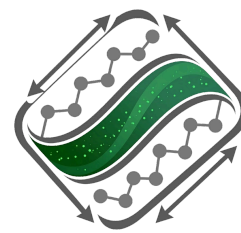


PROGRESS HIGHLIGHT

Reconfigurable Quantum Materials for Low-Energy Electronics

AEA Ignite Team for “From Lab to Fab: Advancing a New Low-Energy Transistor Towards Large-scale Manufacturing” (IG250200225)



From Lab to Fab: Advancing a New Low-Energy Transistor

SUMMARY: This AEA project aims to bring a new low-energy electronic technology from proof of concept towards commercialisation by using quantum materials in thin-film form to create a heterostructure platform with significantly lower energy consumption than current technology. This progress report demonstrates the team’s achievement in completing the first milestone set out in the proposal: Large-Scale Channel-Material Growth, which has successfully increased the project’s TRL by experimentally validating the theoretical concepts in a reproducible laboratory environment.

DEVICE FABRICATION AND PERFORMANCE: To realise the proposed heterostructure transistor channel based on atomically thin films, our team has developed and optimised a device fabrication process for assembling dual-gate field-effect transistors. We demonstrated the effectiveness of the heterostructure transistor channel using MoS_2 with an hBN spacer.

Under an external electric field, MoS_2 with the hBN spacer shows significantly stronger band-gap modulation through the Stark effect compared with conventional bilayer MoS_2 .

THIN FILM QUALITY: Using advanced tunnelling electron microscope (TEM), we have verified the quality and interfacial stability of the MoS_2 -hBN heterostructure film.

ONGOING WORK: Aligned with the project schedule, device modelling and experiments on incorporating ferroelectrics are in progress.

BUSINESS DEVELOPMENT: We are working TQ Transistors to expand the scope of the R&D program through engaging with new external collaborators. □

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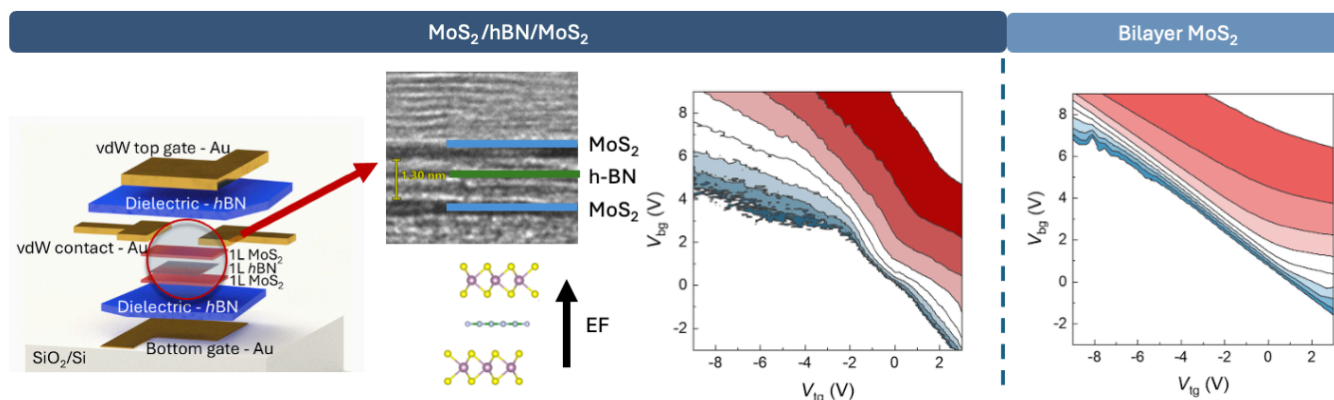


Fig. 1. Reconfigurable heterostructure for enhanced electric field response We have fabricated field-effect transistors using the $\text{MoS}_2/\text{hBN}/\text{MoS}_2$ sandwiched structure as the channel, as confirmed by high-resolution TEM imaging. Under an external electric field, the device with the heterostructure channel shows a much sharper electronic response compared with conventional bilayer MoS_2 .

TECHNICAL REPORT

Reconfigurable Quantum Materials for Low-Energy Electronics

AEA Ignite Team for “From Lab to Fab: Advancing a New Low-Energy Transistor Towards Large-scale Manufacturing” (IG250200225)

Team members: Yuefeng Yin^{1*}, Kaijian Xing², Weiyao Zhao^{1,2}, Mike Klymenko¹, Michael S. Fuhrer^{1,2}, Nikhil V. Medhekar^{1,2}, Wayne Johnson³, Thomas Wrappe³, Stuart Douglas³.

