Density Functional Analysis of Voltage Shifts through Oxide Layers in Si- and MoS_2-based FETs

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We previously showed by density functional theory how oxide layers SrO, La_2O_3, HfO_2, or Al_2O_3 could be used to adjust the electrode Fermi levels (E_F) in either n-type or p-type directions and thereby control the threshold voltages (V_{th}) in high-K/CMOS metal gate stacks, using a combination of dipole effects and band alignments. We now show that these methods can be extended to 2D TMD-channel transistors, such as MoS_2. MoS_2 inevitably contains sulfur vacancies, making it weakly n-type. We find that inserting an Al_2O_3 layer into gate stacks will shift E_F downwards and allow full inversion mode MoS_2 FETs to be regained.

When high-K oxides were introduced, different gate metals were initially suggested for n- and p-type inversion mode FETs [1], with work functions near the Si band edges for n- and p-FETs respectively (Fig. 1a). These were replaced by a single, mid-gap metal such as TiN (Ru, computationally) plus two 'dipole layers' of La_2O_3 or Al_2O_3 to shift the work functions to nearer n- or p-type Si band edges [2], as in Fig. 1(b)[3].

Here, we directly calculate the work function shifts from the band-edge energies of the oxide slab surfaces. Fig. 2 shows a schematic plot of oxide band alignments obtained by the core level or band edge methods. Given the similar band gaps of these oxides, the band alignment diagram exhibits a 'staircase' pattern of staggered band offsets. This staircase pattern of band offsets is crucial as this enables a continuous range of biasing with these oxides. We choose Al_2O_3 and Y_2O_3 as the doping layers to build multiple stacks on Si and show a real-space layer-by-layer local density of states (LDOS) in Fig. 3. It is clear that these oxides cause n- or p-type Si behaviors and the overall alignment can involve both band alignment and dipole voltage effects between interfacial charges.

We then also employ this method to vary the V_{th} shifts in 2D transition metal dichalcogenide (TMD) FETs. MoS_2 is made intrinsic n-type due to the gap states of S vacancies S_{vac}. Pop [4] noted that TMDs have not yet achieved true inversion-mode FETs, mainly due to the unpassivated dangling bonds of S_{vac}. Thus, including a V_{th} shifting layer could allow these FETs to regain full inversion mode. Thus, we first investigated a gate stack model of ideal MoS_2/HfO_2/Ru layers (Fig. 4). We then created an S vacancy in the MoS_2 to shift E_F in a n-type direction (Fig. 5a). After inserting an Al_2O_3 layer between MoS_2 and HfO_2, E_F moves downwards to the valence band maximum (VBM), showing a p-type behavior (Fig. 5b). This is because the Al_2O_3 has a lower VBM than HfO_2 (Fig. 2). Therefore, by oxide interfacial layers, the transition of MoS_2 from n-type to p-type is possible, offering the potential to achieve high-quality n- and p-FETs.

In summary, we show that dipole layers/band offest layers can be used to make MoS_2 FETs inversion mode.

References

[1] R. Chau, et al, Electron Device Lett 25 408 (2004)

[2] K.Kita, A. Toriumi, App Phys Lets 94 132902 (2009)

[3] R Cao, Z Zhang, Y Guo, J Robertson, J. App. Phys. 134 085302 (2023)

[4] E Pop et al, (Stanford), TMD conf, Cambridge (June 2023); to be published.

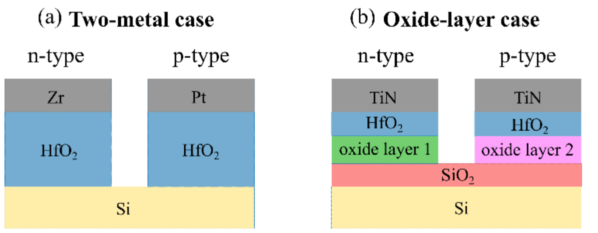

Fig. 1. Different voltage threshold settings in MOS structures (a) two-metal case with n- and p-type metal gates to shift gate voltage, (b) the oxide layer case with single TiN metal gate and an oxide layer to vary the gate voltage, V_{th}.

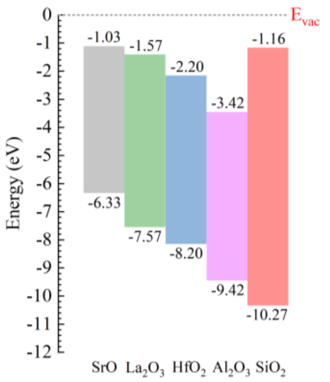

Fig. 2. Band alignments of the four oxides considered here, indicating a 'waterfall' band alignment, with staggered band offsets. E_{vac} is the vacuum level.

