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Online Supporting Information for

Shifting and Breaking Scaling Relations at Transition Metal Telluride Edges for Selective Electrochemical CO_2 Reduction

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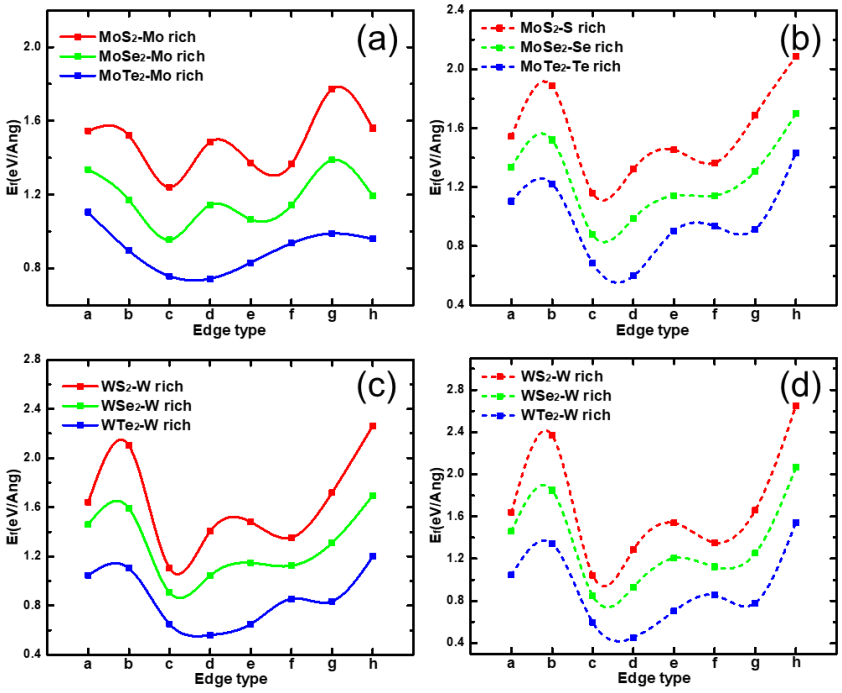

Fig. S1 Comparison of the formation energies for the edges under different chemical environments. (a) MoS_2, $MoSe_2$, and $MoTe_2$ in the Mo-rich condition, (b) MoS_2, $MoSe_2$, and $MoTe_2$ in the X-rich condition, (c) WS_2, WSe_2, and WTe_2 in the W-rich condition, and (d) WS_2, WSe_2, and WTe_2 in the X-rich condition.

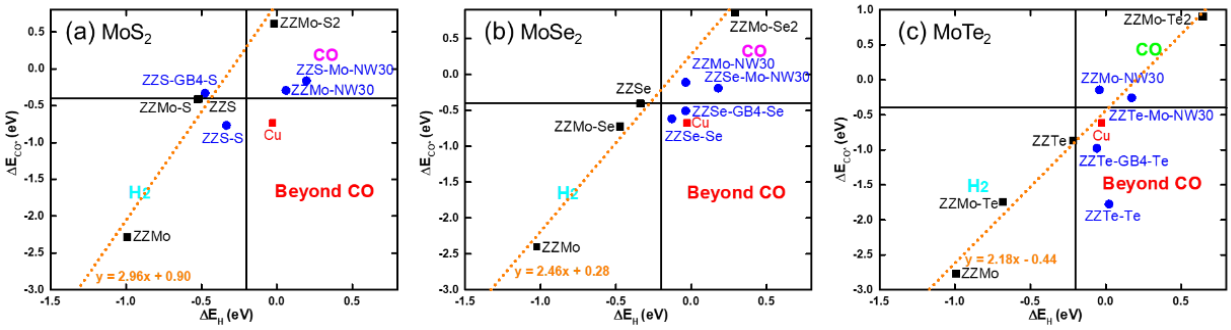

Fig. S2 The CO and H binding energies at the eight edges for (a) MoS_2, (b) $MoSe_2$, (c) $MoTe_2$, where the CO binding energies were computed by using the RPBE functional.

