

Electronic Supplementary Information

**Reactivity of surface oxygen vacancy sites and frustrated Lewis acid-base
pairs of In_2O_3 catalyst in CO_2 hydrogenation †**

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Computational details

All periodic density functional theory (DFT) calculations were carried out with the Vienna ab initio simulation package (VASP)^{1,2} using the Perdew–Burke–Ernzerhof (PBE)³ exchange–correlation functional and the projector-augmented wave (PAW) potentials⁴. An energy cut-off of 400 eV, and a force convergence of 0.03 eV/Å on all unconstrained atoms were enforced. Gaussian smearing with a smearing width of 0.05 eV was used, and the electronic energy of the supercell was converged to 10⁻⁴ eV. In our previous works^{5,6,7}, results from the PBE calculations are in good agreement with the available experimental results, suggesting the PBE functional to be suitable for studying reactivity of the In₂O₃ surface. Here, accuracy of the computational results using these parameters is also found to be sufficient. Transition state (TS) structures were located using the nudged elastic band (NEB) method⁸. The initial images were generated using the Image Dependent Pair Potential procedure⁹ as implemented in the Atomic Simulation Environment (ASE) package.

The In₂O₃(110) and (111) surfaces were built from the optimized primitive unit cell (PUC) of c-In₂O₃ with lattice parameters of a = 10.21 Å, b = 14.44 Å and c = 15.99 Å. The In₂O₃(110) surface was modeled with a rectangular p(1×√2) supercell with four repeated layers, and was optimized using a Γ-centered Monkhorst–Pack¹⁰ (4×3×1) k-point mesh. The In₂O₃(111) surface was modeled with a p(1×1) supercell with three repeated layers, and was optimized using a Γ-centered Monkhorst–Pack (3×3×1) k-point mesh. These catalyst models are shown in Figure 1(a, b), where the distinct V_O and In sites are labeled. In sites near the V_O sites on the In₂O₃ surface and the adjacent OH groups form SFLPs, so four different SFLPs adjacent to the V_{O4} and V_{O3} sites on the In₂O₃(110) surface and three different SFLPs adjacent to the V_{O4} site on the In₂O₃(111) surface were considered, as shown in Figure 1(c, d). The formation energies of the different V_O sites on the In₂O₃ surfaces and the adsorption energies of CO₂ and CH₂ at the different V_O sites were calculated. The energy barriers of CO and HCOO formations were also calculated. Effects of V_O formation energy on the adsorption energies, energy barriers of CO and HCOO formations, and effects of SFLPs on the CO₂ hydrogenation reaction were examined.

V_O formation energy refers to the energy required to generate a specific V_O site on a given surface, denoted as ΔE_{f,V_O}, which can be calculated from the following equation:

$$\Delta E_{f,V_O} = E_{V_O} + \frac{1}{2}E_{O_2} - E_{Surface}$$

Here, E_{V_O} is the energy of the surface with the specified V_O site, E_{O₂} is the energy of an isolated O₂ molecule, and E_{Surface} is the energy of the surface before V_O formation.

The adsorption energy of CX₂ (X = H, O), denoted by E_{ads,CX₂}, indicates the adsorption strength of CX₂ on the surface, where CX₂ is adsorbed at the V_O site, and

can be calculated from the following equation:

$$E_{\text{ads,CX}_2} = E_{\text{CX}_2^*} - E_{\text{CX}_2} - E_{\text{V}_0}$$

Here, $E_{\text{CX}_2^*}$ is the energy of the surface after the adsorption of CX_2 , and E_{CX_2} is the energy of an isolated CX_2 molecule.

The energy barrier of an elementary reaction, for example direct CO_2 dissociation to CO or CO_2 hydrogenation to HCOO , is denoted as E_a , and can be calculated from the following equation:

$$E_a = E_{\text{TS}} - E_{\text{IS}}$$

Here, E_{TS} is the energy of the transition state, and E_{IS} is the energy of the initial state.

Notes and References

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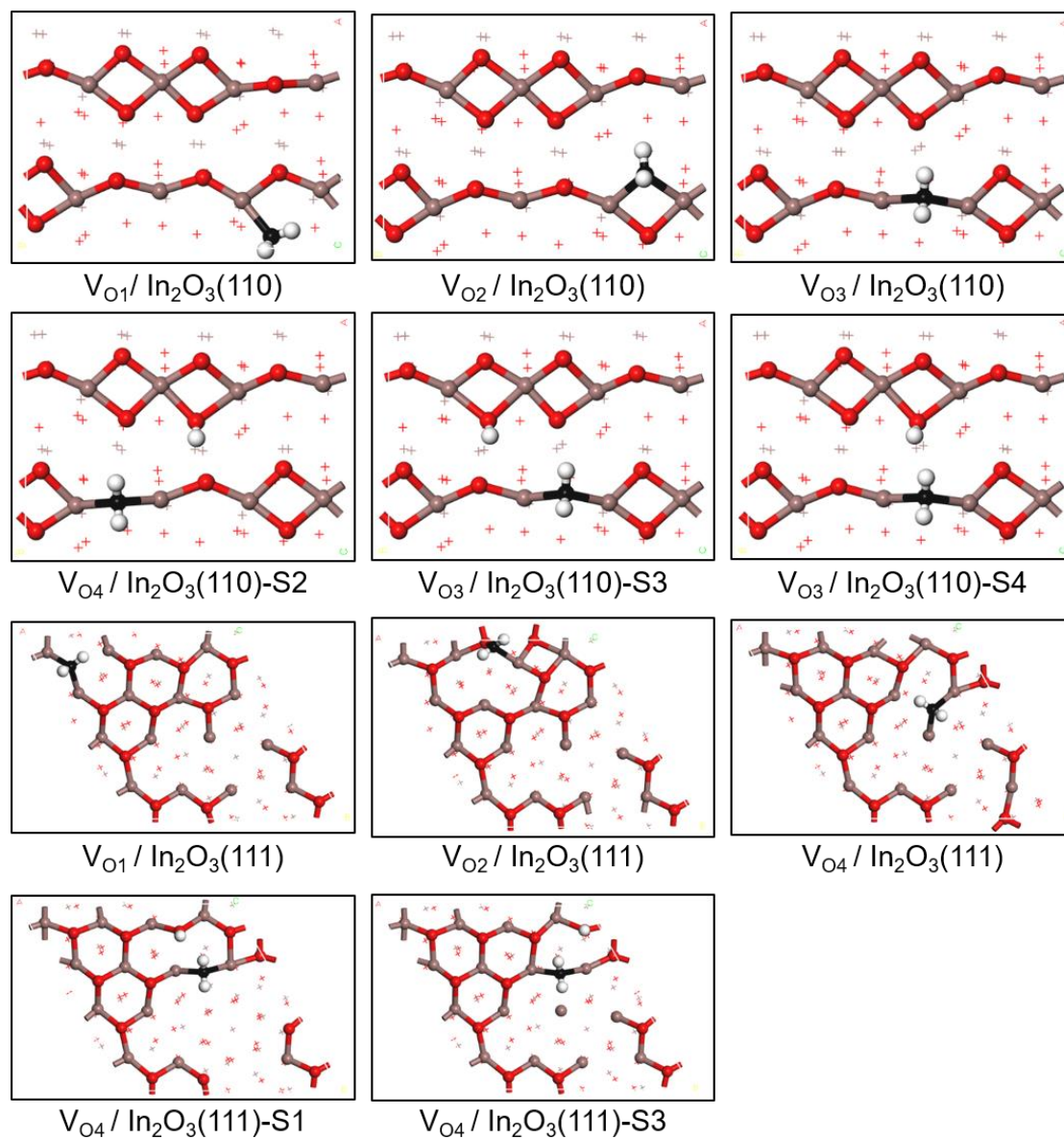


Fig. S1 CH₂ adsorption structures at different oxygen vacancies (red: O, black: C, white: H, grey: In).

