Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Effects of growth substrate on the nucleation of monolayer $MoTe_2$

*David J. Hynek, Raivat M. Singhania, James Hart, Benjamin Davis, Mengjing Wang, Nicholas C. Strandwitz, and Judy J. Cha**

Supplementary Figures:

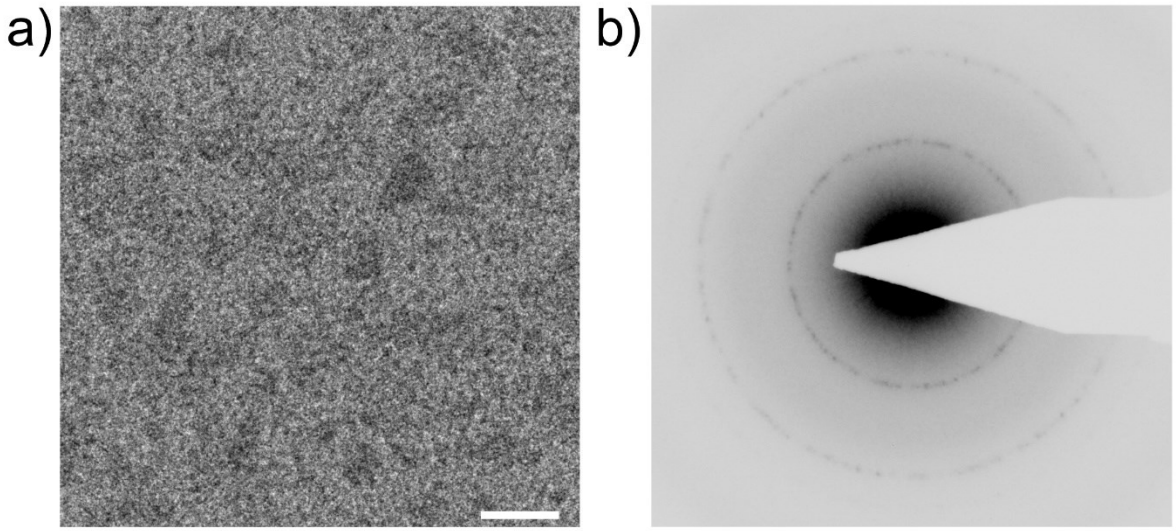

Figure S1: Growth of monolayer $MoTe_2$ from 8 cycle-thick MoO_x. a) TEM image showing 2H monolayer $MoTe_2$ clusters (darker regions) grown on amorphous AlO_x substrate. Scale bar, 20 nm. **b)** Selected area electron diffraction (SAED) taken of (a) showing polycrystalline rings indicating growth of 2H $MoTe_2$.

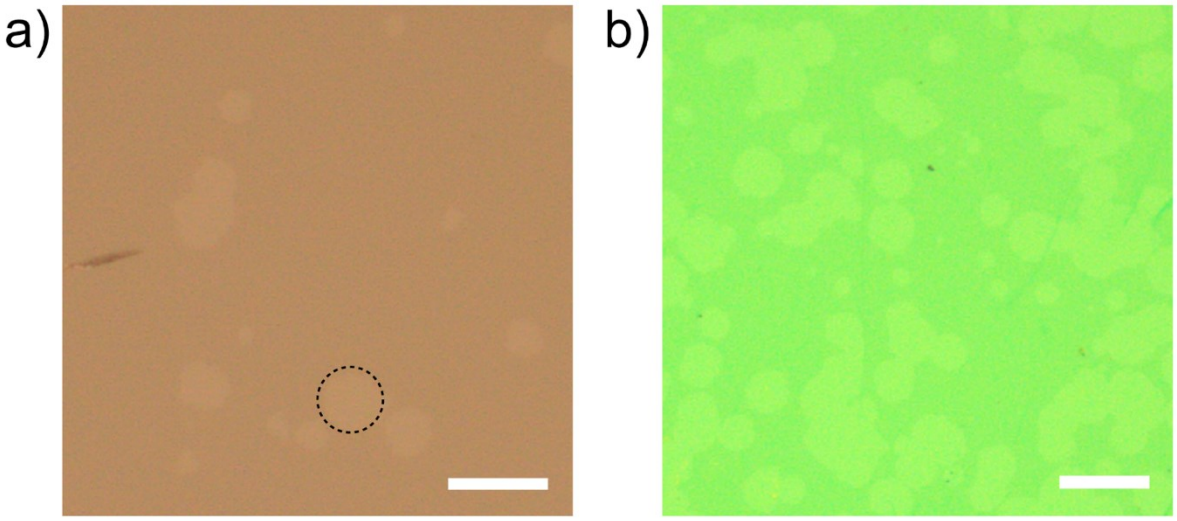

Figure S2: Optical contrast of the 2H and 1T′ phases of $MoTe_2$. Optical images of mixed 1T′/2H phase, 7-8 layer-thick $MoTe_2$ films grown on **a)** sapphire and **b)** SiO_2 at 600 °C. Scale bars are 10 μm and 50 μm respectively. Due to the optical contrast, individual 2H grains (lighter regions) can be tracked as they nucleate out of the initially formed 1T′ film (darker regions); for example, the dotted circle in **a)** encloses a 2H grain.

