Supplementary Materials for

H-Assisted CO_2 Dissociation on $Pd_nPt_{(4-n)}/In_2O_3$ Catalysts: A Density Functional Theory Study

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Table S1. Bader charge (δ) for the COOH-mediated channel on the $Pd_nPt_{(4-n)}/In_2O_3$ catalysts.

		Pt_4	$PdPt_3$	Pd_2Pt_2	Pd_3Pt	Pd_4
CO_2+H	cluster	-0.60	-0.70	-0.72	-0.65	-0.75
	*H	-0.04	0.05	0.06	0.07	0.08
	$*CO_2$	0.53	0.51	0.48	0.42	0.39
TS1	cluster	-0.41	-0.53	-0.50	-0.45	-0.51
	*H	-0.23	-0.25	-0.26	-0.28	-0.27
	$*CO_2$	0.57	0.57	0.55	0.51	0.56
trans-COOH	cluster	-0.35	-0.45	-0.45	-0.41	-0.48
	*COOH	0.19	0.20	0.17	0.15	0.21
TS2	cluster	-0.43	-0.49	-0.50	-0.46	-0.66
	*COOH	0.20	0.21	0.19	0.16	0.38
cis-COOH	cluster	-0.53	-0.54	-0.55	-0.52	-0.58
	*COOH	0.29	0.24	0.22	0.18	0.25
TS3	cluster	-0.48	-0.49	-0.53	-0.73	-0.89
	*CO+*OH	0.36	0.33	0.32	0.41	0.42
CO+OH	cluster	-0.97	-1.01	-1.05	-1.07	-1.17
	*CO+*OH	0.60	0.63	0.62	0.61	0.60

Table S2. Reaction barriers (E_b, eV) and energies (ΔE, eV) of the C-O bond cleavage processes on the In_2O_3 (110) surface.

	E_b	ΔE
R1	1.74	0.77
R2	0.34	-0.11
R3	2.93	2.49
R4	2.86	2.32
R5	2.05	1.21
R6	3.80	2.89

Table S3. Reaction barriers (E_b, eV) and energies (ΔE, eV) of the H-assisted CO_2 dissociation channels on the $Pd_nPt_{(4-n)}/In_2O_3$ catalysts considering the solvation effect.

	R1		*R2*		*R3*		*R4*		*R5*	
	E_b	ΔE	E_b	ΔE	E_b	ΔE	E_b	ΔE	E_b	ΔE
Pt_4	0.38	-0.18	0.58	0.18	2.24	-0.26	1.35	0.29	2.81	1.12
$PdPt_3$	0.67	-0.19	0.54	0.05	1.80	-0.34	0.94	-0.01	2.59	0.74
Pd_2Pt_2	0.66	0.18	0.45	0.11	1.75	-0.56	1.17	0.10	2.39	0.43
Pd_3Pt	0.67	0.16	0.45	0.07	0.90	-0.96	0.85	0.01	1.77	0.69
Pd_4	0.69	0.36	0.60	0.20	0.97	-0.92	1.00	0.24	2.13	0.55

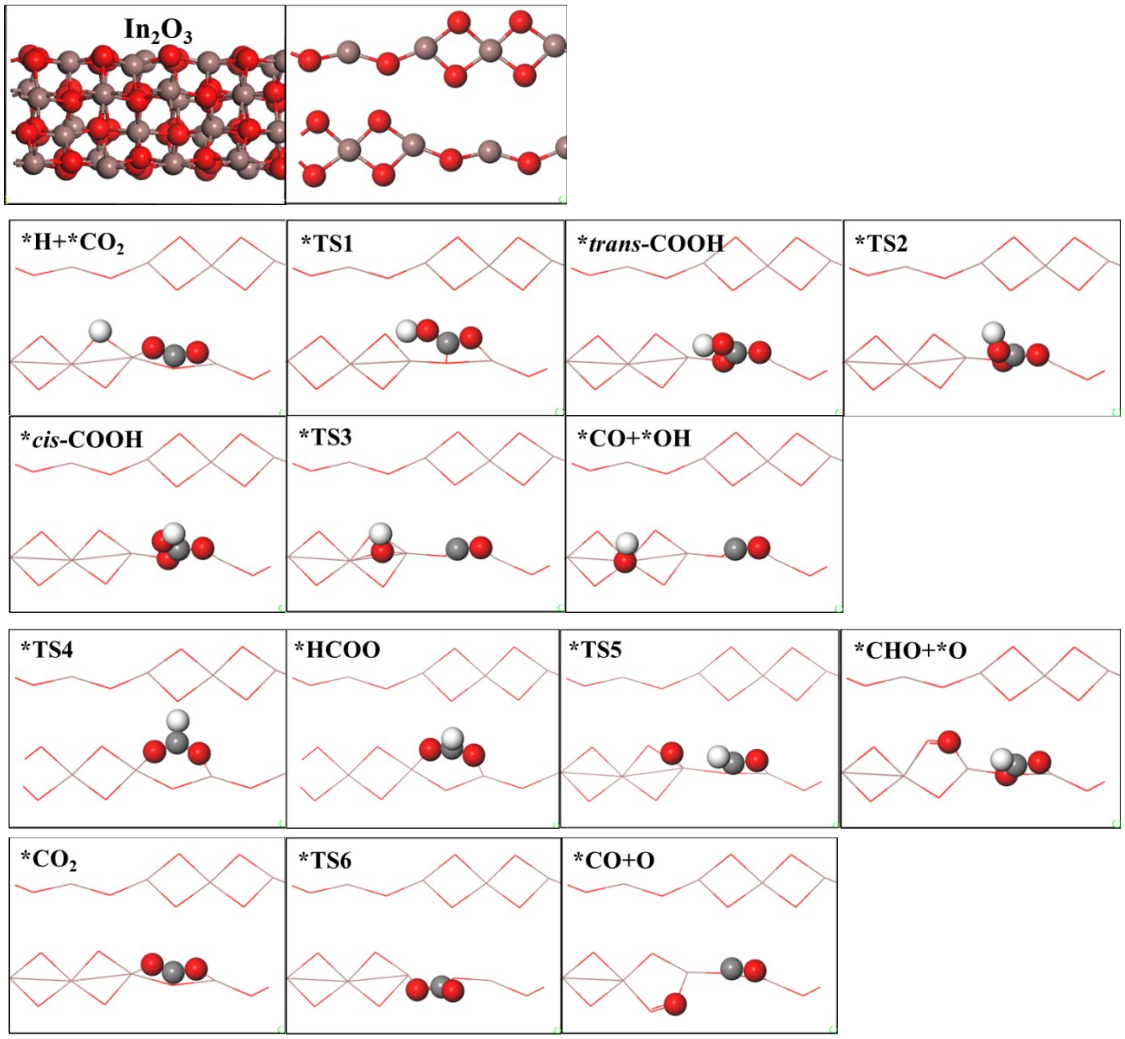

Fig. S1. Structures of the stationary points of the C-O cleavage channels on the In_2O_3 (110) surface.