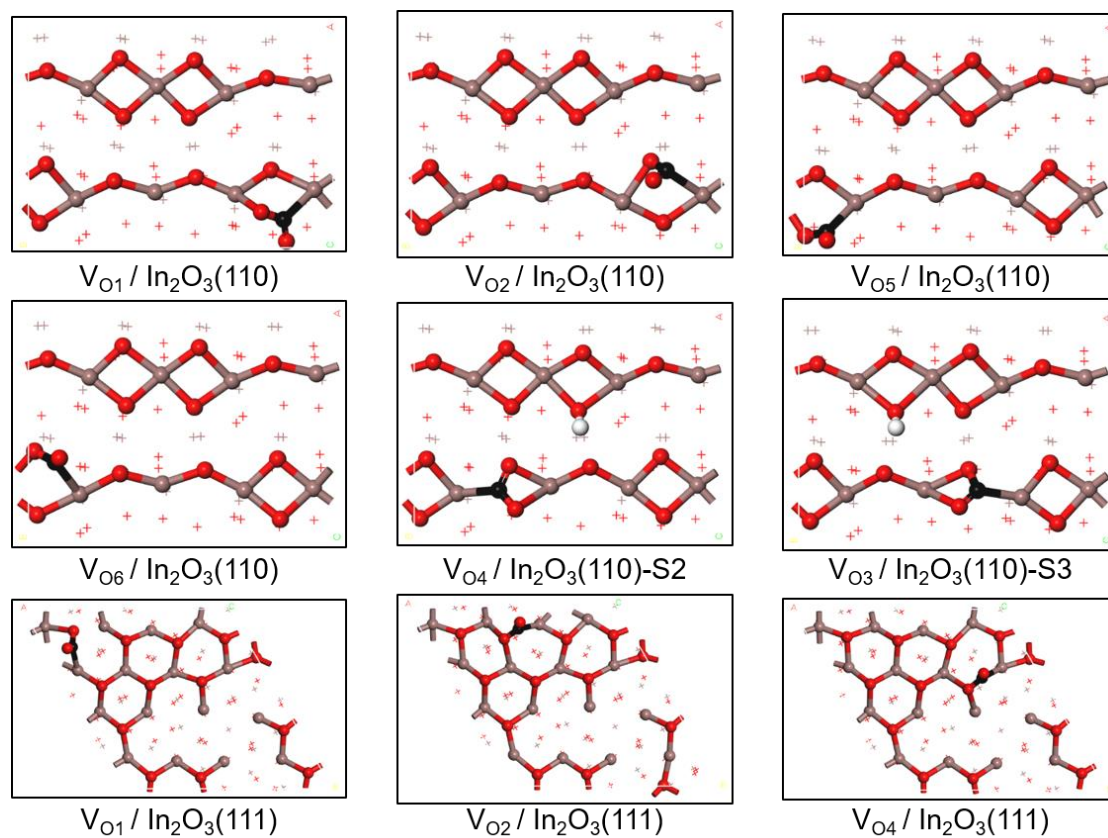


Fig. S2 CO₂ adsorption structures at different oxygen vacancies (red: O, black: C, white: H, grey: In).

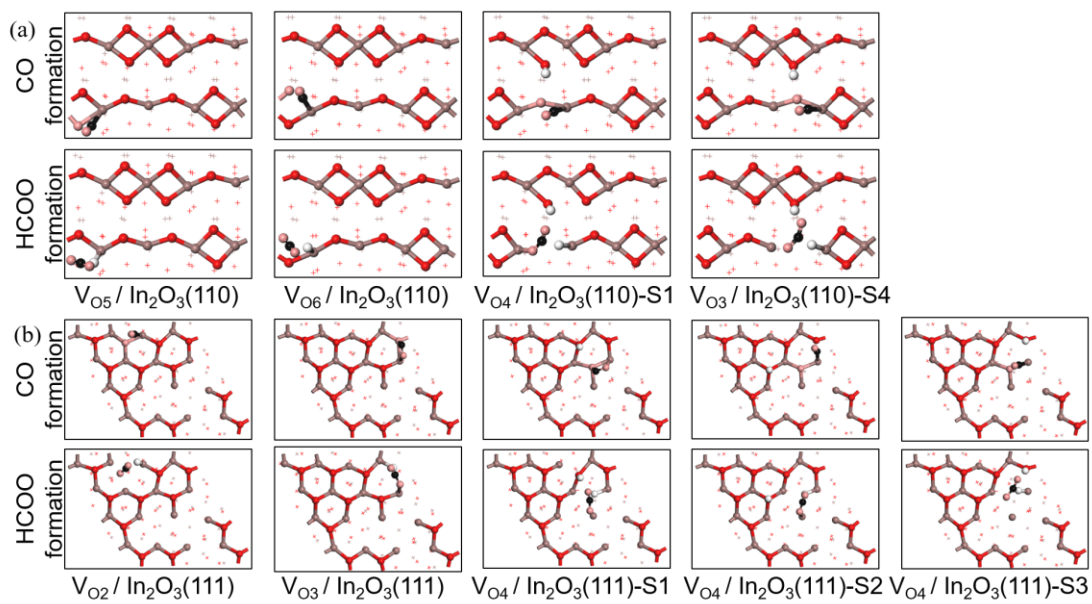


Fig. S3 Transition state structures at different oxygen vacancies (red: O ,black: C, white: H, grey: In).

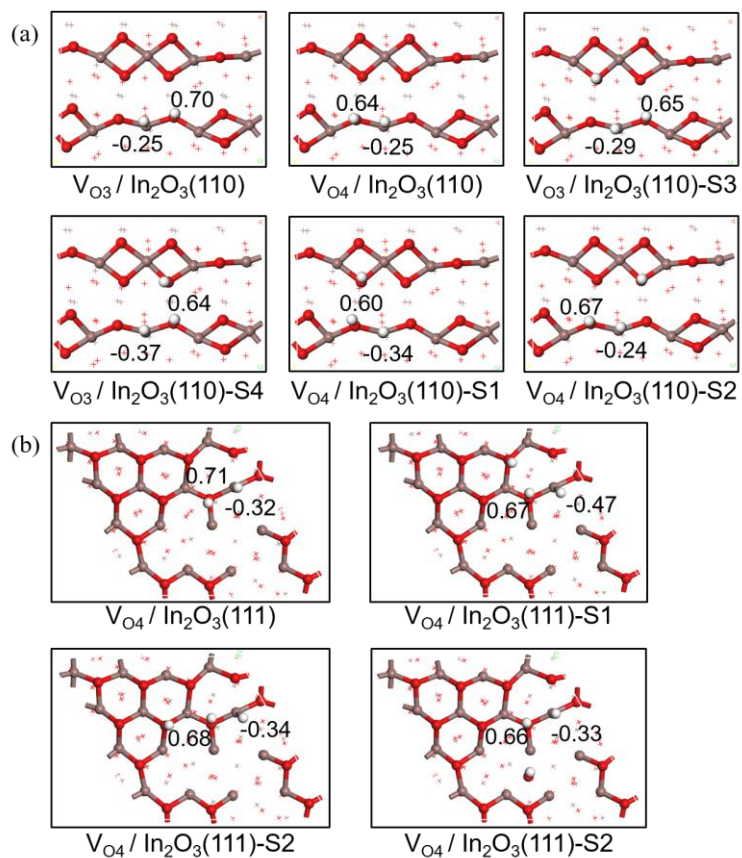


Fig. S4 (a) (b) The structure of H_2 dissociated at different sites. (red: O, black: C, white: H, grey: In)

The charge of H atom after H_2 dissociation has been marked in the figure, H atom in OH has a positive charge, between 0.6 e and 0.7 e, so these H atoms are considered as H^+ . H atom in In-H has a negative charge, between -0.2 e and -0.4 e, so these H atoms are considered as H^- .