We have made a practical advance towards solving one of the pressing challenges of using two-dimensional atomically thin films in transistors as current silicon-based technology approaches its limits: fabricating a semiconducting channel that can respond strongly to an external electric field. Our device, using MoS₂/hBN/MoS₂ as the channel, has shown good interfacial stability when incorporated into a transistor structure, with performance significantly superior to that of conventional van der Waals layers. These results are consistent with our earlier theoretical predictions and demonstrate the effectiveness of this engineering-intuitive and reconfigurable design, as well as its strong potential for commercialisation.

Our background IP and previous calculations established the proof of concept for electric field switching in a bilayer two-dimensional material with the insertion of a middle spacer layer (1–4). The spacer layer not only acts as an interfacial stabiliser to hold the two separated atomically thin films, but also serves as a decoupling layer that drives the electronic structure towards a degenerate, monolayer-like form. As a result, the Stark effect induced by the external electric field becomes more effective because of reduced interlayer screening, leading to an enhanced field response of the transistor channel.

We have also shown that this working principle is general for two-dimensional heterostructures that form a Type-I (straddling) band alignment upon contact. i.e. The valence band maximum (VBM) and conduction band minimum (CBM) of the middle spacer should enclose those of the active thin-film material. Here, we use MoS₂ and hBN, two widely available materials in the field, to form a heterostructure channel and experimentally verify this concept.

In the following, we demonstrate the successful delivery of the first working device incorporating a MoS₂/hBN/MoS₂ channel, whose performance is significantly better than that of a conventional MoS₂ bilayer. Advanced characterisation has confirmed the morphology and stability of the channel. These observations are con-

sistent with our previous density functional theory (DFT) calculations and support the proposed mechanism behind the enhanced electric field response.

Device Fabrication

The metal electrodes (bottom gate – 15nm, source-drain contacts – 20nm, top gate – 50nm) were firstly fabricated on sacrificed SiO₂/Si substrates using standard photolithography, electron-beam evaporation (Au) and lift off process. A bottom gate electrode was picked up and laminated onto a precleaned SiO₂/Si substrate by the PC-assisted dry transfer method, after which a ~20-nm-thick hBN flake was transferred on top via the same technique to form the bottom-gate architecture. Following an annealing step (300 °C in Ar ambient for 2 hours), exfoliated monolayer MoS₂ (bilayer MoS₂ or monolayer MoS₂/monolayer hBN/monolayer MoS₂) were transferred onto the gating area by the PC method. The stack was then annealed at 200 °C in an Ar atmosphere for 2 hours. Finally, a ~20nm hBN and top gate was transferred on the target region to complete the dual gated field-effect transistor. Here it should be noted that we van der Waals integrated all layers including the metal electrodes, which optimised the contact performance and reduced the gate leakage risks, resulting in a higher device yield.

Device Performance

To evaluate Stark-effect bandgap engineering in a decoupled 2D semiconducting system, we compared three dual-gated architectures: monolayer MoS₂ (**Fig. 1a**), bilayer MoS₂ (**Fig. 1c**), and a monolayer MoS₂/few-layer hBN/monolayer MoS₂ heterostructure (**Fig. 1e**). Independent top and bottom gates enable decoupled control over both the carrier density and the out-of-plane electric field across the active channel. We first confirmed the independent functionality of each gate by sweeping one while grounding the other. Next, we mapped the source-drain current across the full V_{tg} - V_{bg} bias space. In the monolayer device (**Fig. 1b**), the constant-current contours maintained a fixed slope across both subthreshold and high-current (linear) regimes, as expected when current depends solely on the net carrier density. Conversely, for bilayer MoS₂, the contour slopes slightly decreased under high out-of-plane electric fields in the subthreshold regime. This slope deviation became significantly more pronounced in the monolayer MoS₂/thin hBN/monolayer MoS₂ heterostructure under high-field conditions. We attribute this phenomenon to Stark-effect-induced bandgap modulation (ΔE_g). Inserting the thin dielectric spacer (such as few-layer hBN) strongly decouples the two semiconductor monolayers, suppressing channel quantum capacitance screening and allowing the out-of-plane field to efficiently shift the bands, thereby altering the bandgap engineering.