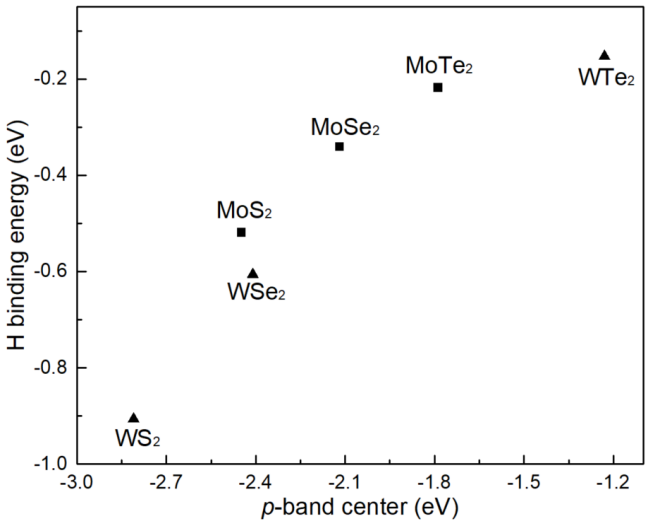

Fig. S3 The H binding energy and *p*-band center for the ZZX edge of six chemical compositions.

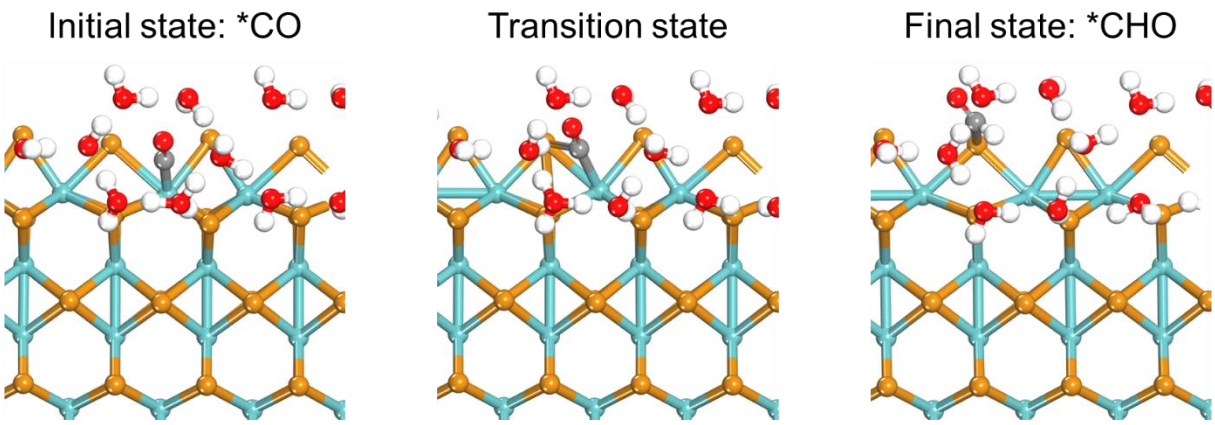

Fig. S4 The initial, transition, and final states for the proton-electron transfer to *CO to form *CHO at the ZZTe-GB4-Te edge of $MoTe_2$. Mo, cyan; Te, brown; C, grey; O, red; H, white.

Table S1 The zero-point energy (ZPE) and entropy (TS) of reaction intermediates and free molecules for CO_2 reduction and HER at the ZZTe-GB4-Te edge.

	ZPE (eV)	**-TS (eV)**
CO_2	0.31	-0.66
COOH*	0.63	-0.22
H_2	0.28	-0.40
H_2O	0.57	-0.67
CO*	0.21	-0.07
CHO*	0.47	-0.18
CH_2O	0.71	-0.68
CH_2OH*	1.11	-0.19
CH_3OH	1.37	-0.81
CH_2*	0.68	-0.05
CH_3*	0.98	-0.11
CH_4	1.20	-0.58
H*	0.23	-0.01