Table S1: Oxygen vacancy formation energy, CH₂ adsorption energy in eV and their absolute/relative errors in eV and %

	$\Delta E_{f,VO}$	$\Delta E_{f,VO}$	Error	E_{ads,CH_2}	E_{ads,CH_2}	Error
	All relaxed	Bottom fixed		All relaxed	Bottom fixed	
<i>In₂O₃ (110)</i>						
(110) VO ₁	2.68	2.80	0.12 (4.48%)	-3.87	-3.94	0.07 (1.81%)
(110) VO ₂	2.94	2.80	0.14 (4.76%)	-3.81	-3.63	0.18 (4.72%)
(110) VO ₃	3.01	3.02	0.01 (0.33%)	-5.45	-5.39	0.06 (1.10%)
(110) VO ₄	2.97	3.05	0.08 (2.69%)	-5.28	-5.29	0.01 (0.19%)
(110) VO ₅	2.69	2.75	0.06 (2.23%)	-3.43	-3.60	0.17 (4.96%)
(110) VO ₆	2.72	2.75	0.03 (1.10%)	-3.41	-3.45	0.04 (1.17%)
SELPs1	3.32	3.43	0.11 (3.31%)	-5.30	-5.29	0.01 (0.19%)
SELPs2	3.10	3.18	0.08 (2.58%)	-5.29	-5.26	0.03 (0.57%)
SELPs3	3.13	3.13	0.00 (0.00%)	-5.46	-5.41	0.05 (0.92%)
SELPs4	3.41	3.48	0.07 (2.05%)	-5.42	-5.38	0.04 (0.74%)
<i>In₂O₃ (111)</i>						
(111) OV ₁	2.92	2.82	0.10 (3.42%)	-3.94	-3.82	0.12 (3.05%)
(111) OV ₂	2.77	2.65	0.12 (4.33%)	-3.49	-3.47	0.02 (0.57%)
(111) OV ₃	3.56	3.50	0.06 (1.69%)	-4.33	-4.24	0.09 (2.08%)
(111) OV ₄	3.22	3.23	0.01 (0.31%)	-4.26	-4.23	0.03 (0.70%)
SELPs1	3.74	3.70	0.04 (1.07%)	-4.50	-4.43	0.07 (1.56%)
SELPs2	3.62	3.58	0.04 (1.10%)	-4.05	-3.99	0.06 (1.48%)
SELPs3	3.37	3.35	0.02 (0.59%)	-4.24	-4.36	0.12 (2.83%)
Max Error			0.14 (4.76%)			0.17 (4.96%)

In Table S1, $\Delta E_{f,VO}$ and E_{ads,CH_2} represent the oxygen vacancy formation energy and CH_2 adsorption energy in the article, $\Delta E_{f,VO-1}$ and E_{ads,CH_2-1} represent the oxygen vacancy formation energy and CH_2 adsorption energy after fixing atoms in the bottom of the slab. Their comparison shows that the absolute (relative) error in the calculated $\Delta E_{f,VO}$ ranges from 0.00 eV to 0.14 eV (<4.8%), and that in E_{ads,CH_2} ranges from 0.01 eV to 0.17 eV (<5.0%). In addition, for the oxygen vacancy formation energy, the absolute (relative) error for the V_{O3} and V_{O4} sites on $In_2O_3(110)$ and the V_{O4} site on $In_2O_3(111)$ is less than 0.08 eV (<2.7%), whereas for the CH_2 adsorption energy, the absolute (relative) error for the V_{O3} and V_{O4} sites on $In_2O_3(110)$ and the V_{O4} site on $In_2O_3(111)$ is less than 0.06 eV (<1.1%). Therefore, the effect of fixing atoms in the bottom layer of the slab on the reaction energies can be expected to be rather small.

Table S2 Oxygen vacancy formation energies and changes in the Bader charges of the In atoms.

Oxygen vacancy	$\Delta E_{f,VO}/eV$	In Charge	In Charge	In Charge	Sum of changes
<i>In₂O₃ (110)</i>					
(110) Vo ₁	2.68	In1: -0.13 (1.74 e→1.61 e)	In2: -0.51 (1.70 e→1.19 e)	/	-0.64
(110) Vo ₂	2.94	In1: -0.13 (1.74 e→1.61 e)	In2: -0.54 (1.70 e→1.16 e)	/	-0.67
(110) Vo ₃	3.01	In2: -0.56 (1.70 e→1.14 e)	In3: -0.46 (1.71 e→1.25 e)	/	-1.02
(110) Vo ₄	2.97	In3: -0.24 (1.71 e→1.47 e)	In4: -0.72 (1.75 e→1.03 e)	/	-0.96
(110) Vo ₅	2.69	In4: -0.14 (1.75 e→1.61 e)	In1: -0.15 (1.74 e→1.59 e)	/	-0.29
(110) Vo ₆	2.72	In3: -0.13 (1.75 e→1.62 e)	In4: -0.13 (1.74 e→1.61 e)	/	-0.26
SELPs1	3.32	In3: -0.74 (1.65 e→0.91 e)	In4: -0.28 (1.73 e→1.45 e)	/	-1.02
SELPs2	3.10	In3: -0.76 (1.65 e→0.89 e)	In4: -0.26 (1.74 e→1.48 e)	/	-1.02
SELPs3	3.13	In2: -0.44 (1.65 e→1.21 e)	In3: -0.68 (1.73 e→1.05 e)	/	-1.12
SELPs4	3.41	In2: -0.48 (1.65 e→1.17 e)	In3: -0.72 (1.74 e→1.02 e)	/	-1.20
<i>In₂O₃ (111)</i>					
(111) Vo ₁	2.92	In1: -0.18 (1.76 e→1.58 e)	In2: -0.11 (1.79 e→1.68 e)	In5: -0.11 (1.75 e→1.64 e)	-0.40
(111) Vo ₂	2.77	In2: -0.08 (1.79 e→1.71 e)	In3: -0.17 (1.75 e→1.58 e)	In6: -0.11 (1.80 e→1.69 e)	-0.36
(111) Vo ₃	3.56	In4: 0.02 (1.76 e→1.78 e)	In8: -0.27 (1.80 e→1.53 e)	In1: -0.21 (1.76 e→1.55 e)	-0.46
(111) Vo ₄	3.22	In7: -0.20 (1.80 e→1.60 e)	In8: -0.43 (1.80 e→1.37 e)	In9: -0.23 (1.74 e→1.51 e)	-0.86
SELPs1	3.74	In7: -0.25 (1.78 e→1.53 e)	In8: -0.49 (1.75 e→1.26 e)	In9: -0.23 (1.73 e→1.50 e)	-0.97
SELPs2	3.62	In7: -0.27 (1.79 e→1.52 e)	In8: -0.44 (1.75 e→1.31 e)	In9: -0.27 (1.74 e→1.47 e)	-0.98
SELPs3	3.37	In7: -0.14 (1.79 e→1.65 e)	In8: -0.69 (1.71 e→1.02 e)	In9: -0.17 (1.74 e→1.57 e)	-1.00

Table S3 Adsorption energies of CH₂ and changes in the Bader charges of the In atoms.

