Electronic Supplementary Information

Effects of oxygen vacancy formation energy and CO_2 hydrogenation activity in Pt-doped In_2O_3 catalysts

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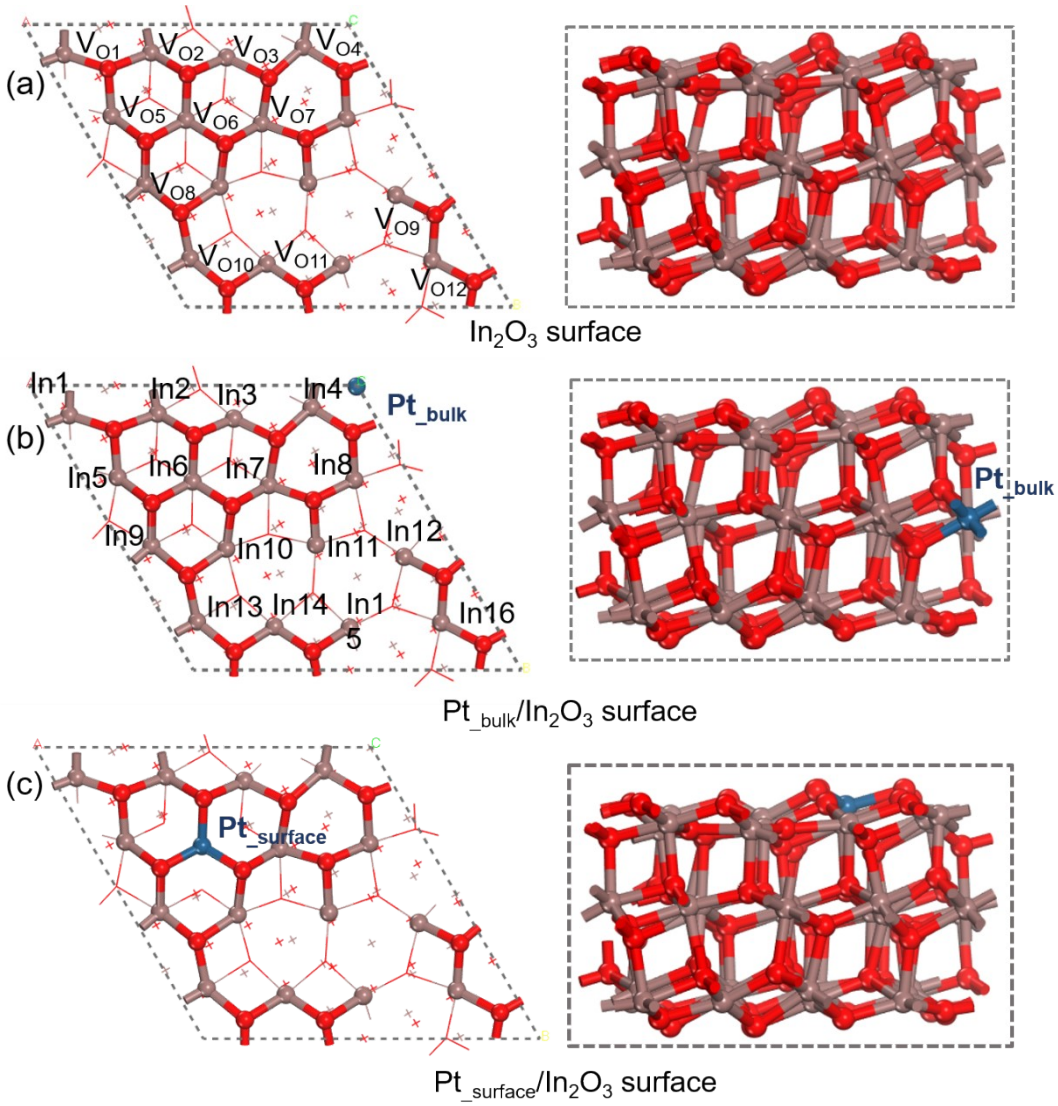

Fig. S1 Models of the (a) In_2O_3 (111), (b) $Pt_{\_bulk}/In_2O_3$ (111) surfaces and (c) $Pt_{\_surface}/In_2O_3$ (111).

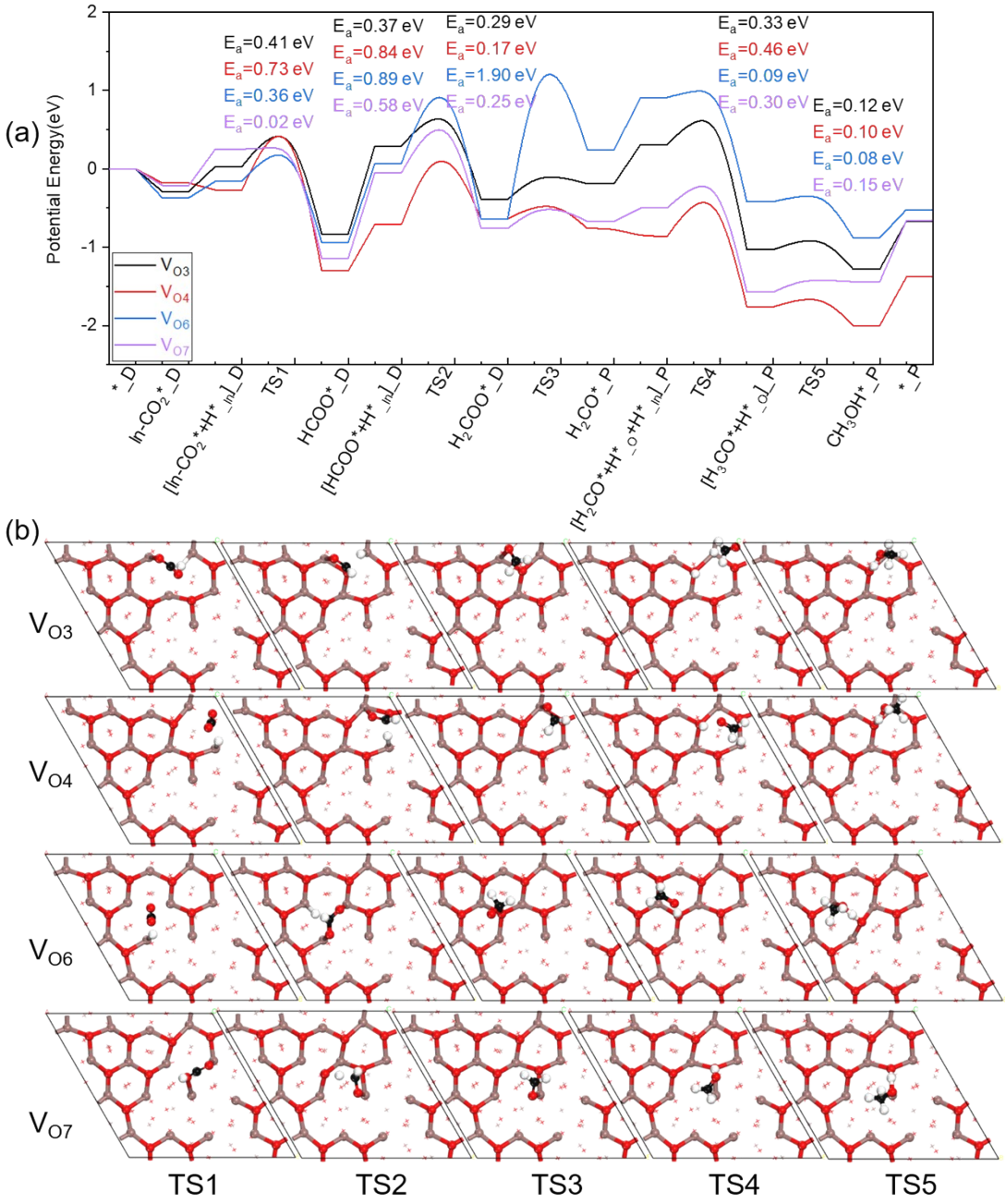

Fig. S2 (a) Energy profiles of CO_2 hydrogenation to methanol on In_2O_3 surface; (b) the structures of transition states. _D represents a defective surface, _P represents a perfect surface, and * represents the adsorption site.

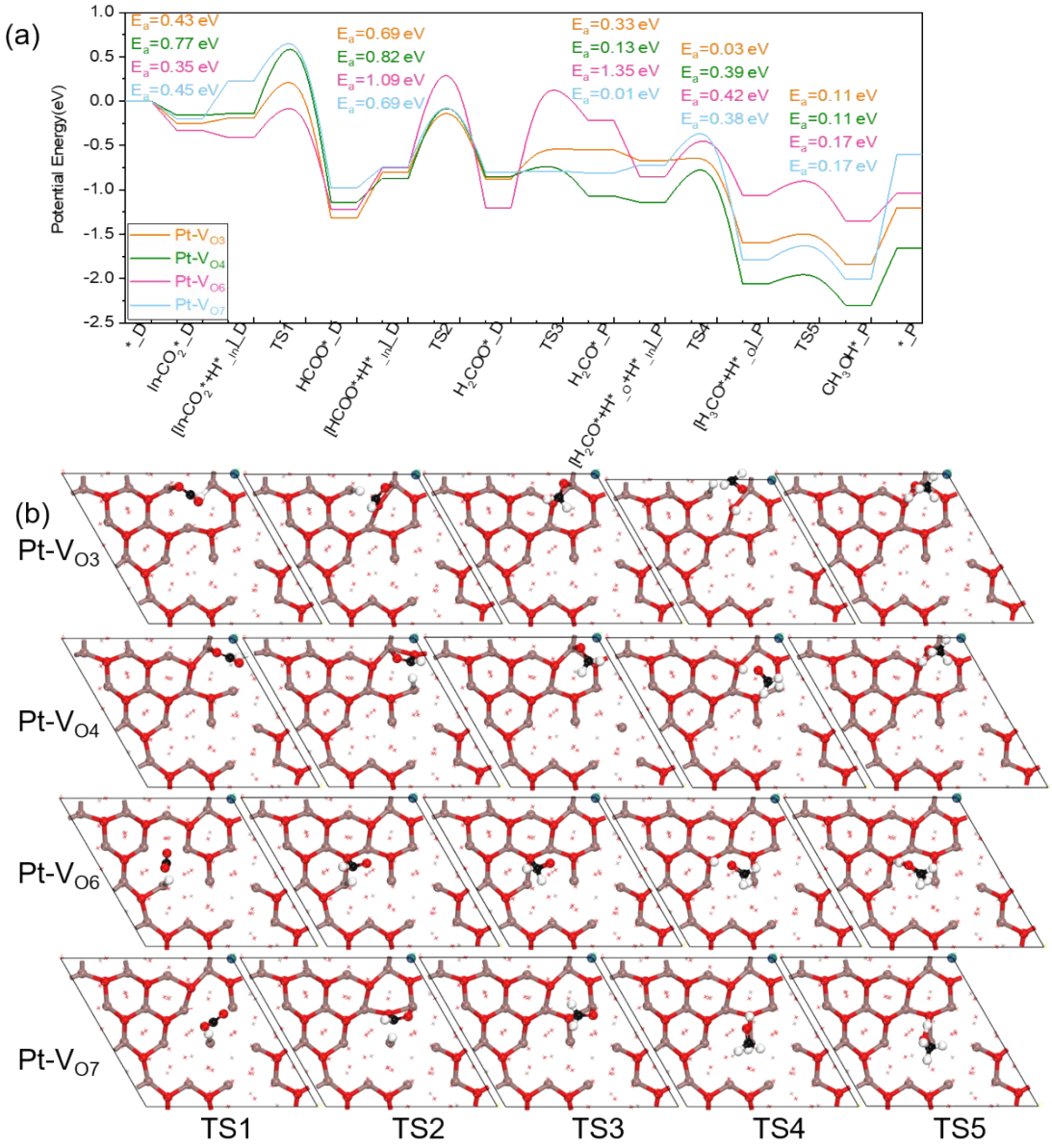

Fig. S3 (a) Energy profiles of CO_2 hydrogenation to methanol on Pt/In_2O_3 surface; (b) the structures of transition states.