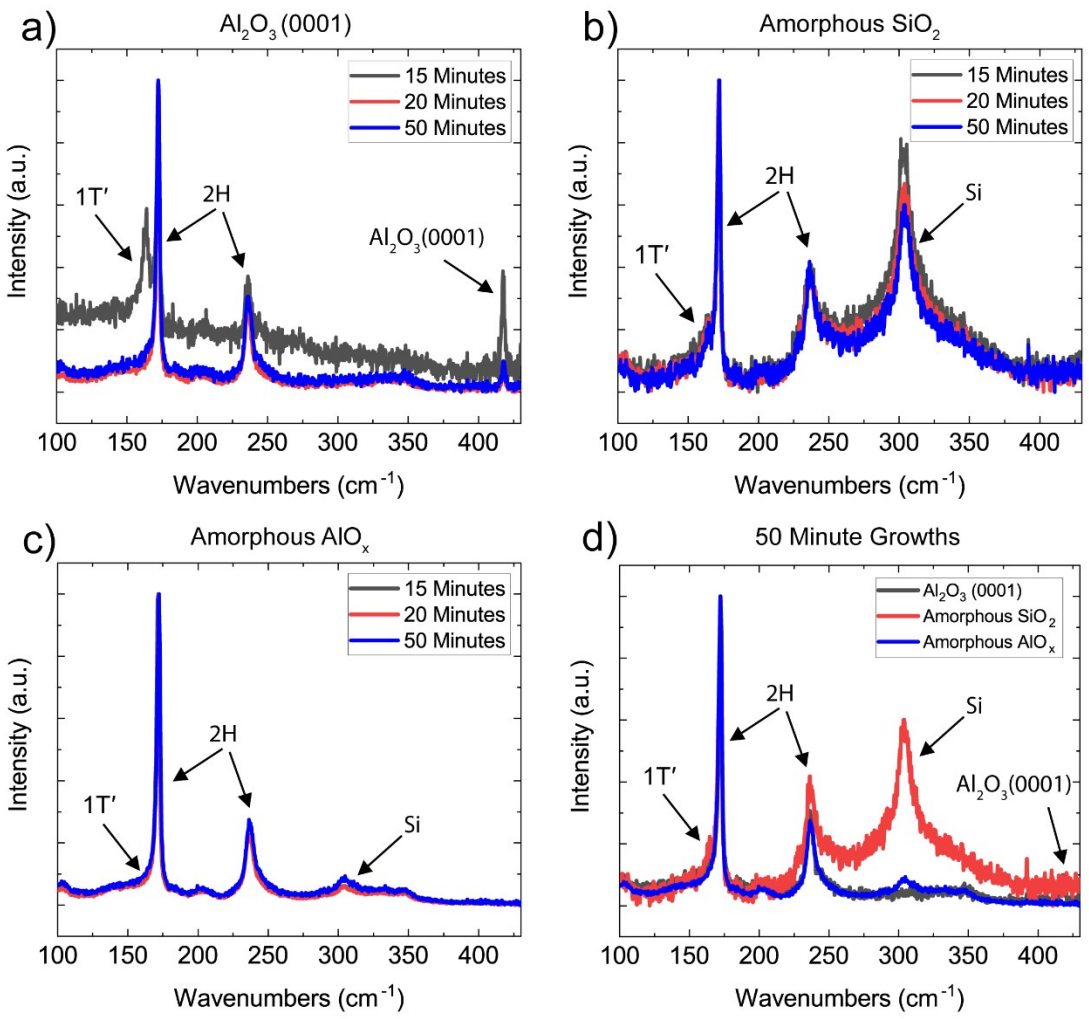

Figure S3: Raman spectroscopy characterization of $MoTe_2$ films converted on different substrates at varying reaction times. Raman spectra of $MoTe_2$ converted from 10 cycle-thick MoO_x deposited on Al_2O_3 (0001) **(a)**, amorphous SiO_2 **(b)**, and amorphous AlO_x **(c)**. Spectra were captured after three different time intervals for each sample: 15 minutes (black), 20 minutes (red), and 50 minutes (blue). Overlaid spectra from all three substrates after 50 minutes of growth are shown in **(d)**.

