Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Atomic defects in monolayer ordered double transition metals carbide ($Mo_2TiC_2T_x$) MXene and CO_2 Activation

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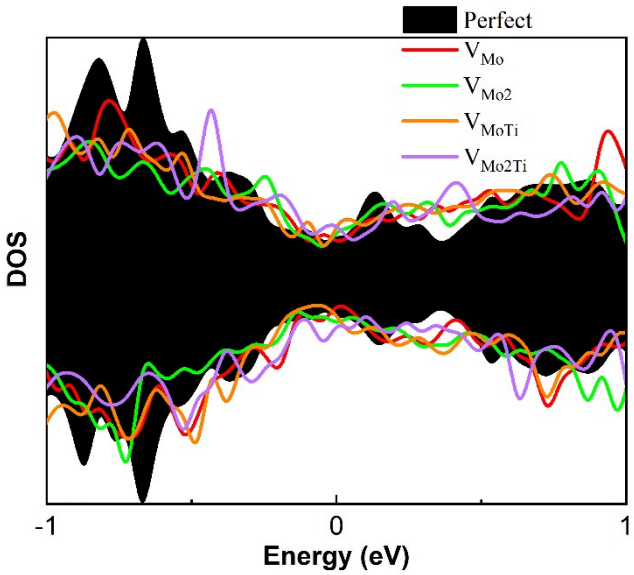

Fig. S1 Calculated total density of states (DOS) of perfect and defected Mo_2TiC_2 MXene.

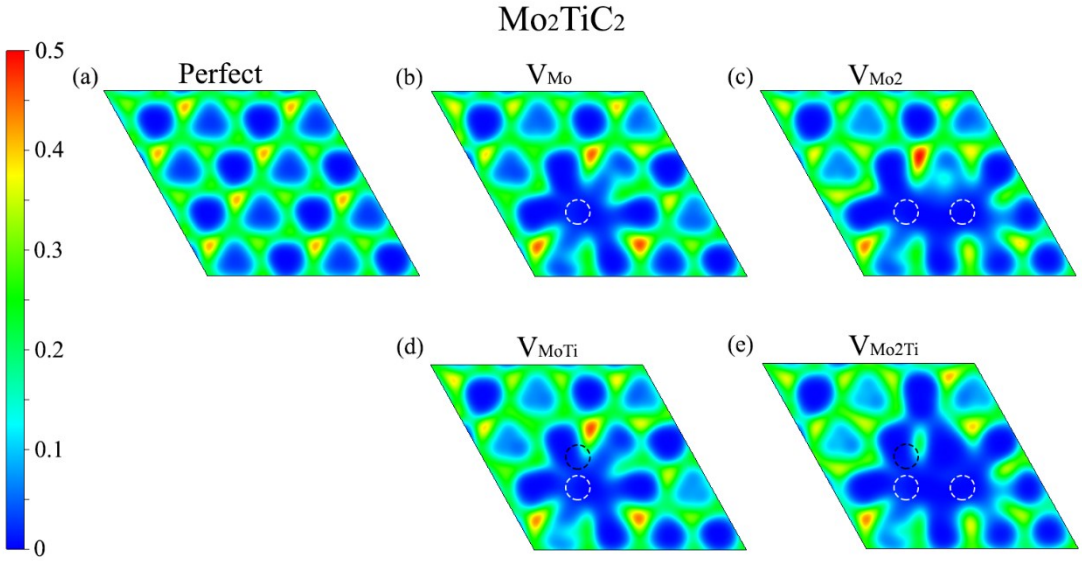

Fig. S2 Electron localization function (ELF) on the plane perpendicular to the *c*-axis at the close distance on top of surface terminations of the defected Mo_2TiC_2 MXenes. Dash circle lines highlight the place of the removed atoms.