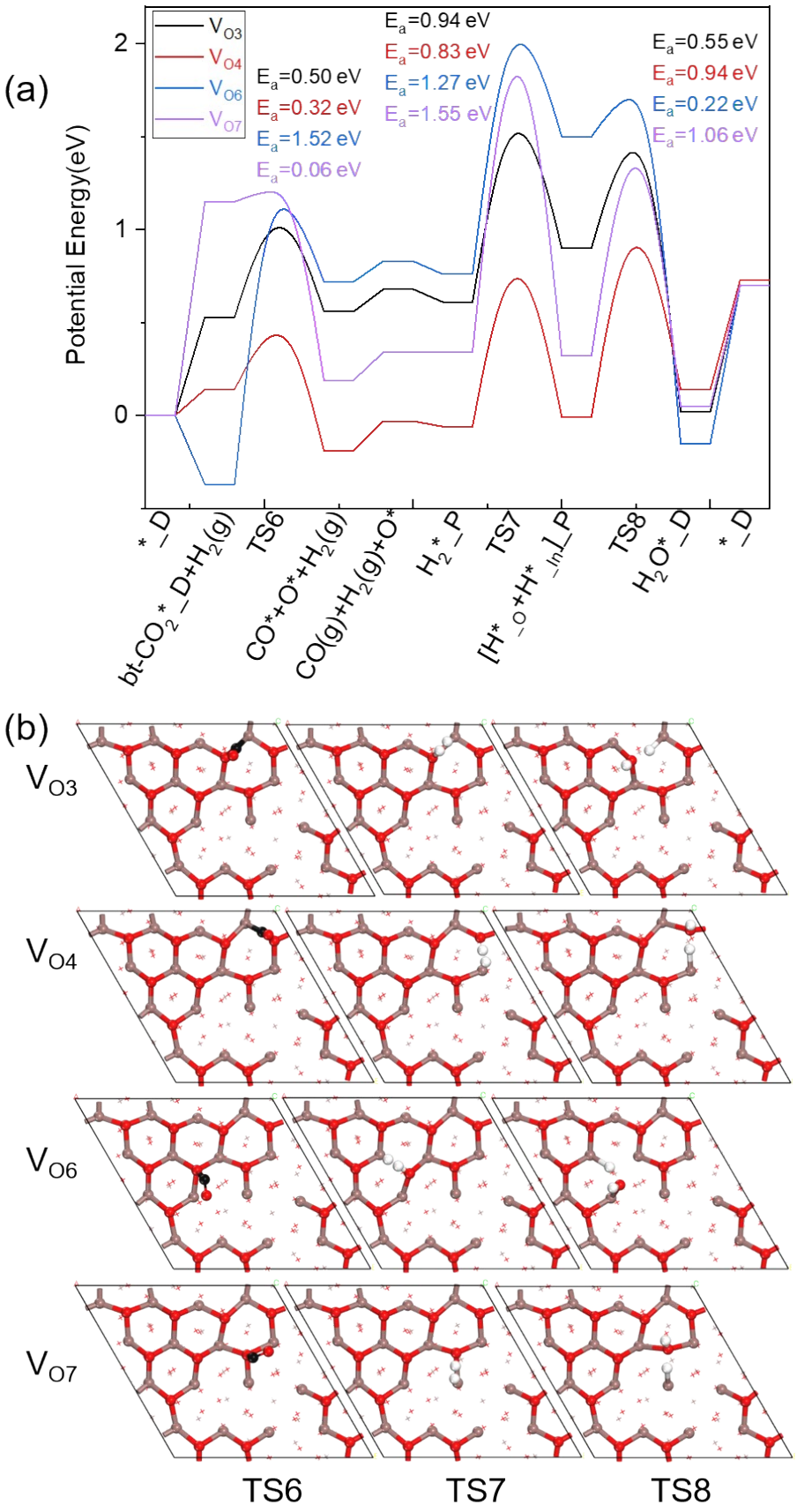

Fig. S4 (a) Energy profiles of RWGS on In_2O_3 surface; (b) the structures of transition states.

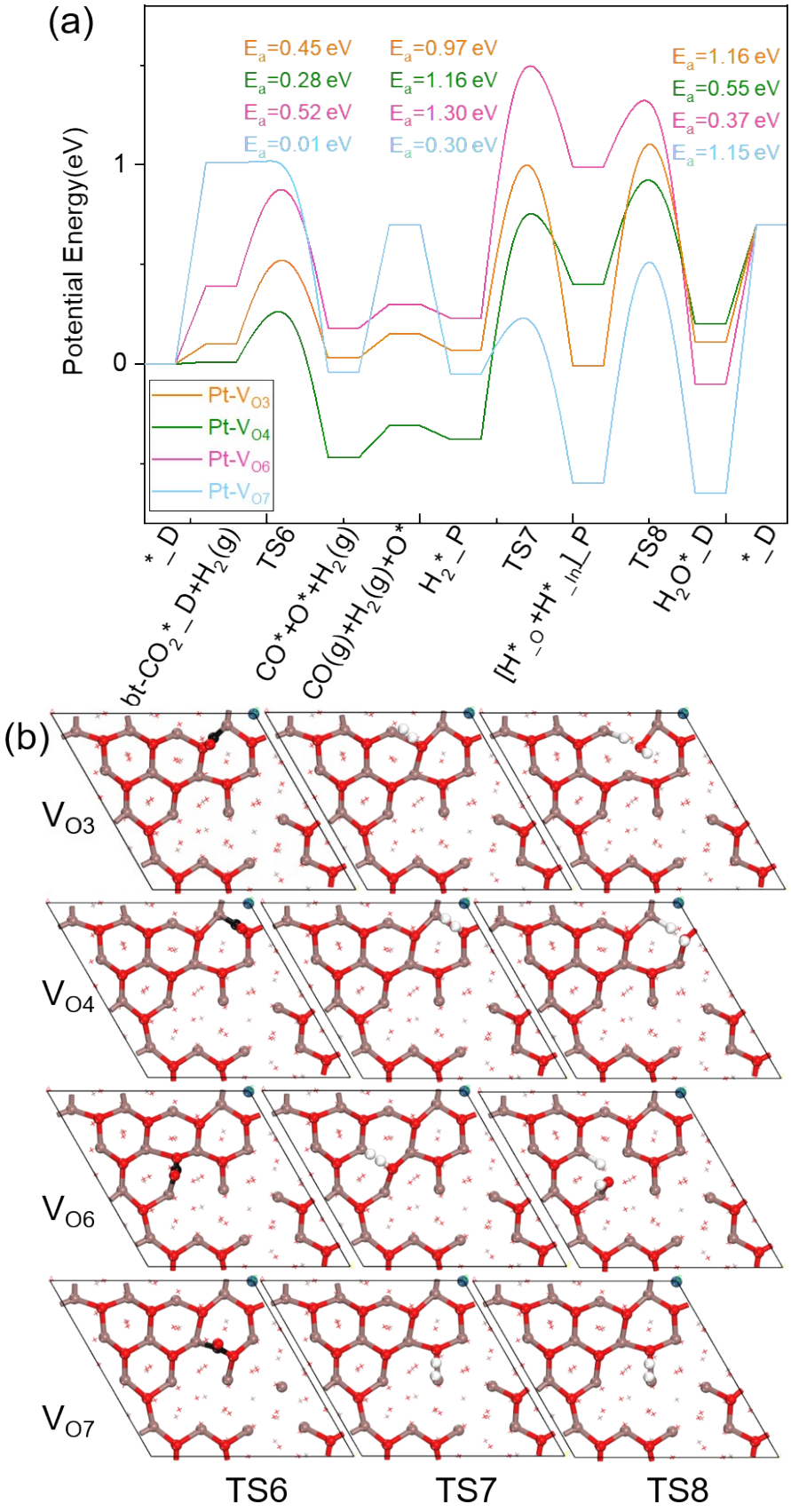

Fig. S5 (a) Energy profiles of RWGS on Pt/In_2O_3 surface; (b) the structures of transition states.