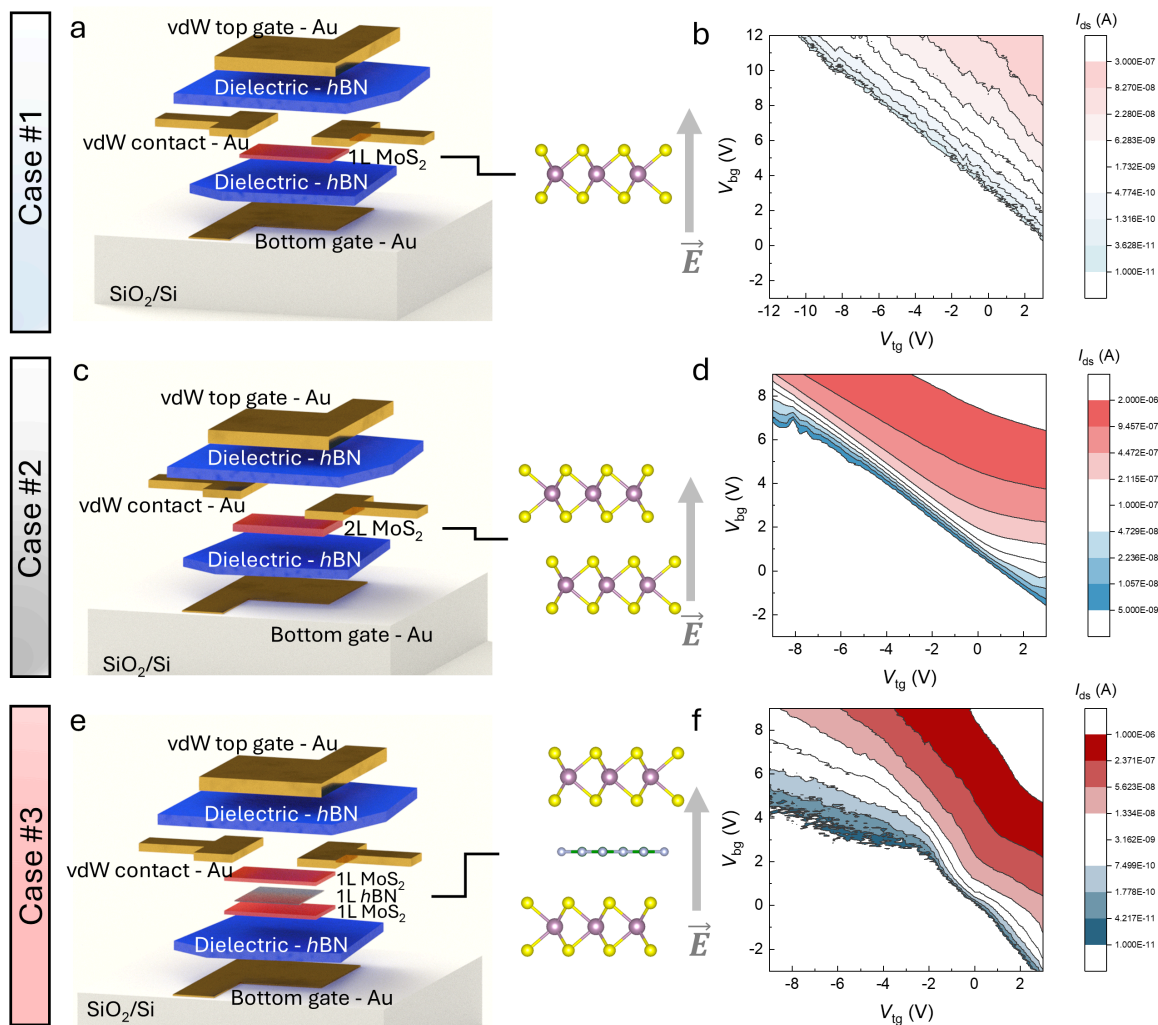


Fig. 1. Band modulation by out-of-plane E field for monolayer MoS₂, bilayer MoS₂ and bilayer MoS₂ with hBN spacer. (a), (c) and (e) represent the architecture dual-gate field-effect transistors for three cases. (b), (d) and (f) show the source-drain current as a function of both top-gate bias, V_{tg} , and bottom-gate bias, V_{bg} .

