Supplementary information

Experimental verification of SO_2 and S desorption contributing to defect formation in MoS_2 by thermal desorption spectroscopy

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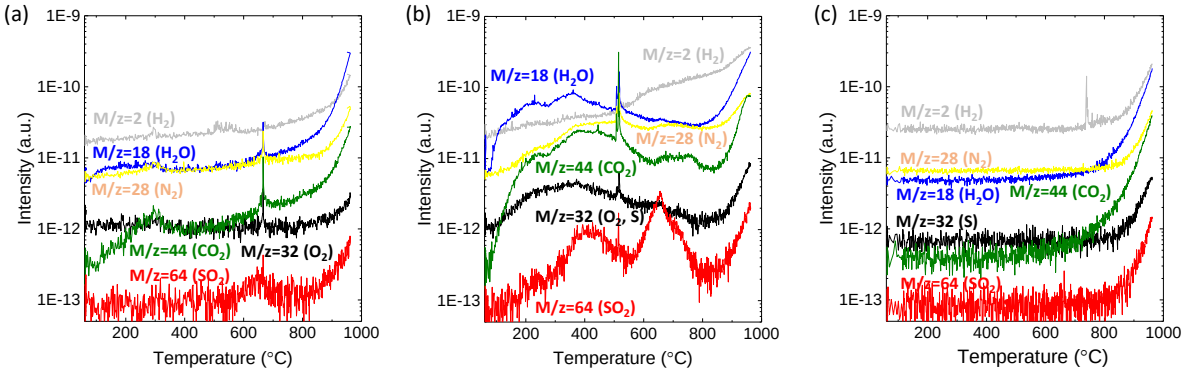

Fig. S1 (a) TDS spectra for the main desorbed species detected from the SiO_2/Si substrate. The spikes at approximately 500 °C result from the fluctuation of the inner pressure in the TDS chamber. (b) TDS spectra for the main desorbed species detected from the MoS_2 flakes on the SiO_2/Si substrate. (c) The second annealing TDS spectra for the MoS_2 flakes on the SiO_2/Si substrate. The removal of adsorbed species on the MoS_2 flakes can be reflected by the flatness of the signal before increasing the inner pressure in the high-temperature region (over 800 °C).

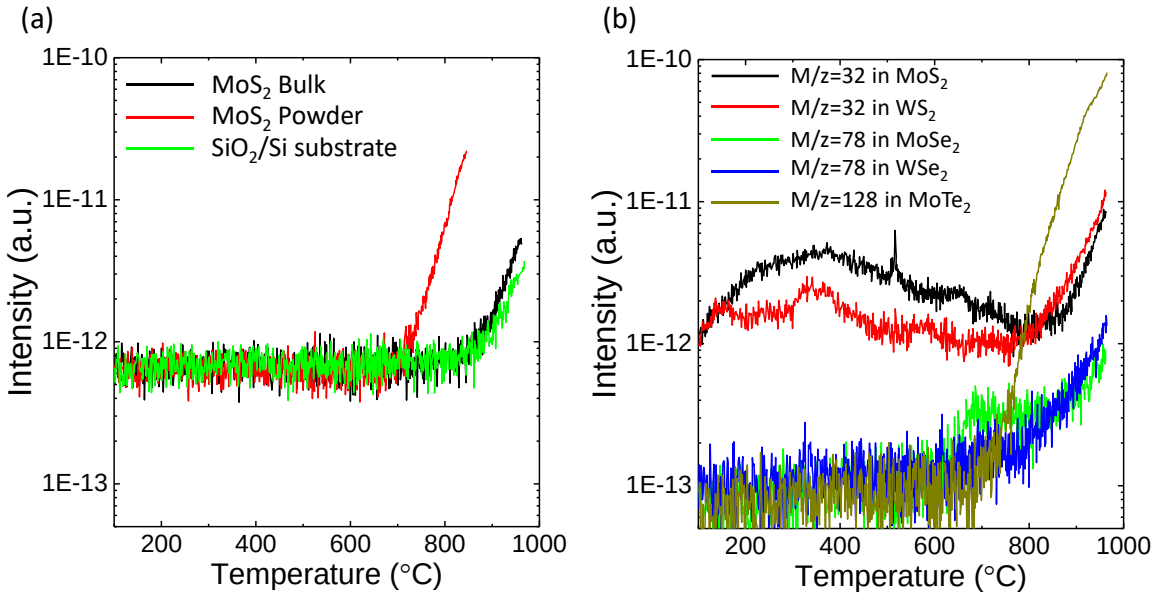

Fig. S2 (a) Comparison of TDS spectra of M/z = 32 for MoS_2 flakes and MoS_2 powder in the second annealing. (b) Comparison of TDS spectra of M/z = 32 for MoS_2 and WS_2, M/z = 78 for $MoSe_2$ and WSe_2, M/z = 128 for $MoTe_2$ in the first annealing.