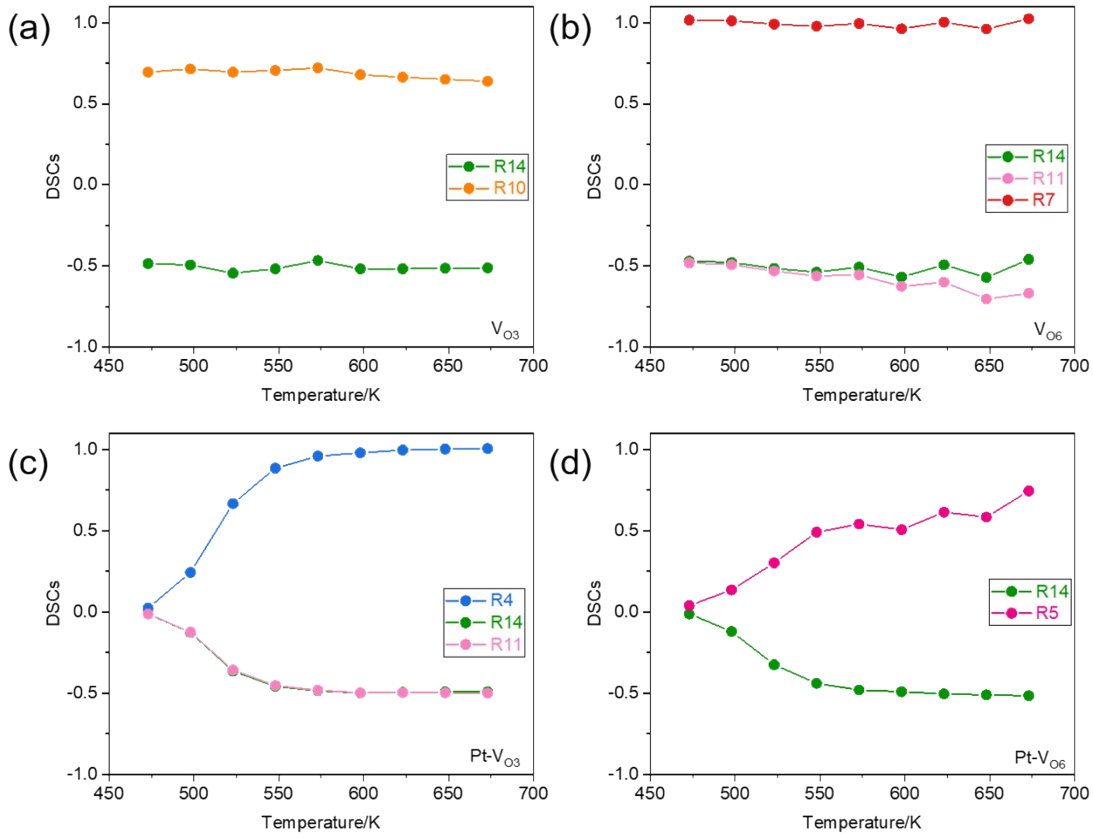

Fig. S6 Calculated DSCs for CO_2 hydrogenation over the (a) V_{O3}, (b) V_{O6}, (c) Pt-V_{O3} and (d) Pt-V_{O6} sites.

Table S1 Oxygen vacancy formation energy (unit eV).

Surface	**In_2O_3**	**$Pt_{\_bulk}/In_2O_3$**	**$Pt_{\_surface}/In_2O_3$**
V_{O3}	2.94	3.47	3.69
V_{O4}	3.65	3.94	3.92
V_{O6}	2.79	3.32	3.18
V_{O7}	3.29	3.53	3.58

Table S2 The charges of surface In atoms on the different model surfaces (unit |e|)

	In_2O_3	$Pt_{\_bulk}/In_2O_3$	In_2O_3-V_{O3_vac}	$Pt_{\_bulk}$-V_{O3_vac}	In_2O_3-V_{O4_vac}	$Pt_{\_bulk}$-V_{O4_vac}	In_2O_3-V_{O6_vac}	$Pt_{\_bulk}$-V_{O6_vac}
In1	1.79	1.78	1.76	1.75	1.57	1.41	1.78	1.76
In2	1.82	1.82	1.81	1.81	1.81	1.81	1.81	1.81
In3	1.77	1.76	1.68	1.58	1.75	1.76	1.75	1.75
In4	1.79	1.78	1.63	1.36	1.44	1.28	1.78	1.76
In5	1.77	1.76	1.76	1.76	1.74	1.74	1.76	1.76
In6	1.82	1.82	1.79	1.80	1.82	1.81	1.72	1.70
In7	1.82	1.82	1.70	1.66	1.81	1.81	1.74	1.72
In8	1.78	1.77	1.76	1.75	1.60	1.56	1.76	1.76
In9	1.82	1.82	1.81	1.82	1.81	1.81	1.81	1.81
In10	1.77	1.75	1.75	1.75	1.76	1.76	1.61	1.42
In11	1.76	1.75	1.75	1.75	1.77	1.77	1.73	1.73
In12	1.77	1.77	1.77	1.78	1.77	1.77	1.77	1.76
In13	1.79	1.78	1.79	1.77	1.77	1.77	1.77	1.76
In14	1.79	1.78	1.78	1.78	1.77	1.78	1.78	1.76
In15	1.79	1.78	1.77	1.78	1.80	1.79	1.78	1.77
In16	1.79	1.78	1.75	1.73	1.77	1.78	1.77	1.77

Table S3 The charges of Pt atoms on different model surfaces (unit |e|).

Surface	Pt charge/e
Pt/In_2O_3	1.39
$Pt\text{-}V_{O3}$	1.39
$Pt\text{-}V_{O4}$	1.39
$Pt\text{-}V_{O6}$	1.39
$Pt\text{-}V_{O7}$	1.39

Table S4 The charges of Pt and oxygen vacancy formation energy in the second layer on Pt/In_2O_3 surface.

Surface	Pt charge/e	V_O formation energy/eV
Pt/In_2O_3	1.39	
$Pt\text{-}V_{O3}$	1.40	4.26
$Pt\text{-}V_{O4}$	1.39	3.54
$Pt\text{-}V_{O6}$	1.40	4.47
$Pt\text{-}V_{O7}$	1.39	3.77

Table S5 Elementary reactions considered in microkinetic simulations of CO_2 hydrogenation to methanol and CO on the In_2O_3 and Pt/In_2O_3 model surfaces.

Step	Elementary reaction [a]
R1	CO_2_g + *_s <-> CO_2_s #ln-CO_2
R2	CO_2_g + *_s <-> O_2C_s #bt-CO_2
R3	CO_2_s + H_h <-> [CO_2-H_s] + *_h <-> HCOO_s + *_h
R4	HCOO_s + H_h <-> [HCOO-H_s] + *_h <-> H_2COO_s + *_h
R5	H_2COO_s <-> [H_2CO-O_s] <-> OH_2CO_s
R6	OH_2CO_s + 2H_h <-> [OHH_2CO-H_s] + 2*_h <-> OH_3COH_s + 2*_h
R7	OH_3COH_s <-> [OH_3CO-H_s] <-> OCH_3OH_s
R8	OCH_3OH_s <-> CH_3OH_g + O_s
R9	H_2_g + 2*_h <-> [H-H_h] + *_h <-> 2H_h
R10	H_2_g + O_s + *_h <-> [OH-H_s] + *_h <-> OH_s + H_h
R11	OH_s + H_h <-> [H-OH_s] + *_h <-> H_2O_s + *_h
R12	H_2O_s <-> H_2O_g + *_s
R13	O_s + H_h <-> OH_s + *_h
R14	CO_2_s + *_s <-> [CO-O_s] + *_s <-> CO_s + O_s
R15	CO_s <-> CO_g + *_s
R16	CH_3OH_s <-> CH_3OH_g + *_s

[a] "_s" and "_h" denote the V_O and "hydrogen reservoir" sites, respectively, "_g" indicates gaseous species, and "#" marks the beginning of a comment.

Table S6 The virtual frequencies of the transition state (unit cm^{-1}).

	V_{O3}	V_{O4}	V_{O6}	V_{O7}	Pt-V_{O3}	Pt-V_{O4}	Pt-V_{O6}	Pt-V_{O7}
TS1	507.622018	384.025355	471.601818	491.682074	546.214602	537.117569	485.787749	494.249525
TS2	678.624361	592.712775	425.916740	641.802480	658.817131	625.541431	327.996085	651.189068
TS3	132.178428	151.448666	205.630970	189.641724	166.846031	160.151975	152.635671	134.667258
TS4	623.965920	642.999521	645.174059	682.466773	687.586652	635.702798	497.513579	519.729332
TS5	873.420659	893.259330	824.667898	773.693810	876.120216	878.122224	891.972661	792.245212
TS6	286.730982	267.095856	338.461100	305.035048	277.372344	265.304315	258.468454	235.503163
TS7	1292.470726	1162.661706	1165.181547	1344.525913	1243.164570	1263.054841	1140.309221	1289.415226
TS8	803.972372	1093.456021	774.875807	1245.060667	1201.703821	1054.519419	1078.606472	1243.305195

Table S7 Optimized factional coordinates of the catalyst model with V_{O3}.

In O

1.00000000000000

12.5091307398836005 -7.2221500000000001 0.0000000000000000

0.0000000000000000 14.4443000000000001 -0.0000000000000248

0.0000000000000000 0.0000000000000000 17.9854999999999983

In O

48 71

Selective dynamics

Direct

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0.5142682570873042	0.7420955417439535	0.5097115493849164	T	T	T
0.1564310591981121	0.0619650681266626	0.6867291437387396	T	T	T
0.8290999999999968	0.9356200000000001	0.3251800000000031	F	F	F
0.4934263782731753	0.2647624177770678	0.4980236421982138	T	T	T
0.1598075603830452	0.6029805369746450	0.6604123466815101	T	T	T
0.3248900000000035	0.4314099999999996	0.3251800000000031	F	F	F
0.9941862097263033	0.7649322081700838	0.4957910548637989	T	T	T
0.6637471858895150	0.0977119024730455	0.6694825533627705	T	T	T
0.8403399999999976	0.6722699999999975	0.3362400000000036	F	F	F
0.5080633114406575	0.0050526634280900	0.5042654014448330	T	T	T
0.1743944841278614	0.3323585563846980	0.6708660145556480	T	T	T
0.1065200000000033	0.6835200000000015	0.3251800000000031	F	F	F
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0.4528704726178415	0.3611599703836351	0.6607896978150951	T	T	T
0.5994799999999998	0.4426500000000004	0.3472999999999971	F	F	F
0.2668381842963090	0.7784373977054264	0.5112277605802050	T	T	T
0.9265903683195437	0.1034567219048912	0.6861588852676462	T	T	T
0.0952800000000025	0.4426500000000004	0.3472999999999971	F	F	F
0.7645660104151422	0.7740523137405820	0.5162507787874046	T	T	T
0.4426507307357744	0.1062337190469328	0.6853224682451556	T	T	T
0.0727899999999977	0.9018900000000016	0.3251800000000031	F	F	F
0.7435530794345807	0.2318573783848827	0.4984283785640387	T	T	T
0.4049885478387517	0.5592587262648488	0.6585920958852827	T	T	T
0.5657599999999974	0.6610299999999967	0.3472999999999971	F	F	F
0.2304054538820196	0.9933968923129922	0.5096228067652528	T	T	T
0.8940806670016154	0.3237114623743447	0.6801217489888898	T	T	T
0.8403399999999976	0.1680700000000002	0.3362399999999965	F	F	F
0.5041570696969010	0.5041016929848836	0.5014244451321177	T	T	T
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0.1065200000000033	0.1793100000000010	0.3251800000000031	F	F	F