Characterisation of the Heterostructure

To evaluate the interfacial quality of the dual-gate MoS₂ devices, we used cross-section tunnelling electron microscope (TEM) to take high-resolution images. The device photo is shown in **Fig. 2a**, in which the channel of MoS₂/hBN/MoS₂ is sandwiched by two multi-layer hBN/Au gates. The black line highlights the area of interest, which has been lifted out using a dual-beam SEM (scanning electron microscope, Thermoscientific FEI Helios 5) with a Ga source focused ion beam. The stackings of 2D materials has been sketched in **Fig. 2b**. The low-resolution cross-section image was taken using the scanning electron tunnelling microscope (STEM) function in Helios 5 (with 30 kV accelerate voltage). The sharp interface across the whole device is shown in **Fig. 2c**. We further show the zoom-in plots in **Fig. 2d**, in which one can see the near comparable thickness of top- and back-dielectric hBN layers. The high-resolution photo (**Fig. 2e**) was taken using the FEI Talos TEM, running at 200 kV and in bright-field mode. The spacer layer in this device is 3 layers of hBN, ~ 1.3 nm.

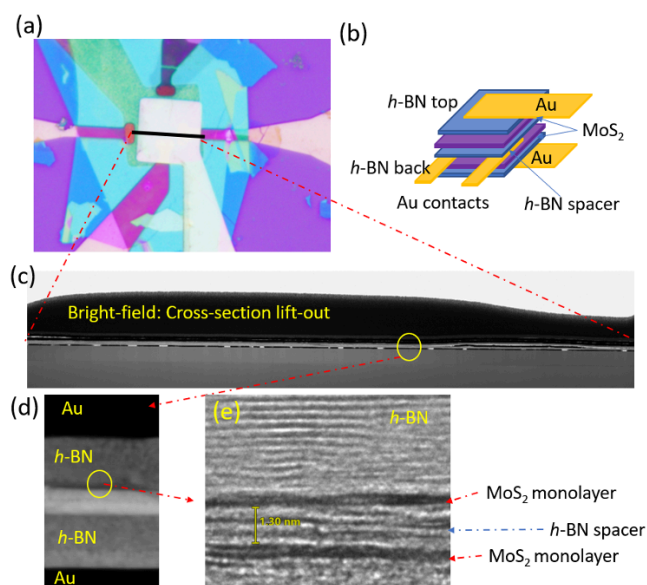


Fig. 2. Structural characterization of dual-gate MoS₂ transistor device. (a) The optical image of the device, in which the area-of-interest is labelled using a black line. (b) The architecture of the device. (c) Broad-area bright-field scanning tunnelling electron microscope (STEM) image of the prepared lamella. (d) The medium-resolution STEM image at the centre of the device channel. (e) High-resolution tunnelling electron microscope (TEM) image of the MoS₂ channel.

Materials Modelling

We have also performed DFT calculations to understand the electronic structure of the $\text{MoS}_2/\text{hBN}/\text{MoS}_2$ heterostructure and its response to an external electric field. As shown in **Fig. 3a**, the band gap of MoS_2 with an hBN spacer is significantly more sensitive to the external electric field compared with monolayer and bilayer MoS_2 .

This enhanced response is also reflected in the maximum switching figure of merit (FOM, $\eta_{\max}$) for the three systems, as shown in **Fig. 3b**. The FOM is a dimensionless metric that quantifies and normalises the electric field response across the channel, defined as $\eta = |dE_g/dE|/t_{\text{channel}}$, where E_g is the band gap and t_{channel} is the channel thickness. A higher η indicates a stronger band-gap response to the electric field for a given channel thickness.

We can also observe clear band separation and shifts in MoS_2 with the hBN spacer under the external electric field, as shown in **Fig. 3c-g**. These results are consistent with our experimental observations and complete the proof-of-concept demonstration and validation of the proposed heterostructure design for enhanced electric field response.