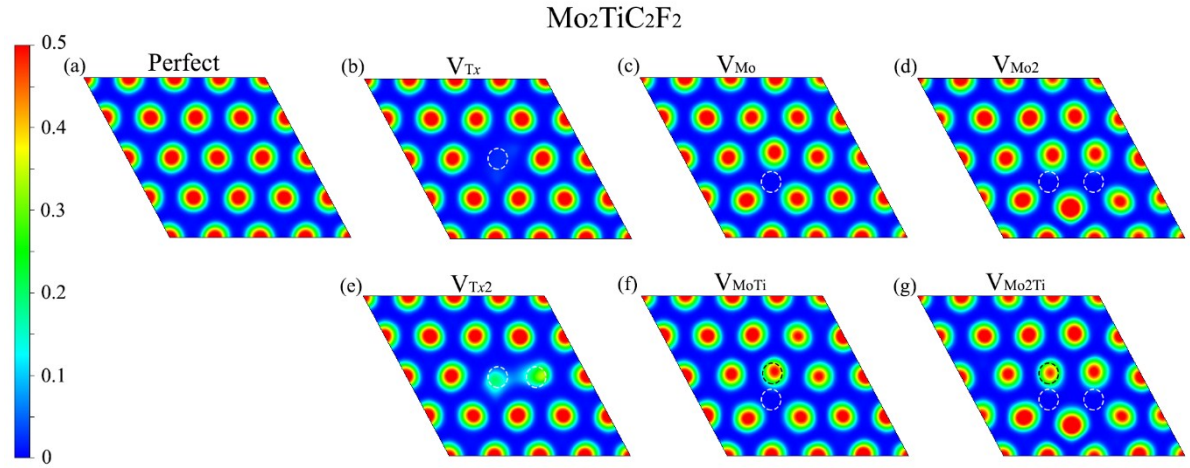

Fig. S3 Electron localization function (ELF) on the plane perpendicular to the *c*-axis at the close distance on top of surface terminations of the defected $Mo_2TiC_2F_2$ MXenes. Dash circle lines highlight the place of the removed atoms.

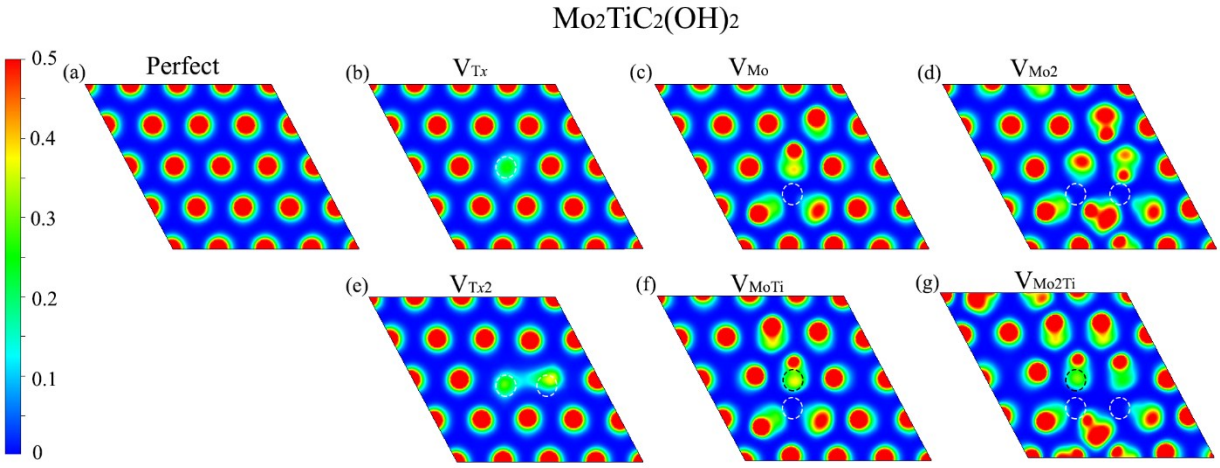

Fig. S4 Electron localization function (ELF) on the plane perpendicular to the *c*-axis at the close distance on top of surface terminations of the defected $Mo_2TiC_2(OH)_2$ MXenes. Dash circle lines highlight the place of the removed atoms.

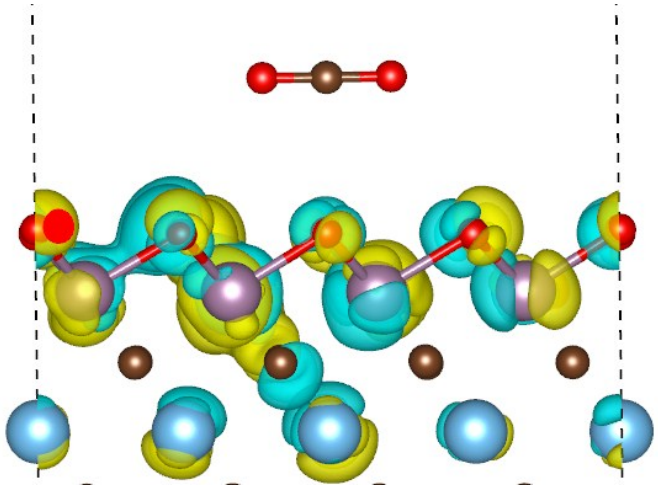

Fig. S5 Electronic density difference plot of CO_2 adsorption structures on MXene-V_{Tx} surface, showing no charge transfer in the regions between the CO_2 and the surface atoms since the molecule is not chemisorbed.