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0.4494037933933415	0.8474258800575661	0.6593408309589031	T	T	T
0.5769999999999982	0.9018900000000016	0.3251800000000031	F	F	F
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0.3473800000000011	0.9131300000000024	0.3472999999999971	F	F	F
0.0147427264191878	0.2441067228509736	0.5182159548126933	T	T	T
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0.3361400000000003	0.6722699999999975	0.3362400000000036	F	F	F
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0.2541799999999981	0.7461800000000025	0.3944800000000015	F	F	F
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0.2346989883807196	0.5095556093001503	0.6662063556704301	T	T	T
0.5217299999999980	0.9989399999999975	0.3799399999999977	F	F	F
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0.3978843580966602	0.5728329506410630	0.5371217328396172	T	T	T
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0.6723300000000023	0.6105200000000011	0.3019099999999995	F	F	F
0.3416211580826519	0.9467262577226331	0.4734429207149943	T	T	T
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0.3997649501527706	0.3403331764339358	0.5378346029363211	T	T	T
0.0726869763819414	0.6713453543226611	0.7078255589904238	T	T	T
0.4919900000000013	0.7542299999999997	0.3944800000000015	F	F	F
0.1635609412787195	0.0819776209181657	0.5677576331803551	T	T	T
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0.5068300000000008	0.2716500000000011	0.3652900000000017	F	F	F
0.1799520602806199	0.6116681722421624	0.5385647420827598	T	T	T
0.8414551551772345	0.9339957121655086	0.7094908179141214	T	T	T
0.1654399999999967	0.0644899999999993	0.3071899999999985	F	F	F
0.8335829925911383	0.3993674088838328	0.4738508971007273	T	T	T
0.4988599223337213	0.7258780669237144	0.6624509906872558	T	T	T
0.9465999999999966	0.3360800000000026	0.3019099999999995	F	F	F
0.6088080830595397	0.6691815422421276	0.4707238014919020	T	T	T
0.2773308082812859	0.0150867201090846	0.6874200436111071	T	T	T
0.6627999999999972	0.8133499999999998	0.2925400000000025	F	F	F
0.3288950208065489	0.1462128483584799	0.4596093220907049	T	T	T
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0.2622300000000024	0.5164199999999965	0.3944800000000015	F	F	F
0.9300864926195578	0.8480496470357484	0.5656188117089808	T	T	T
0.5920445540533085	0.1760215839705467	0.7361016613344079	T	T	T
0.4772099999999995	0.4866799999999998	0.3799399999999977	F	F	F
0.1533757410846848	0.8302041110770222	0.5570174385861383	T	T	T
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0.4180899999999994	0.5983700000000027	0.2779999999999987	F	F	F
0.0827782380941788	0.9281092777762060	0.4471103227710235	T	T	T
0.7450977650087568	0.2602045428739378	0.6159171390885980	T	T	T
0.2743899999999968	0.2743299999999991	0.3705700000000007	F	F	F
0.9470374371006915	0.6122234284223596	0.5415173504430203	T	T	T
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0.1802800000000033	0.5903199999999984	0.2779999999999987	F	F	F
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0.1505500000000026	0.3456100000000006	0.2925400000000025	F	F	F
0.8213404168615087	0.6781379891212236	0.4603595362027573	T	T	T
0.4862799410593152	0.0099877885677162	0.6250770581169891	T	T	T
0.1950599999999980	0.8578600000000023	0.2925400000000025	F	F	F
0.8641819886277291	0.1867494069605935	0.4600091388615598	T	T	T
0.5344723294458629	0.5265750365008622	0.6234123442351741	T	T	T
0.7732299999999981	0.5015799999999970	0.3652900000000017	F	F	F
0.4354420492524970	0.8296418800845834	0.5371304428957596	T	T	T
0.0973050224714412	0.1647883384003139	0.7120162757617871	T	T	T

Table S8 Optimized factional coordinates of the catalyst model with V_{O4}.

In O

1.00000000000000

12.5091307398836005 -7.2221500000000001 0.0000000000000000

0.0000000000000000 14.4443000000000001 -0.0000000000000248

0.0000000000000000 0.0000000000000000 17.9854999999999983

In O

48 71

Selective dynamics

Direct

0.8515799999999984	0.4089299999999980	0.3473000000000042	F	F	F
0.5149990233166554	0.7428080616530326	0.5098463272641417	T	T	T
0.1843580666382897	0.0737361649397346	0.6841553569050361	T	T	T
0.8290999999999968	0.9356200000000001	0.3251800000000031	F	F	F
0.4941053251862303	0.2665901826037373	0.4984375370250552	T	T	T
0.1586688486545680	0.6038946087059446	0.6577924345387669	T	T	T
0.3248900000000035	0.4314099999999996	0.3251800000000031	F	F	F
0.9937069362565175	0.7638609187479671	0.4941975130876368	T	T	T
0.6554651179892720	0.0991562959366657	0.6705560414569639	T	T	T
0.8403399999999976	0.6722699999999975	0.3362400000000036	F	F	F
0.5061131804296303	0.0064690718175148	0.5048205912313559	T	T	T
0.1836748820721856	0.3494679533258775	0.6708915091027603	T	T	T
0.1065200000000033	0.6835200000000015	0.3251800000000031	F	F	F
0.7749604247800389	0.0141661932494103	0.4941893757017904	T	T	T
0.4457243211424951	0.3503163129893044	0.6703378860914831	T	T	T
0.5994799999999998	0.4426500000000004	0.3473000000000042	F	F	F
0.2671128295858441	0.7778910962178234	0.5099900579425301	T	T	T
0.9140881528563943	0.0974694281200542	0.6862199287253025	T	T	T
0.0952800000000025	0.4426500000000004	0.3473000000000042	F	F	F
0.7646581914807949	0.7738317653950539	0.5174305133816433	T	T	T
0.4355061524542749	0.1169083285723086	0.6798550077184921	T	T	T
0.0727899999999977	0.9018900000000016	0.3251800000000031	F	F	F
0.7421399767786604	0.2313462963694210	0.4991018385352823	T	T	T
0.4117081285993067	0.5633682317243957	0.6574447774837775	T	T	T
0.5657599999999974	0.6610299999999967	0.3473000000000042	F	F	F
0.2334209904941849	0.9937172363410687	0.5169532849338699	T	T	T
0.8920885801496300	0.3223419979823625	0.6827482234255083	T	T	T
0.8403399999999976	0.1680700000000002	0.3362399999999965	F	F	F
0.5036616759138343	0.5023785950291298	0.5033157679099141	T	T	T
0.1623622679549648	0.8320262595633152	0.6709406495604809	T	T	T
0.5657599999999974	0.1568299999999994	0.3473000000000042	F	F	F
0.2320483145526137	0.4967127364608228	0.5096734265298722	T	T	T
0.9026866371871530	0.8253446072291560	0.6851994533391705	T	T	T
0.1065200000000033	0.1793100000000010	0.3251800000000031	F	F	F

0.7770372891821231	0.5133767733269278	0.4985703244176635	T	T	T
0.4488434666728597	0.8511451480224920	0.6582374115691593	T	T	T
0.5769999999999982	0.9018900000000016	0.3251800000000031	F	F	F
0.2441398677751724	0.2337011283319960	0.4937472461584972	T	T	T
0.9088928795977106	0.5626442752468587	0.6713133212153211	T	T	T
0.3473800000000011	0.9131300000000024	0.3473000000000042	F	F	F
0.0155955798532133	0.2426119925012491	0.5156995030559189	T	T	T
0.6858960681932245	0.5729895144685381	0.6795539832735090	T	T	T
0.3361400000000003	0.1680700000000002	0.3362399999999965	F	F	F
0.0018756940273994	0.5039036946695492	0.5052497136478931	T	T	T
0.6737219161310161	0.8437886003191407	0.6711746347952220	T	T	T
0.3361400000000003	0.6722699999999975	0.3362400000000036	F	F	F
0.0036591805502722	0.0032315325347718	0.5062618756476039	T	T	T
0.6712076204386068	0.3379939509365142	0.6897718930499546	T	T	T
0.2541799999999981	0.7461800000000025	0.3944800000000015	F	F	F
0.9226348478598790	0.0810032806262124	0.5671832842509296	T	T	T
0.5939463633284054	0.4226488517257991	0.7343359487899489	T	T	T
0.0094700000000003	0.5311999999999983	0.3799399999999977	F	F	F
0.6764931492906964	0.8617903954013848	0.5499099138131547	T	T	T
0.3414580067670765	0.1902069573066768	0.7161492868785984	T	T	T
0.9439199999999985	0.1009499999999974	0.3071899999999985	F	F	F
0.6090246637341016	0.4365401924878508	0.4724910441420572	T	T	T
0.2817459744485556	0.7761385738230853	0.6607177925444565	T	T	T
0.9074600000000004	0.8429700000000011	0.3071899999999985	F	F	F
0.5726889869481916	0.1772302027336016	0.4732578586500206	T	T	T
0.2397596326426580	0.5181390123899720	0.6594690131756259	T	T	T
0.5217299999999980	0.9989399999999975	0.3799399999999977	F	F	F
0.1878374522746549	0.3336640838725558	0.5506067085420190	T	T	T
0.8511804729324217	0.6651000050865498	0.7158118918453577	T	T	T
0.4100400000000022	0.8281300000000016	0.2779999999999987	F	F	F
0.0789235329400360	0.1596789490094486	0.4476081577392707	T	T	T
0.7475798642318706	0.4878006342046997	0.6150704686288698	T	T	T
0.3978899999999967	0.0618100000000013	0.3019099999999995	F	F	F
0.0624200451937423	0.3990730362767277	0.4729942111324351	T	T	T
0.7274430882000924	0.7329225563094782	0.6410094437114989	T	T	T
0.0083500000000001	0.7340200000000010	0.3705700000000007	F	F	F
0.6698819485335642	0.0637639859557397	0.5389460110920550	T	T	T
0.3394222244229990	0.4066747317184655	0.7070070320750419	T	T	T
0.7367599999999968	0.2351799999999997	0.3652900000000017	F	F	F
0.3990551682358240	0.5733466176307767	0.5359517210202084	T	T	T
0.0723974350480446	0.9080510993692298	0.7101741403014246	T	T	T
0.6723300000000023	0.6105200000000011	0.3019099999999995	F	F	F
0.3410253263195972	0.9458645374374500	0.4722008470488638	T	T	T
0.0177133245469693	0.2693616537809603	0.6624761767803953	T	T	T

