Defect and Interface Engineering of 2D Materials by Chemical Vapor Deposition for tunable functional devices

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Defect and interface engineering in two-dimensional (2D) materials offers a powerful route to tailor their electronic and optoelectronic properties for multifunctional device applications. Molybdenum disulfide (MoS_2), a representative 2D semiconductor, intrinsically hosts point defects such as sulfur vacancies (V_s), which can be harnessed to modulate carrier density, light emission, and charge transport. However, precise control over defect concentration during growth, while maintaining crystalline integrity, remains a significant challenge. Here, we present a one-step, in-situ defect engineering strategy for monolayer MoS_2 via a pressure-tunable chemical vapor deposition (CVD) method. Growth under low-pressure (LP-CVD) conditions yields V_s-rich MoS_2 crystals due to oxygen-deficient environments, while atmospheric-pressure (AP-CVD) conditions lead to passivated V_s defects owing to ambient oxygen incorporation. This contrast in defect landscapes enables direct tuning of optoelectronic responses: AP-MoS_2 exhibits enhanced photoluminescence, whereas LP-MoS_2, with its in-gap donor states, demonstrates superior photoresponsivity and detectivity in photodetectors, as well as improved performance in field-effect transistors (FETs). Furthermore, we explore the role of CVD-enabled interface engineering through homo- and heterostructure fabrication to further enhance device functionalities. We investigate bilayer MoS_2 with distinct stacking configurations—2H and 3R phases—revealing stacking-mode-dependent enhancements in electronic and optoelectronic properties, further expanding the tunability of 2D material systems. Our findings establish a scalable approach for the simultaneous engineering of defects, stacking, and interfaces in 2D materials, paving the way for next-generation, tunable electronic, optoelectronic and electrochemical devices.

References

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Figures

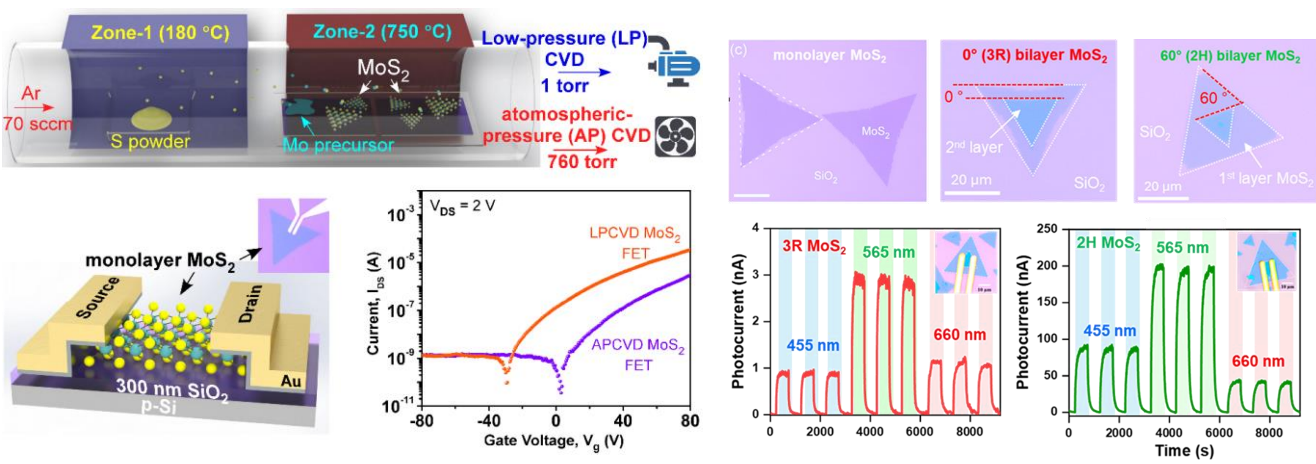

Figure 1: Schematic of CVD configuration used to modulate MoS_2 growth. Schematic and FET characteristics of AP-MoS_2 and LP-MoS_2 based devices. In panel (c) and onwards, stacking dependent (3R and 2H bilayer MoS2) and their photoresponse measurements are shown.