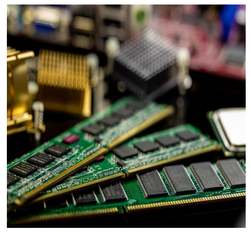
Memristor is a memory device that is more efficient than current devices.



UT Austin is expanding research from previous memristor research.

Traditional Hardware - used in everyday devices

CPU

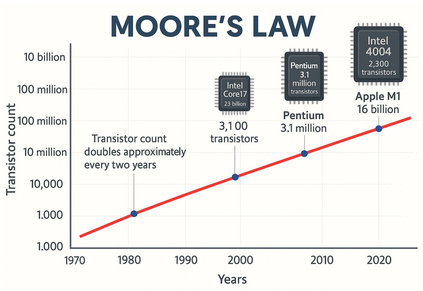


RAM

Computers rely on a CPU for processing and RAM for memory.

Researchers are working to identify a singular device.

Research Barriers

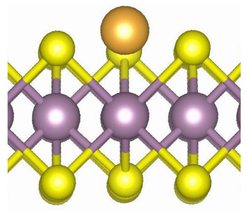


Moore's Law identifies that traditional silicon-based computing is near its scaling limits. → Research is expanding in a new direction using preliminary memristor computations

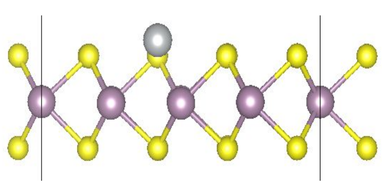
Scientific Question

How do different transition metals (Au, Ag, Fe, and Ni) affect the electronic properties to understand the binding strength of molybdenum disulfide (MoS_2)?

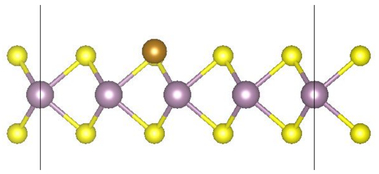
Methods and Results



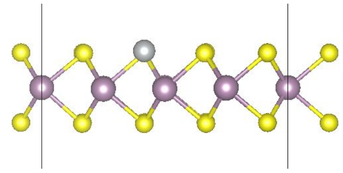
Eads of Au = -2.65671327 eV



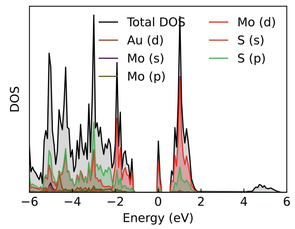
Eads of Ag = -2.14297044 eV



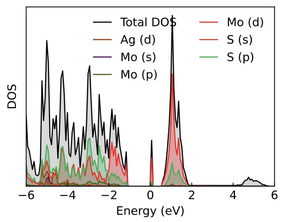
Eads of Fe = -3.60513401 eV



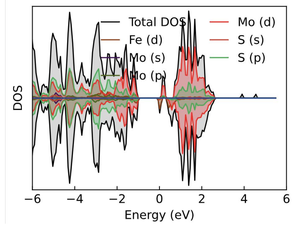
Eads of Ni = -4.937503240 eV



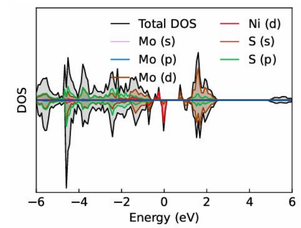
DOS of Au (gold)



DOS of Ag (silver)



DOS of Fe (iron)



DOS of Ni (nickel)

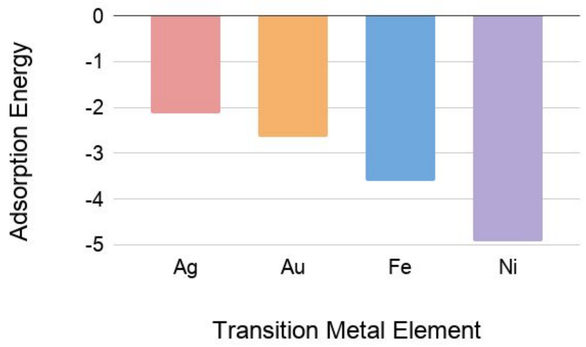
Currently, researchers are testing various metals with Molybdenum Disulfide to determine the optimum combination for the advancement of memristor studies with Gold being the most studied metal.

Adsorption Energy (Eads): Demonstrates the binding strength of each transition metal on the MoS_2 surface in the relax state.

Density of States (DOS): Demonstrates the distribution of electron energy levels to determine how each transition metal altered the electronic properties of MoS_2.

Methods and Results

Adsorption energy of atoms on molybdenum disulfide (MoS_2). More negative values indicate stronger bonding.



Conclusions and Future Work

1. Computational simulations efficiently identified how transition metals influence the electronic properties of MoS_2.
2. Computationally efficient calculations provide a strong foundation for future memristor studies.
3. Contributes to the ongoing development of next-generation electronic materials.

Acknowledgements

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