0.7340799999999987	0.0000599999999977	0.3705700000000007	F	F	F
0.3974593906023621	0.3390016083497778	0.5395158702320482	T	T	T
0.0706325721066450	0.6702751965808893	0.7046118127850254	T	T	T
0.4919900000000013	0.7542299999999997	0.3944800000000015	F	F	F
0.1582981819462456	0.0887257804104741	0.5676250862531925	T	T	T
0.8330367850517658	0.4148282323452948	0.7352280291482206	T	T	T
0.5068300000000008	0.2716500000000011	0.3652900000000017	F	F	F
0.1774282231287453	0.6105887627555564	0.5362075708188521	T	T	T
0.8409331035903725	0.9327013693142870	0.7115982412694291	T	T	T
0.1654399999999967	0.0644899999999993	0.3071899999999985	F	F	F
0.8321587179869120	0.3984320583782845	0.4730225898014767	T	T	T
0.4994735511452422	0.7288731005650684	0.6600801498161354	T	T	T
0.9465999999999966	0.3360800000000026	0.3019099999999995	F	F	F
0.6089150475005091	0.6687307783754296	0.4712544050414884	T	T	T
0.2754552466687241	0.9980533123478725	0.6403975923942706	T	T	T
0.6627999999999972	0.8133499999999998	0.2925400000000025	F	F	F
0.3288265672073034	0.1453051171166040	0.4604529480077387	T	T	T
0.9971378136089177	0.4707678121899500	0.6263710576071274	T	T	T
0.2622300000000024	0.5164199999999965	0.3944800000000015	F	F	F
0.9304866299310866	0.8478980175843058	0.5661171460898767	T	T	T
0.5851991778864267	0.1767145284897717	0.7349603012165379	T	T	T
0.4772099999999995	0.4866799999999998	0.3799399999999977	F	F	F
0.1466906737622366	0.8181752028990663	0.5497473629443860	T	T	T
0.8133174195426405	0.1563977857427856	0.7159632578219376	T	T	T
0.4180899999999994	0.5983700000000027	0.2779999999999987	F	F	F
0.0853035767677959	0.9298321443831534	0.4484221628134067	T	T	T
0.7466092023660805	0.2613999610254240	0.6155995663302544	T	T	T
0.2743899999999968	0.2743299999999991	0.3705700000000007	F	F	F
0.9448379139814714	0.6091547689169616	0.5411916335191426	T	T	T
0.6055322718173781	0.9375550796318572	0.7043386872032661	T	T	T
0.1802800000000033	0.5903199999999984	0.2779999999999987	F	F	F
0.8492109940693141	0.9234267780651133	0.4479637109148874	T	T	T
0.5188309207211310	0.2628966930803271	0.6150509876143280	T	T	T
0.1505500000000026	0.3456100000000006	0.2925400000000025	F	F	F
0.8215553440224140	0.6785143180034984	0.4599791516553160	T	T	T
0.4858328623081304	0.0143661749991254	0.6256972598644751	T	T	T
0.1950599999999980	0.8578600000000023	0.2925400000000025	F	F	F
0.8637215601854377	0.1868742949277953	0.4596942530072318	T	T	T
0.5326219970597968	0.5218189499994355	0.6245796364587243	T	T	T
0.7732299999999981	0.5015799999999970	0.3652900000000017	F	F	F
0.4359386795058534	0.8306580213089910	0.5365753656436388	T	T	T

Table S9 Optimized factional coordinates of the catalyst model with V_{O6}.

In O

1.00000000000000

12.5091307398836005 -7.2221500000000001 0.0000000000000000

0.0000000000000000 14.4443000000000001 -0.0000000000000248

0.0000000000000000 0.0000000000000000 17.9854999999999983

In O

48 71

Selective dynamics

Direct

0.8515799999999984	0.4089299999999980	0.3473000000000042	F	F	F
0.5141925532925935	0.7419197013384988	0.5103325193101471	T	T	T
0.1781414921780414	0.0781005712950788	0.6851584716138206	T	T	T
0.8290999999999968	0.9356200000000001	0.3251800000000031	F	F	F
0.4948275495046375	0.2663115399191428	0.4960542910140632	T	T	T
0.1589140886350291	0.6043299831125067	0.6585566859134935	T	T	T
0.3248900000000035	0.4314099999999996	0.3251800000000031	F	F	F
0.9941659006168786	0.7645410725262597	0.4938754831205310	T	T	T
0.6604135309536290	0.0967734422418557	0.6697262652730297	T	T	T
0.8403399999999976	0.6722699999999975	0.3362400000000036	F	F	F
0.5063655131295643	0.0052443008964012	0.5048745845804046	T	T	T
0.1707697577797966	0.3325436873782238	0.6707606332815154	T	T	T
0.1065200000000033	0.6835200000000015	0.3251800000000031	F	F	F
0.7765006348575767	0.0147370169707819	0.4939542421306986	T	T	T
0.4210894035433554	0.3373804409211386	0.6579338406734250	T	T	T
0.5994799999999998	0.4426500000000004	0.3473000000000042	F	F	F
0.2665710380986376	0.7774155689047565	0.5098189021625538	T	T	T
0.9288027108445768	0.1050079394452689	0.6852488787708763	T	T	T
0.0952800000000025	0.4426500000000004	0.3473000000000042	F	F	F
0.7664713793181972	0.7773293110687680	0.5143274907732568	T	T	T
0.4354162953436856	0.1159965368096227	0.6793969358845542	T	T	T
0.0727899999999977	0.9018900000000016	0.3251800000000031	F	F	F
0.7433708835124259	0.2294575408008300	0.4951086427213606	T	T	T
0.4040794656170409	0.5603597851885608	0.6613484398135180	T	T	T
0.5657599999999974	0.6610299999999967	0.3473000000000042	F	F	F
0.2336106702313199	0.9938165412715348	0.5176647229146970	T	T	T
0.8953737136758612	0.3235908041203784	0.6804139816382840	T	T	T
0.8403399999999976	0.1680700000000002	0.3362399999999965	F	F	F
0.5030435734929976	0.5025966120949061	0.5021465544197324	T	T	T
0.1634682685603070	0.8346072378119898	0.6714577195866556	T	T	T
0.5657599999999974	0.1568299999999994	0.3473000000000042	F	F	F
0.2315322843374992	0.4940351479599676	0.5104115990298604	T	T	T
0.9063697062701104	0.8327925547800683	0.6843537607562018	T	T	T
0.1065200000000033	0.1793100000000010	0.3251800000000031	F	F	F

0.7770659154910923	0.5138599715476235	0.4966917838370417	T	T	T
0.4483596305790315	0.8497621560459632	0.6586882645724377	T	T	T
0.5769999999999982	0.9018900000000016	0.3251800000000031	F	F	F
0.2409331901365772	0.2311286471764132	0.4913793041284149	T	T	T
0.9112149149566391	0.5651506166709712	0.6713639463840854	T	T	T
0.3473800000000011	0.9131300000000024	0.3473000000000042	F	F	F
0.0145924191530356	0.2439549057910406	0.5171475702683890	T	T	T
0.6933860955209147	0.5876980367470963	0.6713741032244053	T	T	T
0.3361400000000003	0.1680700000000002	0.3362399999999965	F	F	F
0.0026013306719207	0.5051965341481149	0.5051560065612113	T	T	T
0.6768256325265942	0.8489934734875746	0.6697247968901917	T	T	T
0.3361400000000003	0.6722699999999975	0.3362400000000036	F	F	F
0.0050005116155343	0.0043115107113030	0.5057096758969211	T	T	T
0.6775946246776201	0.3308299403875045	0.6753580578137882	T	T	T
0.2541799999999981	0.7461800000000025	0.3944800000000015	F	F	F
0.9222068023476675	0.0773211527869937	0.5659663235221480	T	T	T
0.0094700000000003	0.5311999999999983	0.3799399999999977	F	F	F
0.6752406040146071	0.8627777097838605	0.5484987620058012	T	T	T
0.3412571366380032	0.1888535910577747	0.7153381514259297	T	T	T
0.9439199999999985	0.1009499999999974	0.3071899999999985	F	F	F
0.6083238291036938	0.4371041464958193	0.4740140180995582	T	T	T
0.2819003647483735	0.7761204892291402	0.6619909323535222	T	T	T
0.9074600000000004	0.8429700000000011	0.3071899999999985	F	F	F
0.5730318043934377	0.1770420976372283	0.4750266568129999	T	T	T
0.2326043511595277	0.5109011462285888	0.6605881112066452	T	T	T
0.5217299999999980	0.9989399999999975	0.3799399999999977	F	F	F
0.1907482721947558	0.3324072347791976	0.5495603700365586	T	T	T
0.8507620097045151	0.6681331443283963	0.7149046729218134	T	T	T
0.4100400000000022	0.8281300000000016	0.2779999999999987	F	F	F
0.0771949080995711	0.1595889865356447	0.4470608390283979	T	T	T
0.7400007961682702	0.4854930178533039	0.6176603104264515	T	T	T
0.3978899999999967	0.0618100000000013	0.3019099999999995	F	F	F
0.0628042548037139	0.4001925094471486	0.4726323851542375	T	T	T
0.7298146167460757	0.7393928076713271	0.6356843882773678	T	T	T
0.0083500000000001	0.7340200000000010	0.3705700000000007	F	F	F
0.6702274287093608	0.0629991229062482	0.5392797257330330	T	T	T
0.3314236896849930	0.4018041812556653	0.7057776073295395	T	T	T
0.7367599999999968	0.2351799999999997	0.3652900000000017	F	F	F
0.4005214069920771	0.5698741045853020	0.5392761944203808	T	T	T
0.0734891680244481	0.9113183336211655	0.7105181446254306	T	T	T
0.6723300000000023	0.6105200000000011	0.3019099999999995	F	F	F
0.3413276374940263	0.9458942048068104	0.4729990573332817	T	T	T
0.0091039345076855	0.2803162262142489	0.6399040635028214	T	T	T
0.7340799999999987	0.0000599999999977	0.3705700000000007	F	F	F