Oxygen vacancy	E _{ads,CH₂} /eV	In Charge	In Charge	In Charge	Sum of changes
In₂O₃ (110)					
(110) Vo ₁	-3.87	In1: 0.05 (1.61 e→1.66 e)	In2: 0.29 (1.19 e→1.48 e)	/	0.34
(110) Vo ₂	-3.81	In1: -0.01 (1.61 e→1.60 e)	In2: 0.32 (1.16 e→1.48 e)	/	0.31
(110) Vo ₃	-5.45	In2: 0.35 (1.14 e→1.49 e)	In3: 0.24 (1.25 e→1.49 e)	/	0.59
(110) Vo ₄	-5.28	In3: 0.02 (1.47 e→1.49 e)	In4: 0.76 (1.03 e→1.79 e)	/	0.78
(110) Vo ₅	-3.43	In4: -0.05 (1.61 e→1.56 e)	In1: 0.08 (1.59 e→1.67 e)	/	0.03
(110) Vo ₆	-3.41	In4: -0.03 (1.62 e→1.59 e)	In1: 0.09 (1.61 e→1.70 e)	/	0.06
SELPs1	-5.30	In3: 0.54 (0.91 e→1.47 e)	In4: 0.30 (1.45 e→1.57 e)	/	0.84
SELPs2	-5.29	In3: 0.52 (0.89 e→1.45 e)	In4: 0.29 (1.48 e→1.56 e)	/	0.81
SELPs3	-5.46	In2: 0.28 (1.21 e→1.50 e)	In3: 0.63 (1.05 e→1.49 e)	/	0.91
SELPs4	-5.42	In2: 0.33 (1.17 e→1.49 e)	In3: 0.67 (1.02 e→1.51 e)	/	1.00
In₂O₃ (111)					
(111) Vo ₁	-3.94	In1: -0.03(1.58 e→1.55 e)	In2: 0.06 (1.68 e→1.74 e)	In5: -0.07 (1.64 e→1.57 e)	-0.04
(111) Vo ₂	-3.49	In2: 0.02(1.71 e→1.73 e)	In3: -0.12 (1.58 e→1.46 e)	In6: 0.02 (1.69 e→1.71 e)	-0.10
(111) Vo ₃	-4.33	In4: -0.19(1.78 e→1.59 e)	In8: 0.18 (1.53 e→1.71 e)	In1: 0.04 (1.55 e→1.59 e)	0.03
(111) Vo ₄	-4.26	In7: 0.14(1.60 e→1.74 e)	In8: 0.16 (1.37 e→1.53 e)	In9: 0.05 (1.51 e→1.56 e)	0.35
SELPs1	-4.50	In7: 0.03 (1.53 e→1.56 e)	In8: 0.30 (1.26 e→1.56 e)	In9: 0.18 (1.50 e→1.68 e)	0.51
SELPs2	-4.05	In7: 0.09 (1.52 e→1.61 e)	In8: 0.35 (1.31 e→1.66 e)	In9: 0.07 (1.47 e→1.54 e)	0.51
SELPs3	-4.24	In7: 0.14 (1.65 e→1.79 e)	In8: 0.47 (1.02 e→1.49 e)	In9: 0.13 (1.57 e→1.70 e)	0.74

Table S4 Adsorption energies of CO₂ and changes in the Bader charges of the In atoms.

Oxygen vacancy	E _{ads,CO2} /eV	In Charge	In Charge	In Charge	Sum of changes
In₂O₃ (110)					
(110) VO ₁	0.82	In1: 0.03 (1.61 e→1.64 e)	In2: 0.51 (1.19 e→1.70 e)	/	0.54
(110) VO ₂	0.69	In1: -0.03 (1.61 e→1.58 e)	In2: 0.57 (1.16 e→1.73 e)	/	0.54
(110) VO ₃	-0.44	In2: 0.16 (1.14 e→1.30 e)	In3: 0.23 (1.25 e→1.48 e)	/	0.39
(110) VO ₄	-0.42	In3: 0.29 (1.47 e→1.76 e)	In4: 0.43 (1.03 e→1.46 e)	/	0.72
(110) VO ₅	0.47	In4: -0.06 (1.61 e→1.55 e)	In1: 0.15 (1.59 e→1.74 e)	/	0.09
(110) VO ₆	0.65	In4: -0.04 (1.62 e→1.58 e)	In1: 0.13 (1.61 e→1.74 e)	/	0.09
SELPs1	-0.56	In3: 0.54 (0.91 e→1.45 e)	In4: 0.30 (1.45 e→1.75 e)	/	0.84
SELPs2	-0.41	In3: 0.52 (0.89 e→1.41 e)	In4: 0.29 (1.48 e→1.77 e)	/	0.81
SELPs3	-0.42	In2: 0.28 (1.21 e→1.49 e)	In3: 0.63 (1.05 e→1.68 e)	/	0.91
SELPs4	-0.62	In2: 0.33 (1.17 e→1.50 e)	In3: 0.67 (1.02 e→1.69 e)	/	1.00
In₂O₃ (111)					
(111) VO ₁	0.59	In1: 0.19 (1.58 e→1.77 e)	In2: 0.10 (1.68 e→1.78 e)	In5: -0.07 (1.64 e→1.57e)	0.22
(111) VO ₂	0.29	In2: 0.10 (1.71 e→1.81 e)	In3: -0.05 (1.58 e→1.53 e)	In6: 0.12 (1.69 e→1.81 e)	0.17
(111) VO ₃	-0.03	In4: -0.01 (1.78 e→1.77 e)	In8: 0.23 (1.53 e→1.76 e)	In1: 0.02 (1.55 e→1.57 e)	0.24
(111) VO ₄	0.36	In7: 0.18 (1.60 e→1.78 e)	In8: 0.13 (1.37 e→1.50 e)	In9: 0.27 (1.51 e→1.78 e)	0.58

Table S5 Relative energies for CO₂ hydrogenation to form the HCOO species (unit: eV).

Oxygen vacancy	In-CO ₂ *+H*	TS(HCOO)	HCOO*	E _a (HCOO)	Frequency of TS/cm ⁻¹
<i>In₂O₃ (110)</i>					
V _{O1}	1.38	1.42	-0.03	0.04	270.06
V _{O2}	0.85	0.96	-0.61	0.11	231.56
V _{O3}	0.68	1.00	-0.44	0.32	291.56
V _{O4}	0.63	0.78	-0.41	0.15	340.83
V _{O5}	0.54	1.44	-0.33	0.90	390.94
V _{O6}	1.36	1.50	-0.33	0.14	321.95
SFLPs1	0.90	1.20	-0.10	0.30	463.12
SFLPs2	0.93	1.21	-0.07	0.28	323.42
SFLPs3	0.79	1.26	-0.18	0.47	402.86
SFLPs4	0.67	1.39	-0.18	0.72	246.76
<i>In₂O₃ (111)</i>					
V _{O1}	1.08	1.37	0.27	0.29	453.58
V _{O2}	0.94	1.13	-0.48	0.19	383.66
V _{O3}	0.82	1.25	-0.35	0.43	516.19
V _{O4}	1.00	1.43	-0.04	0.43	524.32
SFLPs1	1.06	1.42	0.08	0.36	553.87
SFLPs2	1.11	1.57	0.05	0.46	585.77
SFLPs3	1.18	1.61	0.13	0.42	554.51

Table S6 Relative energies for CO₂ direct dissociation to CO (unit: eV).

