Supporting information

Unveiling the mechanism of thermal catalytic oxidation HCHO from kiln exhaust gas by Sc-decorated Cr2CO2-MXene

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Table S1 The different adsorption site and energy of the Sc/Cr_2CO_2.

	Fcc	Hcp	Top
E_{ads}	-393.40	-393.33	-393.03

Table S2 The O_2 adsorption energies (E_{ads}) of Sc atom on the pristine and defective Cr_2CO_2 at different temperatures.

	$O2_{ads}$	O2+MXene	E_{ads}
298K	-404.88	(-9.27)+(-393.40)=-402.67	-2.21
448K	-406.74	(-9.27)+(-393.58)=-402.85	-3.89

Table S3 The HCHO adsorption energies (E_{ads}) of Sc atom on the pristine and defective Cr_2CO_2 at different temperatures.

	$HCHO_{ads}$	HCHO+MXene	E_{ads}
298K	-416.64	(-22.15) + (-393.40) = -415.56	-1.08
448K	-418.10	(-22.15) + (-393.58) = -415.74	-2.36

Table S4 The O_2 and HCHO co-adsorption energies (E_{ads}) of Sc atom on the pristine and defective Cr_2CO_2 at different temperatures.

	$(O_2+HCHO)_{ads}$	O_2	HCHO	MXene	E_{ads}
298K	-427.82	-8.16	-22.03	-393.36	-4.27
448K	-429.31	-8.16	-22.03	-390.59	-8.53

Table S5 The Gibbs free energy of HCHO oxidation step by ER path.

298K	**$E_{OSZICAR}$**	**ΔG(T)**	**G**
IS	-427.57981	0.012069	-427.567741
MS1	-427.57981	0.012069	-427.567741
MS2	-430.33246	0.527995	-429.804465
MS3	-429.39837	0.639147	-428.759223
MS4	-431.69418	0.850447	-430.843733
FS	-430.61894	0.807055	-429.811885

448K	**$E_{OSZICAR}$**	**ΔG(T)**	**G**
IS	-406.27919	-0.147076	-429.056066
MS1	-406.27919	-0.147076	-429.056066
MS2	-431.89099	0.185723	-431.705267
MS3	-430.81743	0.269499	-430.547931
MS4	-432.68295	0.639670	-432.043280
FS	-431.78008	0.373253	-431.406827

Table S6 The Gibbs free energy of HCHO oxidation step by LH path.

298K	**$E_{OSZICAR}$**	**ΔG(T)**	**G**
IS	-427.81517	0.698875	-427.116295
MS1	-428.36927	0.817818	-427.551452
MS2	-431.70028	0.750686	-430.949594
MS3	-432.39892	0.803076	-431.595844
MS4	-432.21402	0.778342	-430.843733
FS	-430.96599	0.696407	-430.269583

448K	**$E_{OSZICAR}$**	**ΔG(T)**	**G**
IS	-429.31078	0.366372	-428.944408
MS1	-429.35546	0.645282	-428.710178
MS2	-433.15537	0.436081	-432.719289
MS3	-433.44335	0.538733	-432.904617
MS4	-432.85121	0.700359	-432.150851
FS	-431.70910	0.567222	-431.141878