0.3966099379253171	0.3390437687996312	0.5377336967758369	T	T	T
0.0716193502350413	0.6735035615950028	0.7060147135409841	T	T	T
0.4919900000000013	0.7542299999999997	0.3944800000000015	F	F	F
0.1610012030622785	0.0876447608056499	0.5658110392526360	T	T	T
0.8290494043282953	0.4136023627321158	0.7322446682884424	T	T	T
0.5068300000000008	0.2716500000000011	0.3652900000000017	F	F	F
0.1783775880314018	0.6103844030989672	0.5368318246711116	T	T	T
0.8421460997572670	0.9359125954317373	0.7099741594590150	T	T	T
0.1654399999999967	0.0644899999999993	0.3071899999999985	F	F	F
0.8319276755238104	0.3988791925788042	0.4741268055847068	T	T	T
0.4998121598562772	0.7265897122173935	0.6603515669455945	T	T	T
0.9465999999999966	0.3360800000000026	0.3019099999999995	F	F	F
0.6083017068272160	0.6674776798172083	0.4729284149598217	T	T	T
0.2757456653312643	0.9993248263416300	0.6413849787629923	T	T	T
0.6627999999999972	0.8133499999999998	0.2925400000000025	F	F	F
0.3302848214020795	0.1461353472956662	0.4608224129130030	T	T	T
0.9951032769974874	0.4774436076550691	0.6273387600366674	T	T	T
0.2622300000000024	0.5164199999999965	0.3944800000000015	F	F	F
0.9322369998909326	0.8490589370577837	0.5654937054742035	T	T	T
0.5888715352202636	0.1801699671430271	0.7314345524942975	T	T	T
0.4772099999999995	0.4866799999999998	0.3799399999999977	F	F	F
0.1463227335671107	0.8174720536894472	0.5504176477532889	T	T	T
0.8198422525326134	0.1574334308131701	0.7163356309880896	T	T	T
0.4180899999999994	0.5983700000000027	0.2779999999999987	F	F	F
0.0860486316638450	0.9298743807231639	0.4480919763519846	T	T	T
0.7512670805303623	0.2587871310730717	0.6119462876049413	T	T	T
0.2743899999999968	0.2743299999999991	0.3705700000000007	F	F	F
0.9408134484428714	0.6087134054578859	0.5428561716084777	T	T	T
0.6043959635632378	0.9364612893678953	0.7059535674210021	T	T	T
0.1802800000000033	0.5903199999999984	0.2779999999999987	F	F	F
0.8500137742668350	0.9236014180984895	0.4468864988493892	T	T	T
0.5211372261301941	0.2713528822867248	0.6177978034401618	T	T	T
0.1505500000000026	0.3456100000000006	0.2925400000000025	F	F	F
0.8212222377035392	0.6789577669567985	0.4598807999071554	T	T	T
0.4879516648705273	0.0150932515153875	0.6264439805629975	T	T	T
0.1950599999999980	0.8578600000000023	0.2925400000000025	F	F	F
0.8642255988368333	0.1865027241265409	0.4589812693318774	T	T	T
0.5319545225168921	0.5100916723758211	0.6392851794199886	T	T	T
0.7732299999999981	0.5015799999999970	0.3652900000000017	F	F	F
0.4352535589555874	0.8295459654127244	0.5373669257048925	T	T	T
0.0967128506555440	0.1657604442896335	0.7093601303304065	T	T	T

Table S10 Optimized factional coordinates of the catalyst model with Pt-V_{O3}.

In Pt O

1.00000000000000

12.5091307398836005 -7.2221500000000001 0.0000000000000000

0.0000000000000000 14.4443000000000001 -0.0000000000000248

0.0000000000000000 0.0000000000000000 17.9854999999999983

In Pt O

47 1 71

Selective dynamics

Direct

0.8515799999999984	0.4089299999999980	0.3472999999999971	F	F	F
0.5142035697783955	0.7415523605742129	0.5096993486533532	T	T	T
0.1690927113883294	0.0740686755192005	0.6866565085320548	T	T	T
0.8290999999999968	0.9356200000000001	0.3251800000000031	F	F	F
0.4937310800925677	0.2655372039231156	0.4975164031706043	T	T	T
0.1586875382826785	0.6024608010169137	0.6578903816685867	T	T	T
0.3248900000000035	0.4314099999999996	0.3251800000000031	F	F	F
0.9931443370335258	0.7645128327061574	0.4933507707813546	T	T	T
0.6614074298017467	0.0974034977874649	0.6696667985930554	T	T	T
0.8403399999999976	0.6722699999999975	0.3362400000000036	F	F	F
0.5077701135835552	0.0048944703222161	0.5034702716221238	T	T	T
0.1734374578705867	0.3321731076729049	0.6692432943727724	T	T	T
0.1065200000000033	0.6835200000000015	0.3251800000000031	F	F	F
0.7774262744023428	0.0158402420874129	0.4934056131638166	T	T	T
0.4519488375587594	0.3604381772117924	0.6626611624795300	T	T	T
0.5994799999999998	0.4426500000000004	0.3472999999999971	F	F	F
0.2673143616259080	0.7780546092667053	0.5103702334223564	T	T	T
0.9290787855280068	0.1047459003602511	0.6849722820866165	T	T	T
0.0952800000000025	0.4426500000000004	0.3472999999999971	F	F	F
0.7645980126235409	0.7753376765719961	0.5156270265792929	T	T	T
0.4398627726889322	0.1077916987153361	0.6794519497568930	T	T	T
0.0727899999999977	0.9018900000000016	0.3251800000000031	F	F	F
0.7424249474378877	0.2316181309647328	0.4980427675937559	T	T	T
0.4054823906289343	0.5594815710110378	0.6568488093642065	T	T	T
0.5657599999999974	0.6610299999999967	0.3472999999999971	F	F	F
0.2332078089983777	0.9944185292474258	0.5180494350103895	T	T	T
0.8919938847154678	0.3227465079295274	0.6777250973318615	T	T	T
0.8403399999999976	0.1680700000000002	0.3362399999999965	F	F	F
0.5038304762491759	0.5034750483935423	0.5014369053932667	T	T	T
0.1625303083827866	0.8336721229986305	0.6723849766681068	T	T	T
0.5657599999999974	0.1568299999999994	0.3472999999999971	F	F	F
0.2308861133532802	0.4944231079199395	0.5094864259622264	T	T	T
0.9016806452035844	0.8279534794945759	0.6834738226498382	T	T	T
0.1065200000000033	0.1793100000000010	0.3251800000000031	F	F	F

0.7773419333303357	0.5131696828698814	0.4976356582363784	T	T	T
0.4495031155347647	0.8479647474073313	0.6575730856342588	T	T	T
0.5769999999999982	0.9018900000000016	0.3251800000000031	F	F	F
0.2439856434982842	0.2322455189896301	0.4926997066811110	T	T	T
0.9103693922793692	0.5632296622669771	0.6706842872651301	T	T	T
0.3473800000000011	0.9131300000000024	0.3472999999999971	F	F	F
0.0154418168786914	0.2444455653390796	0.5166962123223525	T	T	T
0.6885105265515544	0.5747754209648687	0.6771129126166542	T	T	T
0.3361400000000003	0.1680700000000002	0.3362399999999965	F	F	F
0.0031126111971135	0.5057510595590914	0.5042817370659922	T	T	T
0.6769835299832843	0.8462590458250308	0.6691529797519841	T	T	T
0.3361400000000003	0.6722699999999975	0.3362400000000036	F	F	F
0.6719958243306616	0.3375297578367685	0.6907332112980238	T	T	T
0.0040997264558661	0.0037907392368683	0.5058370150659512	T	T	T
0.2541799999999981	0.7461800000000025	0.3944800000000015	F	F	F
0.9293629879837041	0.0739218283676370	0.5623205610282630	T	T	T
0.5934045097875053	0.4226980689835779	0.7320346334653317	T	T	T
0.0094700000000003	0.5311999999999983	0.3799399999999977	F	F	F
0.6776700214180604	0.8627746770317000	0.5474995319622780	T	T	T
0.9439199999999985	0.1009499999999974	0.3071899999999985	F	F	F
0.6087021106603572	0.4358273372753068	0.4736155144362237	T	T	T
0.2823309720154917	0.7771716422625580	0.6583512184910949	T	T	T
0.9074600000000004	0.8429700000000011	0.3071899999999985	F	F	F
0.5721739679005777	0.1763980132448678	0.4749421234638917	T	T	T
0.2334128063609524	0.5087439202304278	0.6603586871793700	T	T	T
0.5217299999999980	0.9989399999999975	0.3799399999999977	F	F	F
0.1902327833396916	0.3313357236852016	0.5473980557695547	T	T	T
0.8524781261318876	0.6667613930357290	0.7129813875363721	T	T	T
0.4100400000000022	0.8281300000000016	0.2779999999999987	F	F	F
0.0750454853500314	0.1492095545730205	0.4501356593456021	T	T	T
0.7468733507786502	0.4857632963302984	0.6145216540280626	T	T	T
0.3978899999999967	0.0618100000000013	0.3019099999999995	F	F	F
0.0632544243839736	0.4001214907398064	0.4716422000969435	T	T	T
0.7311318101804523	0.7351126388634296	0.6376825640550745	T	T	T
0.0083500000000001	0.7340200000000010	0.3705700000000007	F	F	F
0.6723269903707626	0.0642675203936783	0.5393128894731516	T	T	T
0.3370162243226945	0.3987819447743556	0.7019908142854328	T	T	T
0.7367599999999968	0.2351799999999997	0.3652900000000017	F	F	F
0.3977841852607663	0.5718299996662741	0.5355991752461581	T	T	T
0.0680974053931472	0.9058559945092342	0.7069107309320023	T	T	T
0.6723300000000023	0.6105200000000011	0.3019099999999995	F	F	F
0.3408933020846173	0.9463871007312271	0.4734978914305218	T	T	T
0.0076519793128158	0.2779699003711886	0.6370131548851937	T	T	T
0.7340799999999987	0.0000599999999977	0.3705700000000007	F	F	F

0.3991123802037990	0.3396342819451979	0.5382738330539282	T	T	T
0.0724356448308332	0.6716082331307812	0.7050933641759615	T	T	T
0.4919900000000013	0.7542299999999997	0.3944800000000015	F	F	F
0.1478814140268318	0.0776868233309435	0.5627669112936432	T	T	T
0.8334806194125957	0.4138078675323804	0.7344043326540111	T	T	T
0.5068300000000008	0.2716500000000011	0.3652900000000017	F	F	F
0.1786691935070901	0.6109118624142016	0.5365003614591740	T	T	T
0.8422651074644381	0.9359313649971120	0.7077216511832918	T	T	T
0.1654399999999967	0.0644899999999993	0.3071899999999985	F	F	F
0.8331966819404660	0.3988229737098466	0.4736960891127858	T	T	T
0.4999631788534108	0.7264869522262186	0.6577583363332439	T	T	T
0.9465999999999966	0.3360800000000026	0.3019099999999995	F	F	F
0.6091246420244126	0.6695242218345132	0.4704411435255451	T	T	T
0.2769163523762372	0.0107086613620082	0.6485671851580993	T	T	T
0.6627999999999972	0.8133499999999998	0.2925400000000025	F	F	F
0.3278442207173924	0.1447663731861726	0.4612620292865805	T	T	T
0.9952615084439327	0.4763539859811148	0.6254279913755942	T	T	T
0.2622300000000024	0.5164199999999965	0.3944800000000015	F	F	F
0.9336139864028211	0.8586959305974051	0.5613151175780918	T	T	T
0.5872726682437137	0.1747712418106466	0.7350423544478824	T	T	T
0.4772099999999995	0.4866799999999998	0.3799399999999977	F	F	F
0.1475359516637963	0.8227344596080038	0.5505013062154068	T	T	T
0.8201498002975861	0.1567386703661384	0.7140653300833586	T	T	T
0.4180899999999994	0.5983700000000027	0.2779999999999987	F	F	F
0.0785500189982647	0.9332246774041891	0.4502193688407413	T	T	T
0.7428738829442835	0.2596121435005235	0.6153517721176278	T	T	T
0.2743899999999968	0.2743299999999991	0.3705700000000007	F	F	F
0.9449701225032491	0.6114551631626060	0.5403300897590594	T	T	T
0.6057789899544226	0.9355318120770011	0.7045228734887395	T	T	T
0.1802800000000033	0.5903199999999984	0.2779999999999987	F	F	F
0.8590948049605069	0.9296179028921938	0.4493364796091242	T	T	T
0.5050982074496690	0.2549491138121799	0.6188403619814877	T	T	T
0.1505500000000026	0.3456100000000006	0.2925400000000025	F	F	F
0.8214110206155253	0.6798190309833333	0.4605987005400035	T	T	T
0.4890771379948098	0.0111337483830142	0.6242108410955407	T	T	T
0.1950599999999980	0.8578600000000023	0.2925400000000025	F	F	F
0.8647210004664736	0.1867487410158751	0.4601986738996786	T	T	T
0.5352524301224740	0.5266984988254930	0.6229953208490471	T	T	T
0.7732299999999981	0.5015799999999970	0.3652900000000017	F	F	F
0.4365398223722817	0.8301414587690085	0.5357717763740567	T	T	T
0.0960091062360646	0.1690809012269307	0.7120832254564564	T	T	T

Table S11 Optimized factional coordinates of the catalyst model with Pt-V_{O4}.