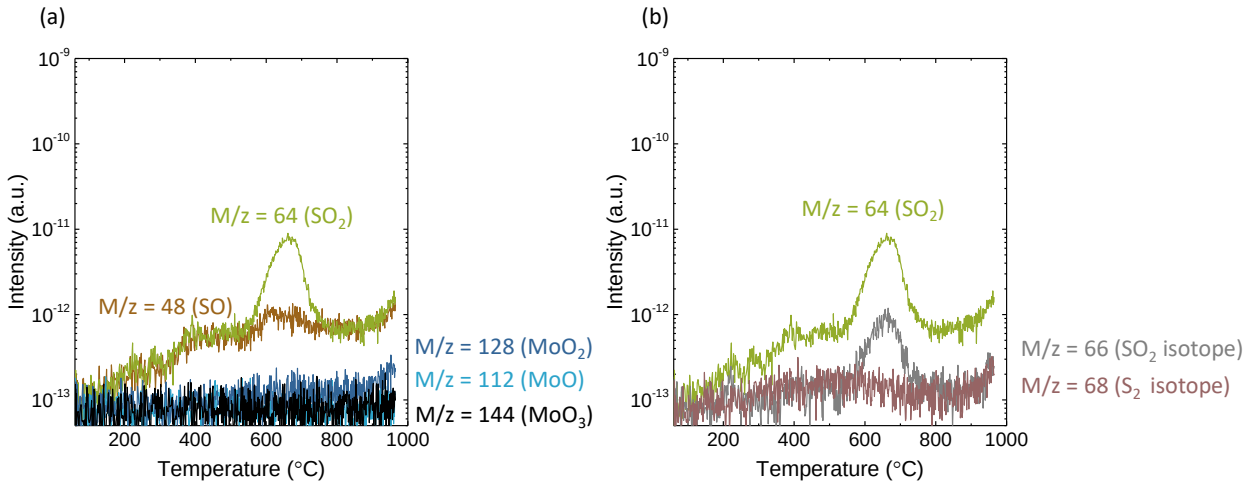

Fig. S3 (a) TDS spectra for bulk MoS_2 repeated for the detection of SO (M/z = 48) and SO_2 (M/z = 64). The Mo oxides including MoO_2 (M/z = 128), MoO (M/z = 112) and MoO_3 (M/z = 144) are included to exclude the desorption from Mo oxides. (b) TDS spectra for the identification of SO_2 desorption by monitoring the desorption signals include sulfur isotopes (M/z = 66 and M/z = 68).

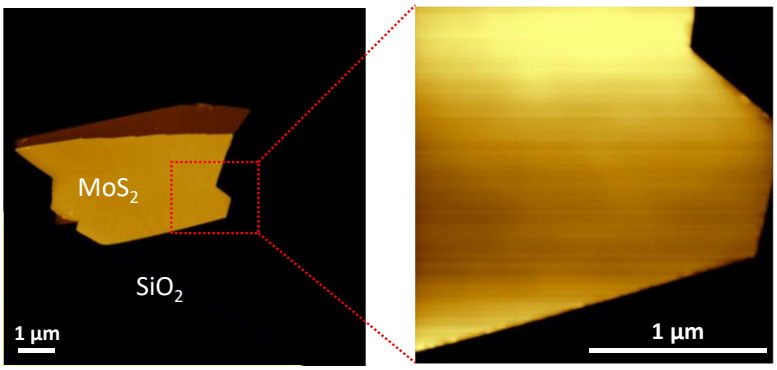

Fig. S4 AFM images for bulk MoS_2 (52 nm) annealed up to 835 °C in the TDS chamber without ALD. No defects can be observed due to the limited resolution of the AFM apparatus.

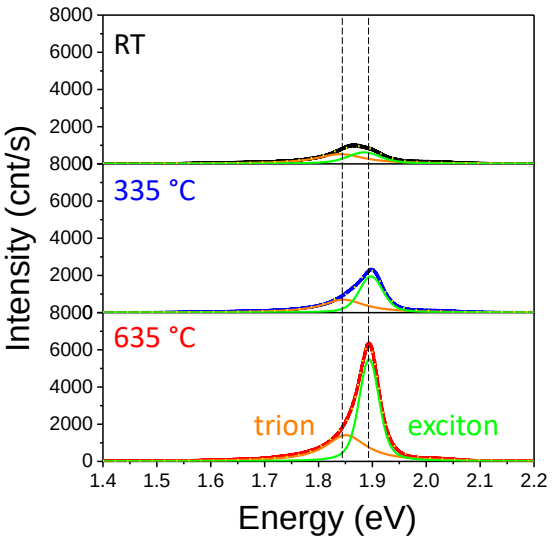

Fig. S5 Deconvolution of PL spectra at different temperatures in **Fig. 4a** to trion (orange) and exciton (green) by Voigt function.