Oxygen vacancy	bt-CO ₂ *	TS(CO)	CO*	O*	E _a (CO)	Frequency of TS/cm ⁻¹
<i>In₂O₃ (110)</i>						
V _{O1}	0.82	1.23	0.99	0.84	0.41	182.75
V _{O2}	0.69	1.14	0.72	0.58	0.45	218.60
V _{O3}	-0.44	0.68	0.57	0.34	1.12	190.82
V _{O4}	-0.42	0.61	0.57	0.29	1.02	230.19
V _{O5}	0.65	1.19	0.92	0.75	0.54	189.87
V _{O6}	0.47	1.22	0.97	0.83	0.75	201.93
SFLPs1	-0.56	0.44	0.32	0.14	1.00	240.81
SFLPs2	-0.41	0.56	0.51	0.31	0.97	193.84
SFLPs3	-0.53	0.50	0.49	0.29	1.03	270.62
SFLPs4	-0.62	0.38	0.22	0.04	1.00	235.51
<i>In₂O₃ (111)</i>						
V _{O1}	0.59	1.37	0.86	0.84	0.78	295.97
V _{O2}	0.29	1.07	0.95	0.86	0.78	215.08
V _{O3}	-0.03	0.68	0.12	-0.01	0.71	262.37
V _{O4}	0.36	0.86	0.56	0.53	0.50	267.69
SFLPs1	/	0.64	-0.04	-0.15	0.64	180.56
SFLPs2	/	0.36	0.14	0.09	0.36	190.39
SFLPs3	/	0.68	0.38	0.32	0.68	249.46

Table S7 Energy barriers of H₂ dissociation (unit: eV).

Oxygen vacancy	E _{a,H2}
<i>In₂O₃ (110)</i>	
V _{O1}	0.54
V _{O2}	0.34
V _{O3}	0.45
V _{O4}	0.62
V _{O5}	0.37
V _{O6}	0.62
SFLPs1	0.48
SFLPs2	0.35
SFLPs3	0.60
SFLPs4	0.60
<i>In₂O₃ (111)</i>	
V _{O1}	0.63
V _{O2}	0.70
V _{O3}	0.53
V _{O4}	0.82
SFLPs1	0.77
SFLPs2	0.56
SFLPs3	0.65

Table S8 Optimized fractional coordinates of the In₂O₃(110) surface.

O In

1.0000000000000000		
10.2136999999999993	0.0000000000000000	0.0000000000000000
0.00000000000000009	14.4443000000000001	0.0000000000000000
0.00000000000000010	0.00000000000000010	15.9873999999999992

O In
48 32

Direct

0.6083428230800030	0.1821215359988391	0.4369380184058317	T	T	T
0.1083428230800027	0.6821215359988391	0.4369380184058317	T	T	T
0.1094363580034473	0.9648884489568584	0.4555553453986410	T	T	T
0.6094363580034472	0.4648884489568584	0.4555553453986410	T	T	T
0.3254848780506642	0.5826213985373794	0.3473318207177140	T	T	T
0.8254848780506642	0.0826213985373793	0.3473318207177140	T	T	T
0.8260020925417190	0.5646746294712682	0.5352225378989747	T	T	T
0.3260020925417190	0.0646746294712684	0.5352225378989747	T	T	T
0.1003999706780155	0.9668908476826428	0.6656460498037335	T	T	T
0.6003999706780154	0.4668908476826428	0.6656460498037335	T	T	T
0.3268381527760965	0.8182488361835055	0.3459993695232036	T	T	T
0.8268381527760965	0.3182488361835055	0.3459993695232036	T	T	T
0.6043109270843865	0.6849245476091186	0.6826411166279759	T	T	T
0.1043109270843867	0.1849245476091188	0.6826411166279759	T	T	T
0.8351846750035605	0.3289409540641913	0.5384322950722678	T	T	T
0.3351846750035606	0.8289409540641913	0.5384322950722678	T	T	T
0.5603190575872750	0.6966087736704329	0.4613955375896568	T	T	T
0.0603190575872748	0.1966087736704329	0.4613955375896568	T	T	T
0.3878793855271461	0.0665096639563859	0.3210391325717529	T	T	T
0.8878793855271462	0.5665096639563859	0.3210391325717529	T	T	T
0.8758499618203253	0.0847275218231312	0.5582585050059113	T	T	T

0.3758499618203254	0.5847275218231311	0.5582585050059113	T	T	T
0.0600052737669815	0.4586098865427559	0.4423391707361337	T	T	T
0.5600052737669815	0.9586098865427558	0.4423391707361337	T	T	T
0.7981607347463098	0.2150341764968214	0.6877865182044192	T	T	T
0.2981607347463097	0.7150341764968214	0.6877865182044192	T	T	T
0.3116026387886767	0.4368160890317112	0.6796880569330696	T	T	T
0.8116026387886767	0.9368160890317183	0.6796880569330696	T	T	T
0.0939569927825695	0.3204464216590973	0.3151540740771181	T	T	T
0.5939569927825694	0.8204464216590971	0.3151540740771181	T	T	T
0.6069820511261995	0.8391767716059221	0.5754984734305879	T	T	T
0.1069820511261997	0.3391767716059221	0.5754984734305879	T	T	T
0.3325098125593699	0.4267397947097418	0.4595683451534162	T	T	T
0.8325098125593700	0.9267397947097420	0.4595683451534162	T	T	T
0.0906216482510172	0.0851911342083012	0.3123923755926927	T	T	T
0.5906216482510172	0.5851911342083013	0.3123923755926927	T	T	T
0.8287523751236080	0.7205200792257886	0.4368591155133884	T	T	T
0.3287523751236079	0.2205200792257886	0.4368591155133884	T	T	T
0.5969658153747263	0.0702687422077286	0.5838934580180218	T	T	T
0.0969658153747263	0.5702687422077287	0.5838934580180218	T	T	T
0.8733359482790036	0.6974254988451853	0.6686327238701679	T	T	T
0.3733359482790036	0.1974254988451854	0.6686327238701679	T	T	T
0.0300060410821778	0.8339050571699889	0.3248364395012205	T	T	T
0.5300060410821777	0.3339050571699890	0.3248364395012205	T	T	T
0.5577861020572096	0.3122064445353567	0.5629169872554650	T	T	T
0.0577861020572095	0.8122064445353567	0.5629169872554650	T	T	T
0.3681068522871402	0.9523514997506451	0.6848400816119061	T	T	T
0.8681068522871401	0.4523514997506453	0.6848400816119061	T	T	T
0.9672588604138499	0.2175917950161028	0.5835113993648092	T	T	T
0.4578642501252143	0.9300149222408519	0.3307345982705630	T	T	T
0.9578642501252141	0.4300149222408519	0.3307345982705630	T	T	T