In Pt In O

1.00000000000000

12.5091307398836005 -7.2221500000000001 0.0000000000000000

0.0000000000000000 14.4443000000000001 -0.0000000000000248

0.0000000000000000 0.0000000000000000 17.9854999999999983

In Pt In O

46 1 1 71

Selective dynamics

Direct

0.8515799999999984	0.4089299999999980	0.3473000000000042	F	F	F
0.5146991917315433	0.7426905165528922	0.5097657926479854	T	T	T
0.1730695572510418	0.0779612298021915	0.6857476679774662	T	T	T
0.8290999999999968	0.9356200000000001	0.3251800000000031	F	F	F
0.4950077877757771	0.2669576574318344	0.4982818554070128	T	T	T
0.1585840932823588	0.6040454220781847	0.6571440741280442	T	T	T
0.3248900000000035	0.4314099999999996	0.3251800000000031	F	F	F
0.9924952252530788	0.7636456126659134	0.4933729854411072	T	T	T
0.6571043977652680	0.0988019799984270	0.6704711556098520	T	T	T
0.8403399999999976	0.6722699999999975	0.3362400000000036	F	F	F
0.5059243182581235	0.0065101069938020	0.5046436098064772	T	T	T
0.1829032606029490	0.3453154678622841	0.6681951233888972	T	T	T
0.1065200000000033	0.6835200000000015	0.3251800000000031	F	F	F
0.7765522686696540	0.0159976906767645	0.4942722712626733	T	T	T
0.4457845875187055	0.3502147842804971	0.6700608913665592	T	T	T
0.5994799999999998	0.4426500000000004	0.3473000000000042	F	F	F
0.2669821522361523	0.7780756488265760	0.5100010019065712	T	T	T
0.9308646023886904	0.0994069582346617	0.6876452230737267	T	T	T
0.0952800000000025	0.4426500000000004	0.3473000000000042	F	F	F
0.7642853690589720	0.7747432111391573	0.5168481659968934	T	T	T
0.4327324968018390	0.1163247767832093	0.6789432722141155	T	T	T
0.0727899999999977	0.9018900000000016	0.3251800000000031	F	F	F
0.7417887621548995	0.2310859079195862	0.4986401029942975	T	T	T
0.4109791657019813	0.5632158996079299	0.6569539039416502	T	T	T
0.5657599999999974	0.6610299999999967	0.3473000000000042	F	F	F
0.2328847061647327	0.9933991916224733	0.5184603068541577	T	T	T
0.8922454351392147	0.3205494550706847	0.6797070763053140	T	T	T
0.8403399999999976	0.1680700000000002	0.3362399999999965	F	F	F
0.5034648300678496	0.5021317010698545	0.5030169423408335	T	T	T
0.1609158057186184	0.8333902851588275	0.6703235722573864	T	T	T
0.5657599999999974	0.1568299999999994	0.3473000000000042	F	F	F
0.2322912377918707	0.4967924188758516	0.5094792513332398	T	T	T
0.9025547863787489	0.8271274573337276	0.6848571062913276	T	T	T
0.1065200000000033	0.1793100000000010	0.3251800000000031	F	F	F

0.7772050293406549	0.5128836552667173	0.4980720033382312	T	T	T
0.4485110979023185	0.8516217533952795	0.6575591098305522	T	T	T
0.5769999999999982	0.9018900000000016	0.3251800000000031	F	F	F
0.2451653511586181	0.2324432642472291	0.4926161686550395	T	T	T
0.9090423807605951	0.5614292373029901	0.6710042641545900	T	T	T
0.3473800000000011	0.9131300000000024	0.3473000000000042	F	F	F
0.0166550062951348	0.2436537012434312	0.5183180188134485	T	T	T
0.6865546978245147	0.5726548592228838	0.6777777029355644	T	T	T
0.3361400000000003	0.1680700000000002	0.3362399999999965	F	F	F
0.0023253553727313	0.5042480597536457	0.5046465465470992	T	T	T
0.6752752157164781	0.8457764954198620	0.6699634128871870	T	T	T
0.3361400000000003	0.6722699999999975	0.3362400000000036	F	F	F
0.0040344277825875	0.0041484440187892	0.5063898380844829	T	T	T
0.6707547381700567	0.3366173313016385	0.6897058943755311	T	T	T
0.2541799999999981	0.7461800000000025	0.3944800000000015	F	F	F
0.9294916928303237	0.0741763241047497	0.5637061432190570	T	T	T
0.5945718932381042	0.4230414669940515	0.7337498811758003	T	T	T
0.0094700000000003	0.5311999999999983	0.3799399999999977	F	F	F
0.6779975949460382	0.8630284081287111	0.5480941416334718	T	T	T
0.3380143401226979	0.1899656766333905	0.7124633988013214	T	T	T
0.9439199999999985	0.1009499999999974	0.3071899999999985	F	F	F
0.6093535100393093	0.4372057656202487	0.4726655921753133	T	T	T
0.2811012235195090	0.7769364981852078	0.6585998615911944	T	T	T
0.9074600000000004	0.8429700000000011	0.3071899999999985	F	F	F
0.5724187176613923	0.1767874378969160	0.4733744298242217	T	T	T
0.2378531068910900	0.5156556747169937	0.6574396977656810	T	T	T
0.5217299999999980	0.9989399999999975	0.3799399999999977	F	F	F
0.1914102507107991	0.3331749551809943	0.5473518356302136	T	T	T
0.8520616791295270	0.6660544050128571	0.7132323315556947	T	T	T
0.4100400000000022	0.8281300000000016	0.2779999999999987	F	F	F
0.0750496756555660	0.1497013969152920	0.4504487144642705	T	T	T
0.7480402951888180	0.4865798272131780	0.6147153124095687	T	T	T
0.3978899999999967	0.0618100000000013	0.3019099999999995	F	F	F
0.0631261455949126	0.3988984755008608	0.4728142916096632	T	T	T
0.7298573941211037	0.7337356013058568	0.6379931864809216	T	T	T
0.0083500000000001	0.7340200000000010	0.3705700000000007	F	F	F
0.6700259517801574	0.0635787364488179	0.5390397991439241	T	T	T
0.3387952083014680	0.4066268200285208	0.7061745799704656	T	T	T
0.7367599999999968	0.2351799999999997	0.3652900000000017	F	F	F
0.3991626142311823	0.5731446338679791	0.5356452315735538	T	T	T
0.0698834823186511	0.9068438091773047	0.7094027490562743	T	T	T
0.6723300000000023	0.6105200000000011	0.3019099999999995	F	F	F
0.3399879135944857	0.9457196084441380	0.4722744736820091	T	T	T
0.0169932342333494	0.2727088222656467	0.6473537651174432	T	T	T

0.7340799999999987	0.0000599999999977	0.3705700000000007	F	F	F
0.3980217394089672	0.3382864865337513	0.5393220904289503	T	T	T
0.0709360642695306	0.6711729083978732	0.7038769116211142	T	T	T
0.4919900000000013	0.7542299999999997	0.3944800000000015	F	F	F
0.1485134744700663	0.0804407532591047	0.5624116570950155	T	T	T
0.8334409723305702	0.4125610978550081	0.7344785413764811	T	T	T
0.5068300000000008	0.2716500000000011	0.3652900000000017	F	F	F
0.1774277119268303	0.6108911486284505	0.5357120914057023	T	T	T
0.8393124710411177	0.9311900419652630	0.7112656584233105	T	T	T
0.1654399999999967	0.0644899999999993	0.3071899999999985	F	F	F
0.8327866146014029	0.3981727826198992	0.4732737256553090	T	T	T
0.5004474940805276	0.7292271680556217	0.6582466986087816	T	T	T
0.9465999999999966	0.3360800000000026	0.3019099999999995	F	F	F
0.6090025850001523	0.6691284994418663	0.4709516950412450	T	T	T
0.2706507886537983	-0.0001136045282533	0.6401295566963985	T	T	T
0.6627999999999972	0.8133499999999998	0.2925400000000025	F	F	F
0.3280896237891725	0.1440976140204423	0.4611457650034722	T	T	T
0.9963788308289925	0.4723195019544538	0.6259803602337504	T	T	T
0.2622300000000024	0.5164199999999965	0.3944800000000015	F	F	F
0.9340049374576197	0.8591053865949680	0.5624225513333083	T	T	T
0.5839900665456661	0.1747945206605981	0.7342353070765031	T	T	T
0.4772099999999995	0.4866799999999998	0.3799399999999977	F	F	F
0.1450741216915488	0.8187847494127027	0.5482198704132279	T	T	T
0.8202676449270502	0.1535254476057135	0.7097424302245120	T	T	T
0.4180899999999994	0.5983700000000027	0.2779999999999987	F	F	F
0.0779884386323637	0.9334166548176026	0.4507590873217243	T	T	T
0.7454822044767432	0.2602021108604211	0.6154032969264231	T	T	T
0.2743899999999968	0.2743299999999991	0.3705700000000007	F	F	F
0.9446031238450741	0.6097217859467187	0.5403560459812449	T	T	T
0.6047509040374296	0.9371632541702735	0.7039776013712933	T	T	T
0.1802800000000033	0.5903199999999984	0.2779999999999987	F	F	F
0.8592070051821541	0.9299919962944975	0.4502075269894798	T	T	T
0.5193611780567239	0.2629192306713781	0.6149853737949247	T	T	T
0.1505500000000026	0.3456100000000006	0.2925400000000025	F	F	F
0.8218105295024148	0.6800856979805214	0.4608116673132495	T	T	T
0.4846077094219561	0.0142769340899942	0.6253777548276285	T	T	T
0.1950599999999980	0.8578600000000023	0.2925400000000025	F	F	F
0.8653253396713378	0.1865540855083086	0.4614065326288142	T	T	T
0.5327087069721398	0.5222014534283375	0.6245074701589339	T	T	T
0.7732299999999981	0.5015799999999970	0.3652900000000017	F	F	F
0.4362003528142600	0.8309279690784750	0.5361086279133498	T	T	T

Table S12 Optimized factional coordinates of the catalyst model with Pt-V_{O6}.