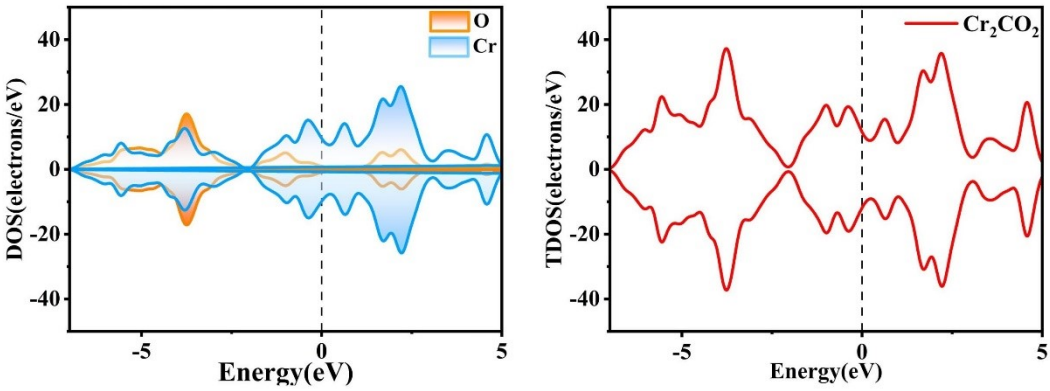

Fig. S1 Density of states for Cr_2CO_2-MXene.

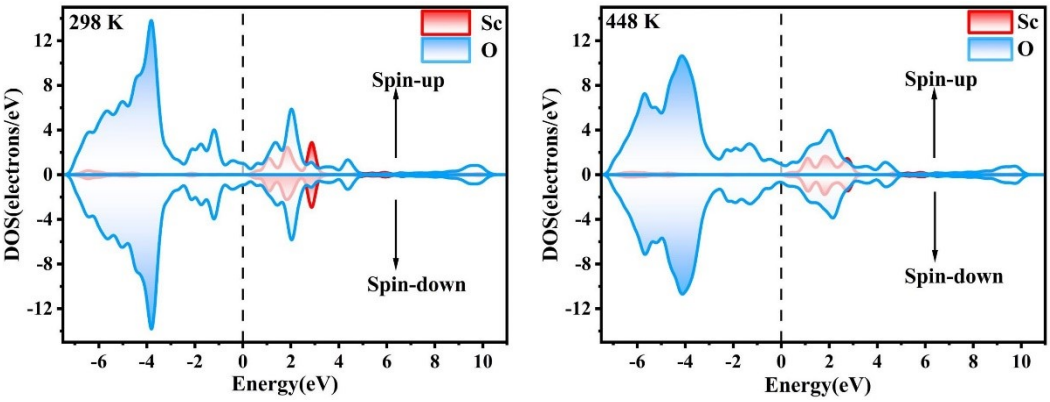

Fig. S2 Density of states for Sc/Cr_2CO_2-MXene.

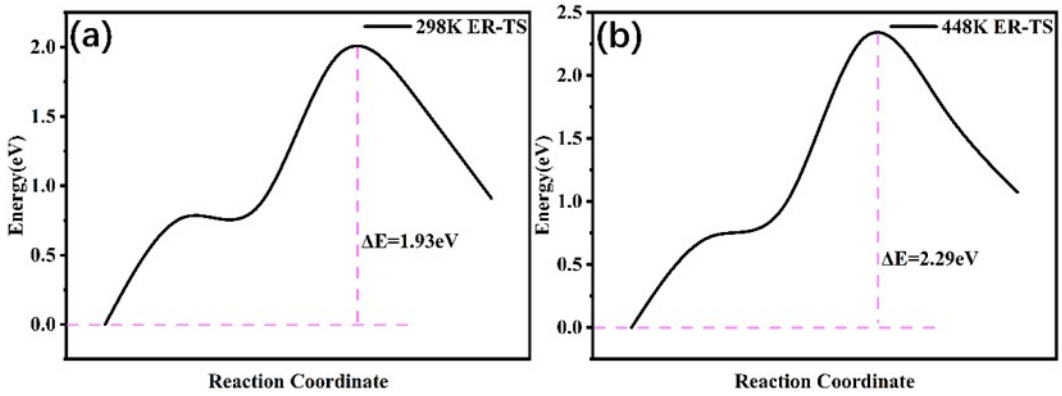

Fig.S3 Transition state search of ER path using CI-NEB method.

