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## Chemically Functionalized Top-contact Electrodes: Boosting the Performance of MoS<sub>2</sub> Field-Effect Transistors by Tuning the Charge Injection

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The interface between electrodes and semiconductors plays a critical role in the (opto-)electronic performance of devices based on ultrathin two-dimensional layered materials. Unfortunately, a lack of interfacial modulation in the top-contact configuration impedes the performance of these devices. Here, we propose a contact engineering method to functionalize the electrodes of top-contact field-effect transistors (FETs) by transferring chemically pre-modified electrodes. We systematically tuned the electrodes of molybdenum disulfide ( $MOS_2$ )-based FETs using conventional thiol molecules with different dipoles. Notably, we observed significant improvements in device performance when we modified the Au electrode with electron-donating molecules. Using this facile approach, we fabricated a high-performance Schottky diode with asymmetrically functionalized electrodes by utilizing dipole-opposed molecules on two electrodes, resulting in a rectification ratio of ~10<sup>3</sup>. Our results demonstrate a powerful and unprecedented strategy for tuning the interfacial properties in top-contact MoS2 FETs and tailoring device performance on demand.

## References

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## **Figures**



Figure 1: Schematic diagram and the output curve of asymmetric MoS<sub>2</sub> FETs device with electrodes functionalized by PFBT and DABT respectively.