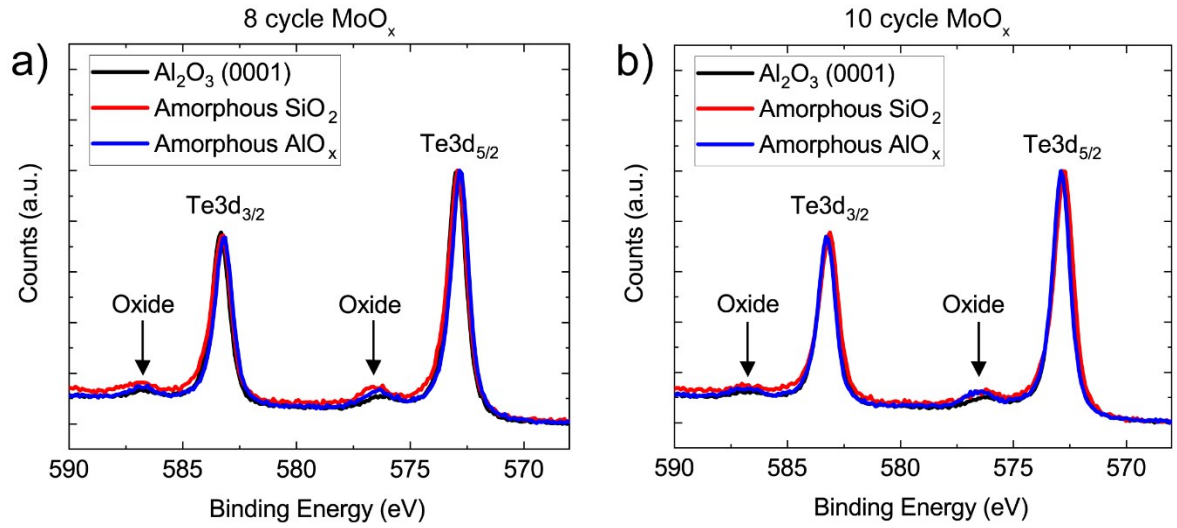

Figure S4: XPS analysis of Te 3*d* peaks in $MoTe_2$ films converted on different substrates at varying reaction times. XPS of Te 3*d* peaks in $MoTe_2$ films converted from 8 **(a)** and 10 **(b)** cycle-thick MoO_x deposited on Al_2O_3 (0001) (black), amorphous SiO_2 (red), and amorphous AlO_x (blue). Spectra were captured after 50 minutes of total tellurization time at 600 °C for all films.

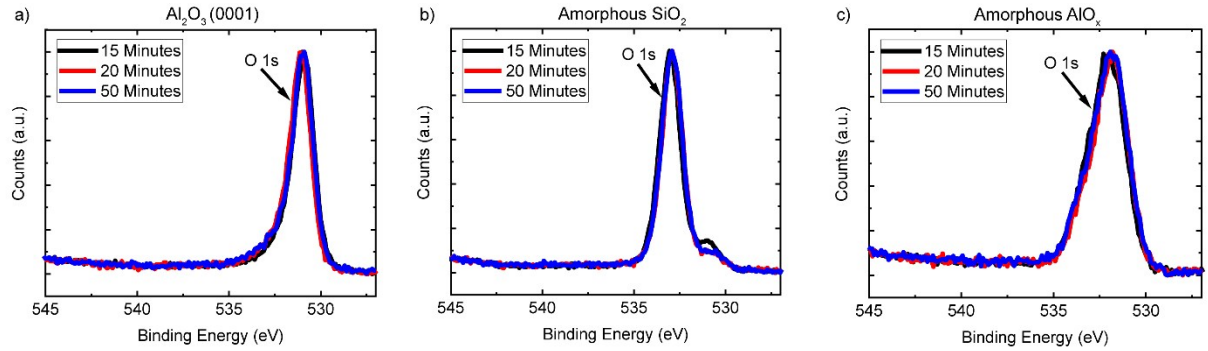

Figure S5: XPS analysis of O 1s peaks in $MoTe_2$ films converted on different substrates at varying reaction times. XPS of O 1s peaks in $MoTe_2$ films converted from 8 cycle-thick MoO_x deposited on Al_2O_3 (0001) (a), amorphous SiO_2 (b), and amorphous AlO_x (c). Spectra were captured after three different time intervals for each sample: 15 minutes (black), 20 minutes (red), and 50 minutes (blue).