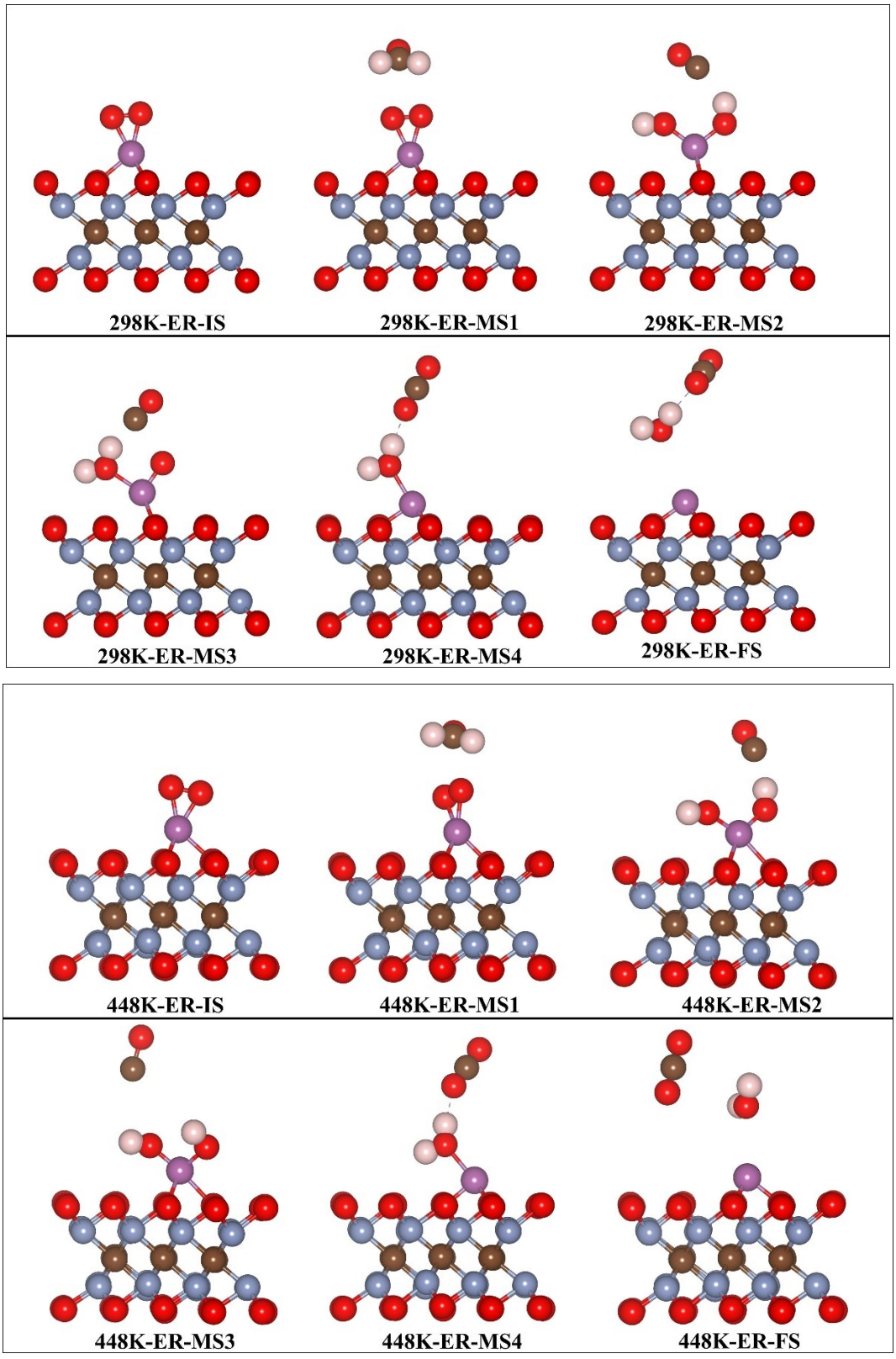

Fig.S4 The configuration of HCHO oxidation step by ER path.

