Supporting Information

## Nanoscale Investigation of Defects and Oxidation of HfSe<sub>2</sub>

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Figure S1. STM topography images of two different regions across the sample. (a) in Location I; (b) in Location II. The image size is 100 nm  $\times$  100 nm, sample bias voltage is -0.4 V and tunnel current is 0.6 nA.



Figure S2. STM topography images of three different TMD surfaces, obtained by the same scanning tunneling microscopy settings. The image size is 100 nm  $\times$  100 nm, sample bias voltage is -0.3 V and tunnel current is 0.6 nA.



Figure S3. Height of the depression for dark defects. Panel (a): three different positions, marked by the blue, red, and black rings. The heights are 0.3, 0.5, and 0.8nm, respectively. Panel (b): The exact height of the same dim dark defect marked by the dashed red contour, depends on the sample bias voltage.



Figure S4. The three types of dark defects. (a) STM topography image of  $HfSe_2$  surface, the image size is 40 nm × 40 nm, sample bias voltage is -0.4 V and tunnel current is 0.6 nA. The three types of defects, marked by the blue, black, and green contours, are corresponding to the dim dark defect, less dark defects and very dark defects, respectively; (b) The depth and size of the defect marked by the dashed white line; (c) Depth of the dark defects from (a); (d) Size of the dark defects from (a).



Figure S5. dI/dV spectra of the bright defect in Figure 1f, the dark defect in Figure 1e and the pristine surface.



Figure S6. (a) STM topography image for the dI/dV maps shown in Figure 2b and Figure 3; (b) corresponding grid *I-V* map recorded simultaneously with (a), under  $V_s$ = -0.78 V.