In Pt In O

1.00000000000000

7.2221500012007906 -12.5091307391902902 0.0000000000000060

0.0000000000000000 8.3394204937178671 -11.7937215635675585

14.6850992550548085 8.4784460098618144 5.9951666679957052

In Pt In O

46 1 1 71

Selective dynamics

Direct

0.8515836378845805	0.4089291826345161	0.3472970745831390	F	F	F
0.5138774281850954	0.7414815708031497	0.5101873675033112	T	T	T
0.1768198674770328	0.0767968513058676	0.6843384219480754	T	T	T
0.8291001228075459	0.9356178259191950	0.3251822334614900	F	F	F
0.4952215789173156	0.2664414026139793	0.4960865270142480	T	T	T
0.1588393052158884	0.6036221813838484	0.6574284918173996	T	T	T
0.3248949945999087	0.4314126977115507	0.3251822334614900	F	F	F
0.9924195334836363	0.7633115888697333	0.4931795822608191	T	T	T
0.6600596454912132	0.0969641956242143	0.6698291985182783	T	T	T
0.8403418803460667	0.6722735042768520	0.3362396540223145	F	F	F
0.5066557073075106	0.0054167528912604	0.5044218973676239	T	T	T
0.1714812398071595	0.3322312790071765	0.6693725548579043	T	T	T
0.1065177031116420	0.6835152618153728	0.3251822334614900	F	F	F
0.7768216912713122	0.0157621099738446	0.4932720568349137	T	T	T
0.4241223162004544	0.3398664743129202	0.6580654186827660	T	T	T
0.5994810737807654	0.4426544552500715	0.3472970745831390	F	F	F
0.2671226745540508	0.7774021635480027	0.5099460505562008	T	T	T
0.9302505998258498	0.1041477408487896	0.6844292391097953	T	T	T
0.0952759455731211	0.4426544552500715	0.3472970745831461	F	F	F
0.7654573785568706	0.7766648787777600	0.5148242772901956	T	T	T
0.4355109372011883	0.1168340675441873	0.6783390566937584	T	T	T
0.0727924304960865	0.9018925533036395	0.3251822334614900	F	F	F
0.7430501773176872	0.2302226363967577	0.4955341195803835	T	T	T
0.4054409198513591	0.5600102764798401	0.6594007422095816	T	T	T
0.5657558011652100	0.6610317467383382	0.3472970745831461	F	F	F
0.2327848921163903	0.9924039750498298	0.5171275005452062	T	T	T
0.8951470971441430	0.3228418318354797	0.6796798912598105	T	T	T
0.8403418803460667	0.1680683760692148	0.3362396540223145	F	F	F
0.5039434601503653	0.5028029916625659	0.5028795964681543	T	T	T
0.1627015944144111	0.8341069333230289	0.6701279944911974	T	T	T
0.5657558011652100	0.1568266185306939	0.3472970745831461	F	F	F
0.2315007659939720	0.4944999976066441	0.5103315728327782	T	T	T
0.9065709338660191	0.8336355193588122	0.6836848618529590	T	T	T
0.1065177031116420	0.1793101336077285	0.3251822334614900	F	F	F

0.7761627123556268	0.5133609031448948	0.4984128215689396	T	T	T
0.4488976784899731	0.8502647136186694	0.6575677841641415	T	T	T
0.5769975587037308	0.9018925533036395	0.3251822334614900	F	F	F
0.2418080979905710	0.2301614248309529	0.4908105069218357	T	T	T
0.9112582228441454	0.5651936198023965	0.6718601492655181	T	T	T
0.3473785096769433	0.9131343108421603	0.3472970745831461	F	F	F
0.0158194125328951	0.2442678704794031	0.5163803085413124	T	T	T
0.6906911353112963	0.5851536871393359	0.6798010120441086	T	T	T
0.3361367521384224	0.1680683760692148	0.3362396540223145	F	F	F
0.0022690576560052	0.5052006110815108	0.5047610901443779	T	T	T
0.6768724127600425	0.8473304993987976	0.6687542219794521	T	T	T
0.3361367521384295	0.6722735042768520	0.3362396540223145	F	F	F
0.0046306742079199	0.0039865049519307	0.5058899361739662	T	T	T
0.6779526242388638	0.3327674357086196	0.6770811530502355	T	T	T
0.2541842590098113	0.7461778751490158	0.3944775844339503	F	F	F
0.9294932802735969	0.0740444926555031	0.5621144678085971	T	T	T
0.0094723336752622	0.5311979178146160	0.3799386832336822	F	F	F
0.6774237788043171	0.8635206148570492	0.5468009719457188	T	T	T
0.3396967722053547	0.1884228200220724	0.7128309389927936	T	T	T
0.9439217482440156	0.1009536314534927	0.3071906159917361	F	F	F
0.6084365646025516	0.4370382321519304	0.4739756161020519	T	T	T
0.2818591961599293	0.7768727745330773	0.6577514368957554	T	T	T
0.9074566249617817	0.8429681167905230	0.3071906159917361	F	F	F
0.5724310125686120	0.1765183640472009	0.4752083322643387	T	T	T
0.2324545739475431	0.5098372502966165	0.6566876060987852	T	T	T
0.5217255841393538	0.9989379227400192	0.3799386832336822	F	F	F
0.1900877659270539	0.3301841217541661	0.5474978146867030	T	T	T
0.8562551466775935	0.6718258322998428	0.7133529306125416	T	T	T
0.4100411230105863	0.8281303682776340	0.2780017236106858	F	F	F
0.0741266252260893	0.1488266263954454	0.4494390789853888	T	T	T
0.7410854689792284	0.4871068092695400	0.6190167046707671	T	T	T
0.3978860819165106	0.0618058007524454	0.3019131806672561	F	F	F
0.0630814090766997	0.3998686749645772	0.4722476835276559	T	T	T
0.7328283279588097	0.7385722139996294	0.6349425427939029	T	T	T
0.0083537854409172	0.7340228340549402	0.3705661273773728	F	F	F
0.6711498351778253	0.0636735246591927	0.5394839307627411	T	T	T
0.3314236796714683	0.4018425869504173	0.7053346720829871	T	T	T
0.7367620124481107	0.2351831206849297	0.3652886920528999	F	F	F
0.3998247256408935	0.5697979297963410	0.5374117269281968	T	T	T
0.0736231174467899	0.9110304822411650	0.7093970972954418	T	T	T
0.6723299752512091	0.6105241744987708	0.3019131806672561	F	F	F
0.3405901871471277	0.9454468274350172	0.4726092623406218	T	T	T
0.0081246875284025	0.2771634242998440	0.6378357441052994	T	T	T
0.7340793050292973	0.0000564709743571	0.3705661273773728	F	F	F

0.3958473949179252	0.3369536268406112	0.5374350053130610	T	T	T
0.0732310635452386	0.6733214052003645	0.7055607000106210	T	T	T
0.4919936161392044	0.7542259974054701	0.3944775844339503	F	F	F
0.1494433990647129	0.0791513822420519	0.5619892948124823	T	T	T
0.8308968260647347	0.4132705335142347	0.7328383893828151	T	T	T
0.5068313646520934	0.2716482439671637	0.3652886920528999	F	F	F
0.1772842463515446	0.6104360202004864	0.5357324406473510	T	T	T
0.8426376223444167	0.9366749244688486	0.7084934385380831	T	T	T
0.1654421396247585	0.0644885081712587	0.3071906159917361	F	F	F
0.8320650589148419	0.3991509097698991	0.4745618917651197	T	T	T
0.5003682436134845	0.7270944584220468	0.6565312797545936	T	T	T
0.9466044556628361	0.3360802811640724	0.3019131806672561	F	F	F
0.6086869387994827	0.6683112953351542	0.4719697645211601	T	T	T
0.2743475573853980	0.0003129275834443	0.6388725211398214	T	T	T
0.6628011706015897	0.8133490907390950	0.2925406248109539	F	F	F
0.3286005217561188	0.1444765689384716	0.4614730602812622	T	T	T
0.9951260983441805	0.4765375072540876	0.6266979808701224	T	T	T
0.2622323812662657	0.5164166402760770	0.3944775844339503	F	F	F
0.9357239254265917	0.8600064309720358	0.5617494803542972	T	T	T
0.5884218568099484	0.1800828941324652	0.7313909656173233	T	T	T
0.4772123386006655	0.4866846722759277	0.3799386832336822	F	F	F
0.1446993173953786	0.8180510734213786	0.5483405331516555	T	T	T
0.8205853065417834	0.1560766276066192	0.7144533026687410	T	T	T
0.4180892452670406	0.5983691334046952	0.2780017236106858	F	F	F
0.0785210335652271	0.9331730008768689	0.4502270977557718	T	T	T
0.7501731023797580	0.2588701882883244	0.6124865068997367	T	T	T
0.2743874223603413	0.2743309513859842	0.3705661273773728	F	F	F
0.9409471372925988	0.6091889293076098	0.5427972338688901	T	T	T
0.6049898618574819	0.9360280076636686	0.7046987764201736	T	T	T
0.1802798881376475	0.5903210111482409	0.2780017236106858	F	F	F
0.8603708581296990	0.9301825537541495	0.4495863326329861	T	T	T
0.5217261254759084	0.2713773634329418	0.6174960894080816	T	T	T
0.1505479201374982	0.3456090858136918	0.2925406248109539	F	F	F
0.8215710699529126	0.6800108323303651	0.4606969044697543	T	T	T
0.4874958730520458	0.0152742542391515	0.6260384936426063	T	T	T
0.1950611656761865	0.8578623362777833	0.2925406248109539	F	F	F
0.8650383835707429	0.1862978656352900	0.4600501876074425	T	T	T
0.5309646499211992	0.5118486675055224	0.6335297061631294	T	T	T
0.7732271357303446	0.5015788917631880	0.3652886920528999	F	F	F
0.4365710251032552	0.8309562783883737	0.5361574274840634	T	T	T
0.0975949167250010	0.1656028200398918	0.7079163870469315	T	T	T