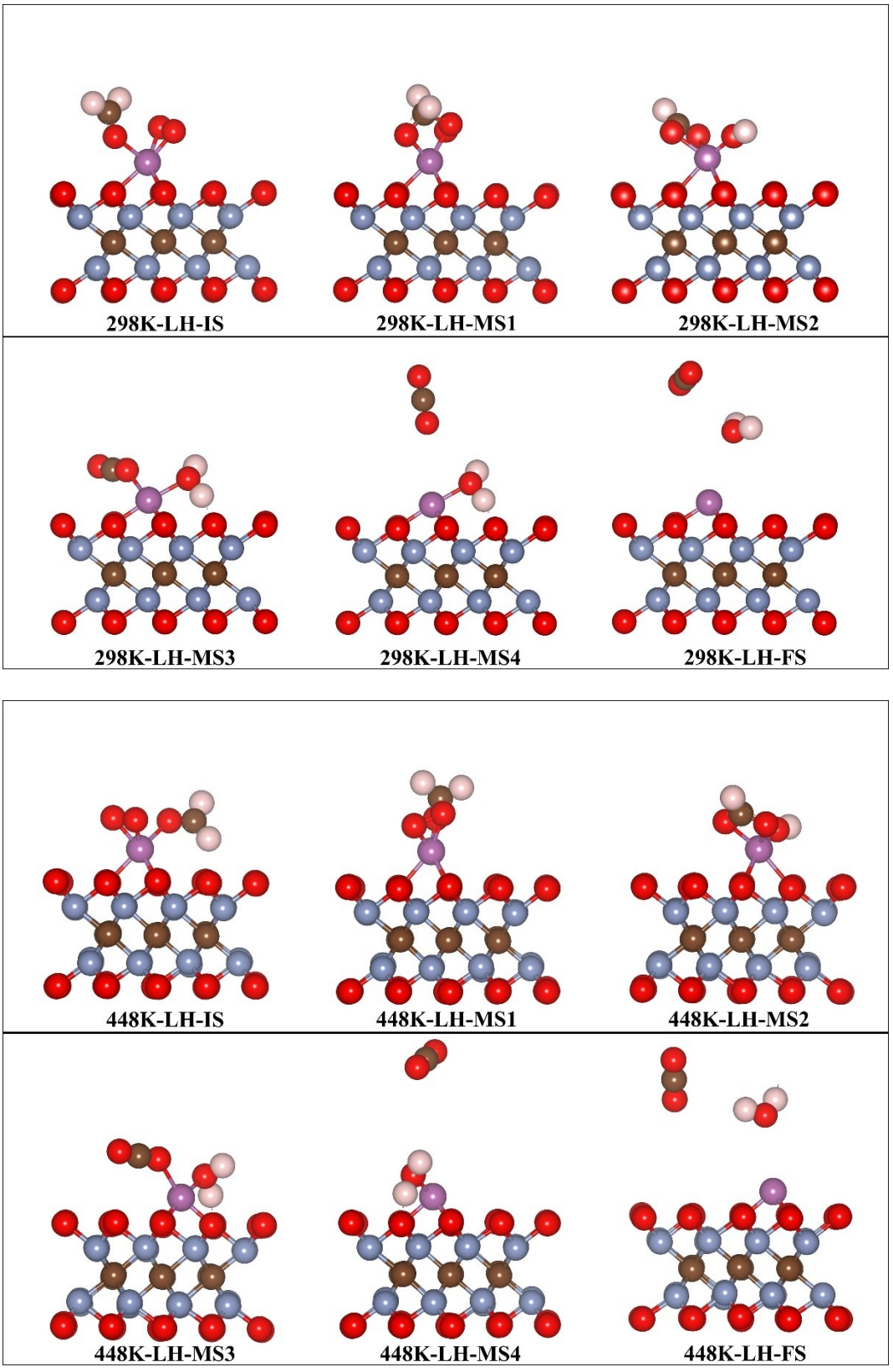

Fig.S5 The configuration of HCHO oxidation step by LH path.