0.4672588604138498	0.7175917950161028	0.5835113993648092	T	T	T
0.2197158900674743	0.5582751364735336	0.4603161767097189	T	T	T
0.2136161334356610	0.0915235569049950	0.4218755434027682	T	T	T
0.7136161334356611	0.5915235569049951	0.4218755434027682	T	T	T
0.7197158900674743	0.0582751364735337	0.4603161767097189	T	T	T
0.7442861692658064	0.5736695727439871	0.6646181053776383	T	T	T
0.1810881729654220	0.8248200329316175	0.4406828766877843	T	T	T
0.6810881729654290	0.3248200329316176	0.4406828766877843	T	T	T
0.2442861692658065	0.0736695727439869	0.6646181053776383	T	T	T
0.4637166537784854	0.1824930474386829	0.5476518254178890	T	T	T
0.9666118805511511	0.9710102516312472	0.3526602059708915	T	T	T
0.4666118805511510	0.4710102516312472	0.3526602059708915	T	T	T
0.9637166537784855	0.6824930474386831	0.5476518254178890	T	T	T
0.2199060471478881	0.8461676448981347	0.6541776092766940	T	T	T
0.2326413378491865	0.3025360939495086	0.6742496541390306	T	T	T
0.7326413378491865	0.8025360939495090	0.6742496541390306	T	T	T
0.7199060471478880	0.3461676448981346	0.6541776092766940	T	T	T
0.6775384794461232	0.8257264735290554	0.4430394862328090	T	T	T
0.2531722875519335	0.5763511875231372	0.6678045626850462	T	T	T
0.7531722875519337	0.0763511875231372	0.6678045626850462	T	T	T
0.1775384794461231	0.3257264735290553	0.4430394862328090	T	T	T
0.9610153159705757	0.1997457020641322	0.3405082226888251	T	T	T
0.4647989539034962	0.9512713887214392	0.5655840289924665	T	T	T
0.9664998574227760	0.6993789979417215	0.3396506785460203	T	T	T
0.4659791417273259	0.4474354420490636	0.5667694777237950	T	T	T
0.9659791417273259	0.9474354420490634	0.5667694777237950	T	T	T
0.4610153159705755	0.6997457020641322	0.3405082226888251	T	T	T
0.9647989539034963	0.4512713887214390	0.5655840289924665	T	T	T
0.4664998574227758	0.1993789979417215	0.3396506785460203	T	T	T

Table S9 Optimized fractional coordinates of the $\text{In}_2\text{O}_3(110)$ -S1 surface.

O In H

1.0000000000000000		
10.2136999999999993	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.4443000000000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	15.9873999999999992

O	In	H
47	32	1

Selective dynamics

Direct

0.6095686820254770	0.1825114159645722	0.4381487546460453	T	T	T
0.1087755503256958	0.6837267130630117	0.4380760929483463	T	T	T
0.1104294540235488	0.9630634557161379	0.4562199416361755	T	T	T
0.6101560773873370	0.4669528846377826	0.4570635829020565	T	T	T
0.3266539379042760	0.5848428137919939	0.3513660417451590	T	T	T
0.8257243504928218	0.0813297348010074	0.3466417621759503	T	T	T
0.8288436381236814	0.5635665508648882	0.5339327126279299	T	T	T
0.3285786075623168	0.0621782484463505	0.5352262153034306	T	T	T
0.0993096973212565	0.9732814086921442	0.6641499747218254	T	T	T
0.6045400519654289	0.4705413993896739	0.6680745866612290	T	T	T
0.3318388234254163	0.8177085036304803	0.3489235124782502	T	T	T
0.8282280883024253	0.3174220783425004	0.3455766306097673	T	T	T
0.5843373546081168	0.6914487117635293	0.6911891883668372	T	T	T
0.1063778739625133	0.1863009871044712	0.6828143100028783	T	T	T
0.8372614679959249	0.3297141393924857	0.5371836788037235	T	T	T
0.3310291285695274	0.8231023682765823	0.5435581068209631	T	T	T
0.5675363313296302	0.6955409886803833	0.4551778260792210	T	T	T
0.0627322035562031	0.1946856467834246	0.4609770327509996	T	T	T
0.3894827107164080	0.0663701676419853	0.3230685179263911	T	T	T
0.8902642247123460	0.5650115738695870	0.3195316220643138	T	T	T

0.8741017712469671	0.0862542654574298	0.5578269791827184	T	T	T
0.3733470368224049	0.5896293842688191	0.5673777080091194	T	T	T
0.0636025601043780	0.4591420296240140	0.4405135683244523	T	T	T
0.5619842398437710	0.9547271995863184	0.4436499126616033	T	T	T
0.8025170943944021	0.2172656978427500	0.6883848192717004	T	T	T
0.3150162304177613	0.4331068385863817	0.6755101978372721	T	T	T
0.8139624003881055	0.9412269171459934	0.6827625451317587	T	T	T
0.0970576866089496	0.3185370078578923	0.3154008655653363	T	T	T
0.5963151283999035	0.8208150118032621	0.3118673486395753	T	T	T
0.6087734706105764	0.8330187214499214	0.5750309230839526	T	T	T
0.1099538420656946	0.3375184400508470	0.5735714823033832	T	T	T
0.3341759310236440	0.4291815027625749	0.4626179287615615	T	T	T
0.8343592807071639	0.9265028173522089	0.4593199853076924	T	T	T
0.0921685292815338	0.0839277281266352	0.3124955412833726	T	T	T
0.5907181721806120	0.5832975917714009	0.3092193616211075	T	T	T
0.8321389493782224	0.7187390398341894	0.4346047159141810	T	T	T
0.3312048039532282	0.2202072859270919	0.4384504220523315	T	T	T
0.5975079332706037	0.0682401186146862	0.5847906967827290	T	T	T
0.0991933899927908	0.5710901008850312	0.5843648098486605	T	T	T
0.8537304451054462	0.6957578031432488	0.6662524738335371	T	T	T
0.3769075864639577	0.1951434561849290	0.6685592851418450	T	T	T
0.0324801680597876	0.8336669843283414	0.3243587959243004	T	T	T
0.5303842841142344	0.3352711379718472	0.3275553062026847	T	T	T
0.5597583548098124	0.3138970693904501	0.5651757325996579	T	T	T
0.0525526297980516	0.8117906033901623	0.5696225399610874	T	T	T
0.3683927568421850	0.9486866534691396	0.6857058429398595	T	T	T
0.8748977351599391	0.4487759814773148	0.6839049709243311	T	T	T
0.9699343982332935	0.2180700852325546	0.5826746927001843	T	T	T
0.4602802974825161	0.9303608039543115	0.3300754501046473	T	T	T
0.9608806927618003	0.4280310840553849	0.3295013586690471	T	T	T