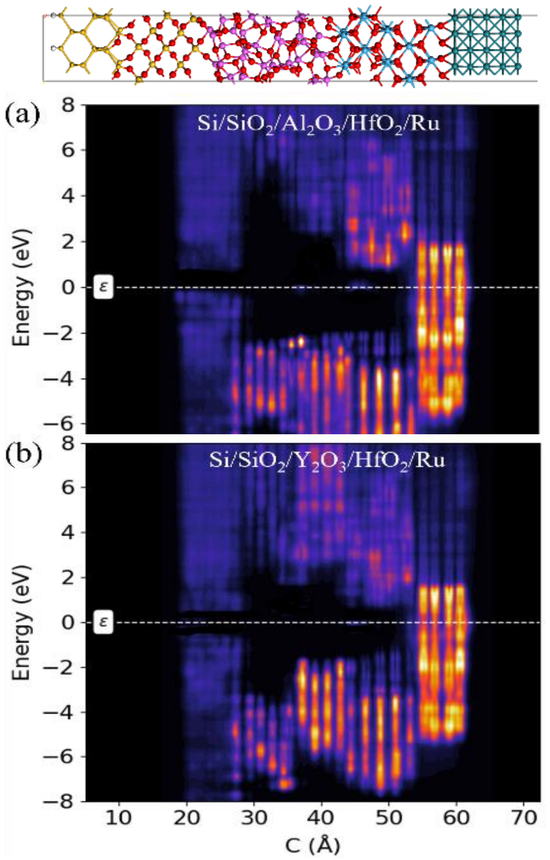

Fig. 3. GGA calculation of band edge energies vs atomic layers along the z axis for V_{th} shifting (a) p-type Al_2O_3 and (b) n-type Y_2O_3 gate stacks with Ru midgap metal, moving E_F next to (a) CBM and (b) VBM respectively. Y_2O_3 is used rather than La_2O_3 for better lattice matching.

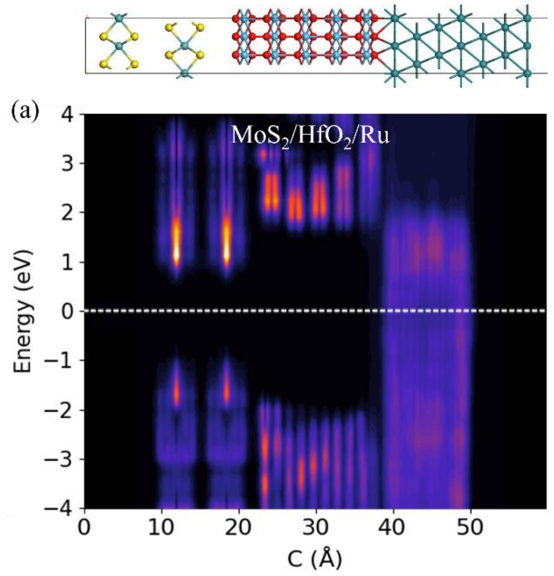

Fig. 4. Atomic model and LDOS of band edge energies vs atomic layers along the z axis for $MoS_2/HfO_2/Ru$.

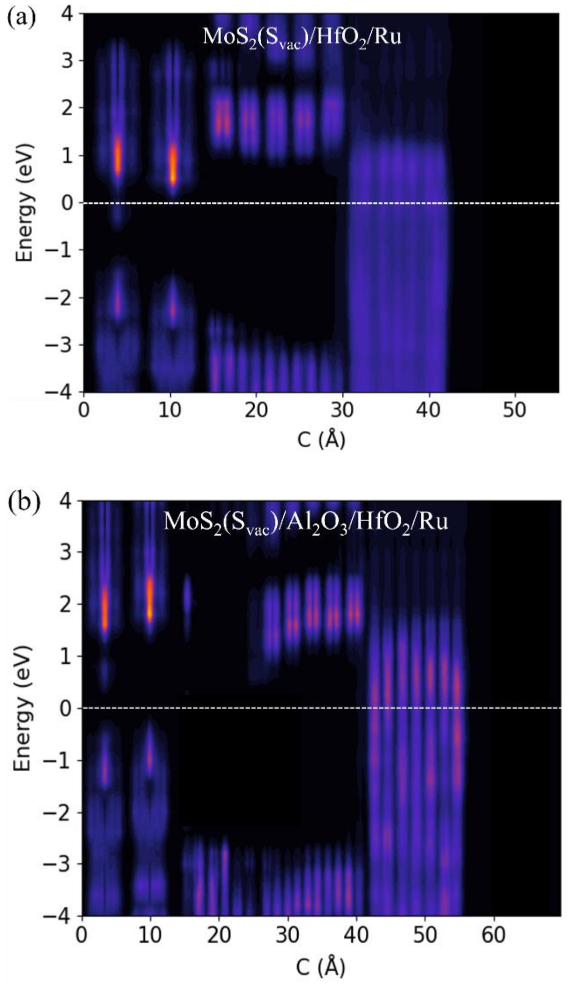

Fig. 5. GGA calculation of band edge energies vs atomic layers along the z axis for V_{th} shifting (a) $MoS_2/HfO_2/Ru$ layers with S_{vac}, and (b) $MoS_2/Al_2O_3/HfO_2/Ru$ layers with S_{vac}, moving E_F from CBM to nearer VBM, respectively.