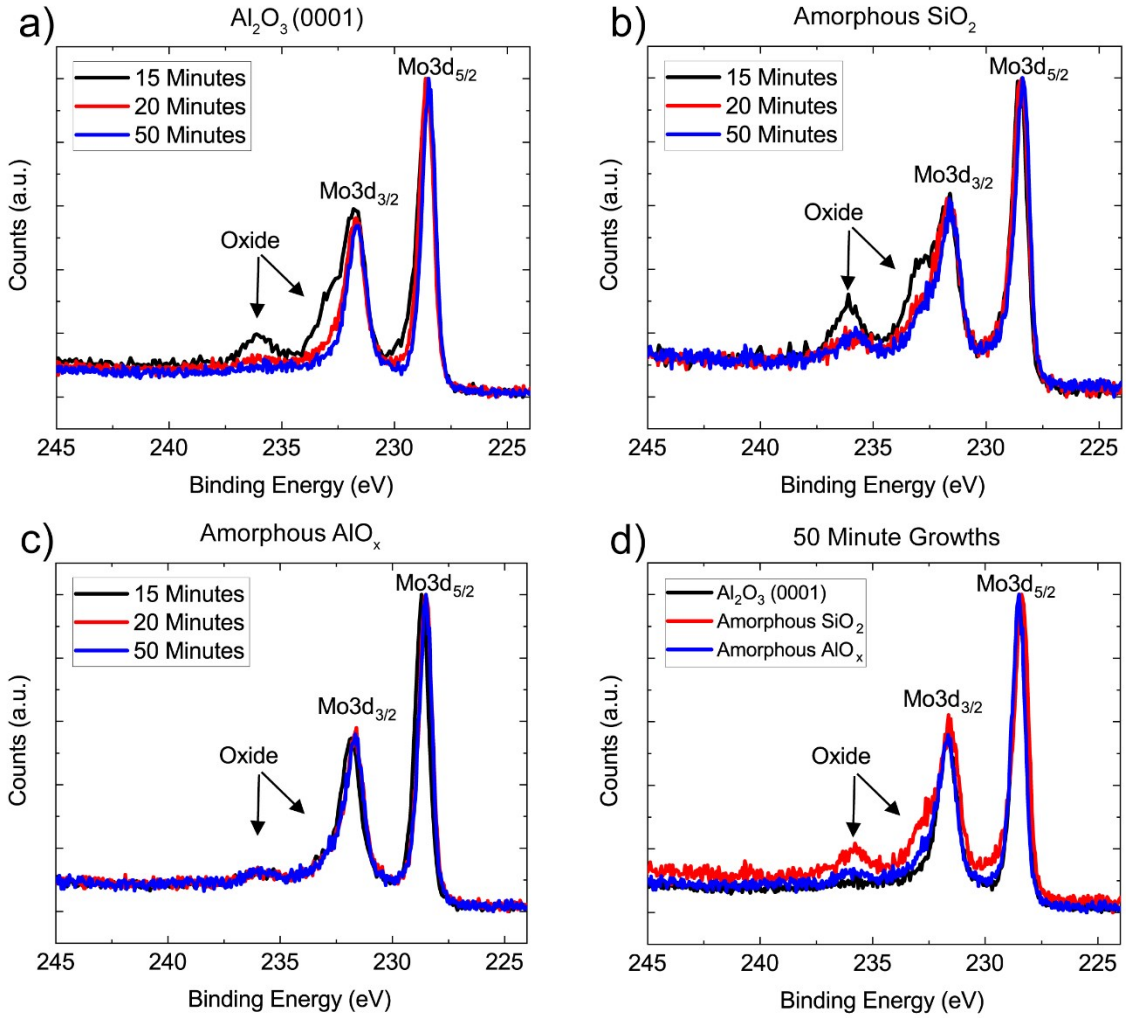

Figure S6: XPS analysis of Mo 3*d* peaks in $MoTe_2$ films converted on different substrates at varying reaction times. XPS of Mo 3*d* peaks in $MoTe_2$ films converted from 10 cycle-thick MoO_x deposited on Al_2O_3 (0001) **(a)**, amorphous SiO_2 **(b)**, and amorphous AlO_x **(c)**. Spectra were captured after three different time intervals for each sample: 15 minutes (black), 20 minutes (red), and 50 minutes (blue). Overlaid spectra from all three substrates after 50 minutes of growth are shown in **(d)**.