0.4718456293876815	0.7162054720961553	0.5690356587758626	T	T	T
0.2210727527121934	0.5596448587745998	0.4650531429070570	T	T	T
0.2160551900157550	0.0906985844125315	0.4216227433168199	T	T	T
0.7198073080926195	0.5880953923007968	0.4166321539304130	T	T	T
0.7199809717312891	0.0582348139135238	0.4599142640794607	T	T	T
0.7541110633758343	0.5671586516619401	0.6627886963139418	T	T	T
0.1804537847222987	0.8243617253286918	0.4386013573198021	T	T	T
0.6818465330502508	0.3264570205423368	0.4405745060960595	T	T	T
0.2467884059282460	0.0758251409452030	0.6640940895425119	T	T	T
0.4666550225871691	0.1826580228413016	0.5477674175447644	T	T	T
0.9679348668655058	0.9708179362778236	0.3510499683816460	T	T	T
0.4657702049540661	0.4719075641715568	0.3549600677781467	T	T	T
0.9641523173816748	0.6812137591698525	0.5465611317359045	T	T	T
0.2131453657898163	0.8514684073886558	0.6552989715168217	T	T	T
0.2357021072055678	0.3016381106153945	0.6739726222426455	T	T	T
0.7343307658093936	0.8107775764183430	0.6759401292688404	T	T	T
0.7226115299502337	0.3460486108162925	0.6531873315191220	T	T	T
0.6840746601102794	0.8250794857443519	0.4380698758820298	T	T	T
0.2458218580033192	0.5780554399171043	0.6831734373068362	T	T	T
0.7533399272694584	0.0803285020411364	0.6688923662045777	T	T	T
0.1809857707891052	0.3256408579870759	0.4426590498978161	T	T	T
0.9620792475202256	0.1987647227008275	0.3407450977467305	T	T	T
0.4664387628552888	0.9498217898713996	0.5661893235217931	T	T	T
0.9707396290424530	0.6979204138636090	0.3372015295390568	T	T	T
0.4627630389826733	0.4480659584594089	0.5717583805528610	T	T	T
0.9663271446948107	0.9506326473695527	0.5652624204389221	T	T	T
0.4638074840213340	0.6990290699852859	0.3356362451887697	T	T	T
0.9711635574503381	0.4500330209274394	0.5637353202265214	T	T	T
0.4678857751602116	0.2000547804561949	0.3397954827116389	T	T	T
0.5261372081412165	0.6763532813608948	0.7379284034407385	T	T	T

Table S10 Optimized fractional coordinates of the In₂O₃(110)-S2 surface.

O In H

1.0000000000000000		
10.2136999999999993	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.4443000000000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	15.9873999999999992

O	In	H
47	32	1

Selective dynamics

Direct

0.6091085439923705	0.1843363085505927	0.4394681387796644	T	T	T
0.1081972113103023	0.6830949060102905	0.4375882644904662	T	T	T
0.1115686132259114	0.9639151433546352	0.4560162043075416	T	T	T
0.6066782372940802	0.4669826888258562	0.4587884538252157	T	T	T
0.3258457053777851	0.5847946907141761	0.3503920949489518	T	T	T
0.8256903496598379	0.0829509006333808	0.3467825524025669	T	T	T
0.8229171252582268	0.5650647897119760	0.5366699405172679	T	T	T
0.3293223641769994	0.0620185819101196	0.5353075790701763	T	T	T
0.0998439094680252	0.9726992018112537	0.6639584017488318	T	T	T
0.5910046816623628	0.4688555761940915	0.6765861826574461	T	T	T
0.3309726415978233	0.8185668996930843	0.3491859960704950	T	T	T
0.8278982721000288	0.3183788705902972	0.3458447500355569	T	T	T
0.6029021513950520	0.6846011964747032	0.6815342703064940	T	T	T
0.1084251858676314	0.1865160850796762	0.6831926610515067	T	T	T
0.8360011032372627	0.3284091914434518	0.5384220293780415	T	T	T
0.3359851692880759	0.8195845937685499	0.5453182817544324	T	T	T
0.5669244628316878	0.6956325945559534	0.4551396438478212	T	T	T
0.0619834888502303	0.1958805555522612	0.4615200737732760	T	T	T
0.3884230523715776	0.0675465066281198	0.3228586598473288	T	T	T
0.8885885628526127	0.5661395278746344	0.3209838622873479	T	T	T

0.8753001664710450	0.0860224151616127	0.5580742191209650	T	T	T
0.3731668988321864	0.5876405669564826	0.5652534334785133	T	T	T
0.0592604655712402	0.4585474847329098	0.4414186098045622	T	T	T
0.5617588918287103	0.9573762865195553	0.4419702618881632	T	T	T
0.8024793850130962	0.2135595332178840	0.6907011035452638	T	T	T
0.3241491544197035	0.4330184205520236	0.6783322088229555	T	T	T
0.8146266485418353	0.9364083178457249	0.6791803960408092	T	T	T
0.0957544540752075	0.3192810887433598	0.3148705222331851	T	T	T
0.5953374079071080	0.8209968840334464	0.3119623717368330	T	T	T
0.6117314948494778	0.8369822783435210	0.5721201431130664	T	T	T
0.1075678199659807	0.3400571040723840	0.5765083186938544	T	T	T
0.3298610797663590	0.4281035905673463	0.4584981890554497	T	T	T
0.8348723129458236	0.9276050490436294	0.4581526652298754	T	T	T
0.0919215824550402	0.0850914926070946	0.3127274415732229	T	T	T
0.5910225778205559	0.5832542195571420	0.3099288929776988	T	T	T
0.8322823478068538	0.7197023655622468	0.4362671506256715	T	T	T
0.3306415373905224	0.2211819360948866	0.4395986086527902	T	T	T
0.5984892731509838	0.0684978621219808	0.5847439100075182	T	T	T
0.0980681676384485	0.5686736634539123	0.5839042723738963	T	T	T
0.8749346919338202	0.6989393017703059	0.6694014149052644	T	T	T
0.3783384881845775	0.1953391418350961	0.6688609971610935	T	T	T
0.0324337662938101	0.8342500847359982	0.3247234327144568	T	T	T
0.5311394545167579	0.3359071926985310	0.3277666748419225	T	T	T
0.5589946045978196	0.3157710032200963	0.5678139872770209	T	T	T
0.0587207190851156	0.8126559688626053	0.5654938698904073	T	T	T
0.3692971146322558	0.9495948748627969	0.6853525062423336	T	T	T
0.8550364721719718	0.4517467274110533	0.6825053631028699	T	T	T
0.9713218706309037	0.2168947271908311	0.5836975864937218	T	T	T
0.4595303584889600	0.9311126057077928	0.3294563882908160	T	T	T
0.9598358426348365	0.4292631332752011	0.3288621261545500	T	T	T

0.4813365840638010	0.7132568704700084	0.5734878203650707	T	T	T
0.2184562541047324	0.5595381174691119	0.4636742087989343	T	T	T
0.2164352592176957	0.0909378217649585	0.4217101170368571	T	T	T
0.7180279148260591	0.5898367680435880	0.4182528371876089	T	T	T
0.7204397139597797	0.0590831976722568	0.4599255699455979	T	T	T
0.7493075334827267	0.5779156731709408	0.6657487888530641	T	T	T
0.1816364182060746	0.8243021942578498	0.4401325105691620	T	T	T
0.6819503597876715	0.3272143861514774	0.4398617522893441	T	T	T
0.2479498691202760	0.0751905078463661	0.6642040975659025	T	T	T
0.4668757105751198	0.1820284057726663	0.5480897402768868	T	T	T
0.9684019563334028	0.9715225761046269	0.3514902722068873	T	T	T
0.4651982066454124	0.4725069713268799	0.3527298092040024	T	T	T
0.9659904192014825	0.6816342379256872	0.5473163751800636	T	T	T
0.2156326409331293	0.8517410671907585	0.6539453244977665	T	T	T
0.2377918745913976	0.3021233002282183	0.6739829498720874	T	T	T
0.7343511697618612	0.8040304863505260	0.6736391370200115	T	T	T
0.7216211051334023	0.3402223560143636	0.6533997072293884	T	T	T
0.6831838271696661	0.8263311327057850	0.4382155882575742	T	T	T
0.2463584953963387	0.5810260312357964	0.6821232082762595	T	T	T
0.7545959269537483	0.0757275080264907	0.6689232683199814	T	T	T
0.1768513430077337	0.3253902561811681	0.4430463846341915	T	T	T
0.9616806499168369	0.1994788305713363	0.3403147943129727	T	T	T
0.4679190039904228	0.9489934045054850	0.5655701057909700	T	T	T
0.9690342576991116	0.6993653996231654	0.3378098634088213	T	T	T
0.4570548552828174	0.4470753872276068	0.5648253681673867	T	T	T
0.9658496350757373	0.9490732107621355	0.5653778851541238	T	T	T
0.4628338474766877	0.6996327230682788	0.3364844046992401	T	T	T
0.9647847380899376	0.4513402748323037	0.5645146425642301	T	T	T
0.4670284722101288	0.2008252610057442	0.3404513056724052	T	T	T
0.5178823717515557	0.4684269686229706	0.7169072920003807	T	T	T

Table S11 Optimized fractional coordinates of the In₂O₃(110)-S3 surface.

