Supplementary Information

for

Optimizing Crystalline MoS_2 Growth on Technologically Relevant Platinum Substrates Using Ionized Jet Deposition: Interface Interactions and Structural Insights

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XRD on interface film

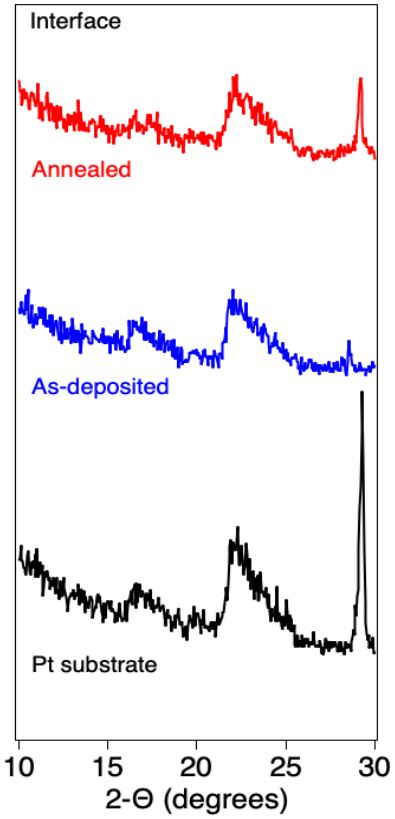


Figure S1 XRD pattern of as-deposited and annealed MoS_2 interface film; the lower panel shows the corresponding reference spectrum of the bare Pt substrate.

The XRD spectra of bare Pt substrate, as well as as-deposited and annealed MoS_2 interface film are shown in Figure S1. The crystalline contributions stemming from the Pt substrate are dominant in

all XRD spectra while the ones stemming from MoS_2 are not detectable. Since the interface film has an estimated thickness of less than 5 nm, the XRD spectra are consistent with the fact that the deposition first fills the roughness of the substrate in an amorphous manner, therefore we cannot observe any crystalline contribution from MoS_2. Any contribution from crystalline layers is below the detection limit of XRD analysis.

XPS spectra fitting

The XPS spectra were fitted using a passive Shirley background to account for inelastic scattering. Peak shapes were modeled with a mixed Gaussian-Lorentzian (GL) profile, using a GL(30) ratio—i.e., 30% Lorentzian contribution, as implemented in the XPSPEAK41 software. For metallic platinum components observed in the interface film (Figure 6), an asymmetric peak shape was applied to better capture the characteristic line shape of metallic states. All fits were performed with constraints based on known chemical shifts and spin-orbit splitting values where applicable.

Table 1 presents the binding energies (BE) of the fitted XPS core levels, along with a comparison to our previous results [1], [2].

	Present Work	**Previous Work on Pt [1]**	**Previous Work on SiO_2/Si [2]**
Core Level	**BE (eV)**	**BE (eV)**	**BE (eV)**
S $2p_{3/2}$ (MoS_2)	161.65	161.80	161.54
S $2p_{3/2}$ (defective MoS_2)	162.75	-	-
S $2p_{3/2}$ (Pt–S interface interaction)	162.73	-	-
S $2p_{3/2}$ (Elemental)	163.90	163.70	~163.00
S 2s (MoS_2)	226.32	226.30	~226.30
S 2s (defective MoS_2)	227.57	-	-
S 2s (Pt-S interface interaction)	227.55	-	-
S 2s (Elemental)	228.62	228.00	~227.80
Mo $3d_{5/2}$ (MoS_2)	228.85	228.90	228.72
Mo $3d_{5/2}$ (MoO_2)	230.50	-	-
Mo $3d_{5/2}$ (MoO_3)	232.64	-	-
Pt $4f_{7/2}$ (Metallic)	71.03	-	-
Pt $4f_{7/2}$ (Pt-S interaction)	71.80	-	-

References

1. Timpel, M.; Ligorio, G.; Ghiami, A.; Gavioli, L.; Cavaliere, E.; Chiappini, A.; Rossi, F.; Pasquali, L.; Gärisch, F.; List-Kratochvil, E.J.; et al. 2D-MoS_2 goes 3D: Transferring optoelectronic properties of 2D MoS_2 to a large-area thin film. *npj 2D Mater. Appl.* **2021**, *5*, 64.
2. Ghiami, A.; Timpel, M.; Chiappini, A.; Nardi, M.V.; Verucchi, R. Synthesis of MoS_2 Thin Film by Ionized Jet Deposition: Role of Substrate and Working Parameters. *Surfaces* **2020**, *3*, 683–693.