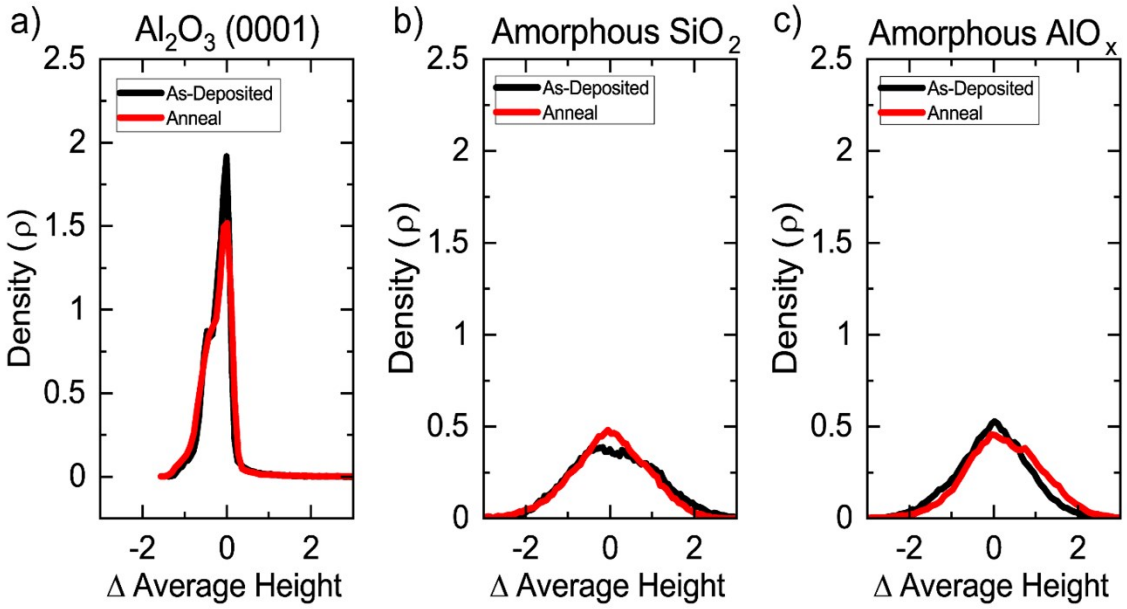

Figure S7: Effects of H_2 annealing on surface morphology of ALD deposited MoO_x films. 10 μm^2 AFM scans were taken on MoO_x films deposited on **(a)** Al_2O_3 (0001), **(b)** amorphous SiO_2, and **(c)** amorphous AlO_x substrates before (black) and after annealing under an H_2/Ar environment for 5 minutes at 600 °C (red).

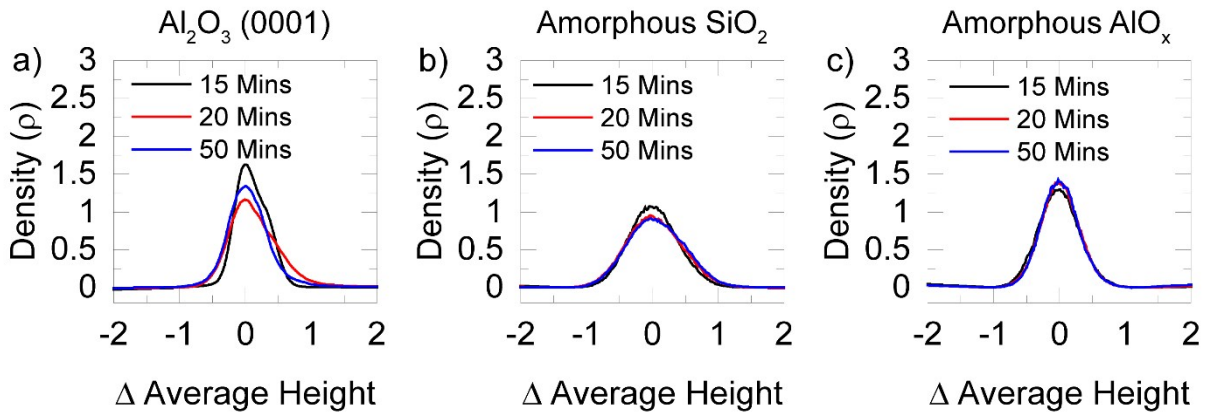

Figure S8: AFM characterization of $MoTe_2$ films converted on different substrates at varying reaction times. AFM height distributions of $MoTe_2$ converted from 10 cycle-thick MoO_x deposited on Al_2O_3 (0001) **(a)**, amorphous SiO_2 **(b)**, and amorphous AlO_x **(c)** at different reaction times. Height profiles for the three substrates were obtained by averaging the height distributions of four AFM images taken from each sample, 8 μm distance from one another after each time interval: 15 minutes (black), 20 minutes (red), and 50 minutes (blue).