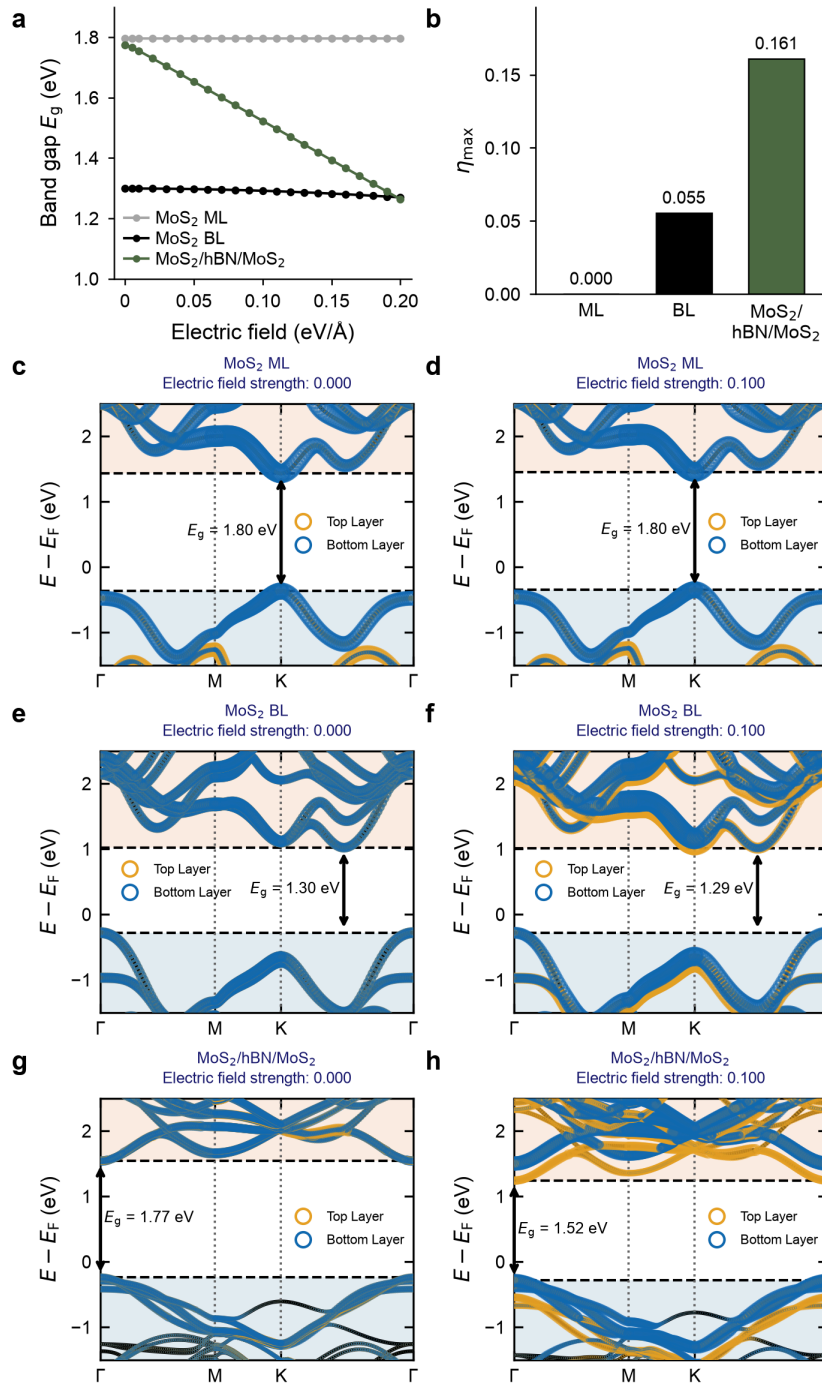


Fig. 3. DFT modelling of monolayer MoS_2 (MoS_2 ML), bilayer MoS_2 (MoS_2 BL), and $\text{MoS}_2/\text{hBN}/\text{MoS}_2$ under external electric field. (a) Electronic band gap evolution with respect to the external electric field for three systems. (b) Maximum switch figure of merit (FOM, $\eta_{\max}$) for three systems. (c)-(g) Electronic band structures of MoS_2 ML, MoS_2 BL, and $\text{MoS}_2/\text{hBN}/\text{MoS}_2$ under $E = 0$ V/nm and $E = 0.1$ eV/Å, respectively.

Next Steps

1. Ferroelectric incorporation and device modelling.

The next step is to incorporate ferroelectric materials into the heterostructure channel to achieve non-volatile switching. We will also perform device modelling to predict the performance of devices incorporating ferroelectric materials.

2. Engagement with new collaborators.

We are currently engaging with new collaborators to expand the scope of the R&D program, particularly in large-scale crystal growth and device fabrication.

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