O In H

1.0000000000000000		
10.2136999999999993	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.4443000000000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	15.9873999999999992

O	In	H
47	32	1

Selective dynamics

Direct

0.6093595752629349	0.1821033078725542	0.4362021308187917	T	T	T
0.1097336680146565	0.6821899620486447	0.4368255579133498	T	T	T
0.1086387357914821	0.9654253546145296	0.4559101211125159	T	T	T
0.6177095227839565	0.4635131053058318	0.4482490038451482	T	T	T
0.3264877465435439	0.5821969757916166	0.3489995435202032	T	T	T
0.8272920451994878	0.0831291909389608	0.3488325706920898	T	T	T
0.8261732959274620	0.5630135653822951	0.5349454924967666	T	T	T
0.3266984380667814	0.0653183256222889	0.5355155177742388	T	T	T
0.1017525811896484	0.9664413618048102	0.6661289818727572	T	T	T
0.5959181596662677	0.4686778021080418	0.6640552473977142	T	T	T
0.3269409383200048	0.8171524858192690	0.3445501253435044	T	T	T
0.8321629783806593	0.3176214207205609	0.3429065528327085	T	T	T
0.5947027074508637	0.6857351577686273	0.6944101842847290	T	T	T
0.1017947125342245	0.1807303959553364	0.6832125191713198	T	T	T
0.8403207208536467	0.3292814046868675	0.5376524846350488	T	T	T
0.3324271400416313	0.8326052958626914	0.5351637561367198	T	T	T
0.5594778189284041	0.6930242776806994	0.4626261576326673	T	T	T
0.0637753944646382	0.1980374503324785	0.4623626519733278	T	T	T
0.3893029261093647	0.0653088094496129	0.3227576875123411	T	T	T
0.8910460018941021	0.5654280684659968	0.3213461812150382	T	T	T

0.8759745200829179	0.0855636649009197	0.5588496095297064	T	T	T
0.3744652402151722	0.5786289623770549	0.5654452804026873	T	T	T
0.0641750755637951	0.4575333804731286	0.4438346387651216	T	T	T
0.5617857850962580	0.9562344544593434	0.4442965677731359	T	T	T
0.7998425764029899	0.2173063373147036	0.6887308800965040	T	T	T
0.3073123849313029	0.7180953456913833	0.6835627100405001	T	T	T
0.8125699868477201	0.9409428766137554	0.6830913306286240	T	T	T
0.1007133538631829	0.3204987564363142	0.3162894588036401	T	T	T
0.5956402208141826	0.8189416648981751	0.3173346646830593	T	T	T
0.6023106193687342	0.8327874362522050	0.5790507480099690	T	T	T
0.1171085280787739	0.3416194065409806	0.5800360247367169	T	T	T
0.3380374466117717	0.4272984216779601	0.4577140660752463	T	T	T
0.8320891829126180	0.9257631079613208	0.4618652691915695	T	T	T
0.0924399813582480	0.0850939227795607	0.3127065753794667	T	T	T
0.5907625903147973	0.5861986623020410	0.3096622999713509	T	T	T
0.8296829612321747	0.7192177739893623	0.4357456577781376	T	T	T
0.3319599426305056	0.2205853086334532	0.4366243483453552	T	T	T
0.5972760698900410	0.0716238889054015	0.5838920624042246	T	T	T
0.0987046585400818	0.5720032032035091	0.5851197821968760	T	T	T
0.8561216842152071	0.6965032115196174	0.6654004904083977	T	T	T
0.3731332966317887	0.1988014467943582	0.6684564274267611	T	T	T
0.0301965068826353	0.8348138103032650	0.3252786808405403	T	T	T
0.5321233583468684	0.3336031203393244	0.3220066227518978	T	T	T
0.5623926983194395	0.3139812455303513	0.5607488831503303	T	T	T
0.0550830950155577	0.8114049337780356	0.5649959179017310	T	T	T
0.3706603913155618	0.9529844120160335	0.6848962418021201	T	T	T
0.8669453017543493	0.4501141373790788	0.6850568018065472	T	T	T
0.9707564675823965	0.2175053473176978	0.5837865732517004	T	T	T
0.4588939906174104	0.9287571789332564	0.3317932890883711	T	T	T
0.9645875071875548	0.4295362262089489	0.3305318101591688	T	T	T

0.4549355547289781	0.7178590631590207	0.5782448568863878	T	T	T
0.2217309505574999	0.5583118877322932	0.4633247593956359	T	T	T
0.2163199703397375	0.0910255713157582	0.4215840333503286	T	T	T
0.7187502558121199	0.5909079371812304	0.4170798662327969	T	T	T
0.7204255123153520	0.0581612678178854	0.4612290580341468	T	T	T
0.7474988952623131	0.5692820582924116	0.6633567709611874	T	T	T
0.1794261209385675	0.8256255078643082	0.4387158385695688	T	T	T
0.6878044266357082	0.3219862404000488	0.4370408465500584	T	T	T
0.2457938622289920	0.0735154858011318	0.6648418607179858	T	T	T
0.4630558080315885	0.1844719639141685	0.5474485043137503	T	T	T
0.9660992757476515	0.9716292343097211	0.3528661171095869	T	T	T
0.4674843175999666	0.4705553009424163	0.3467781878880353	T	T	T
0.9638998118308421	0.6818836706616822	0.5466421894963575	T	T	T
0.2213103894345924	0.8473853111369696	0.6541423375460824	T	T	T
0.2268493742413826	0.3004398935205557	0.6866597574720390	T	T	T
0.7335925906612972	0.8098841556985440	0.6761769790902614	T	T	T
0.7203707779358544	0.3452050434263058	0.6525427592862911	T	T	T
0.6785545148557605	0.8239905066278890	0.4444129760258343	T	T	T
0.2482488964523235	0.5726666630431729	0.6805181908934923	T	T	T
0.7526155857541030	0.0798148085122095	0.6687226141794166	T	T	T
0.1824946753822858	0.3255327852057262	0.4450112123756998	T	T	T
0.9655992946655141	0.1998158593269153	0.3403837053967476	T	T	T
0.4654176679406749	0.9523410572946176	0.5658566165947400	T	T	T
0.9694699390881176	0.6992455431624333	0.3382685202634647	T	T	T
0.4836112708474546	0.4519144232884131	0.5534426328449465	T	T	T
0.9682764212282036	0.9489111444531397	0.5667742301977416	T	T	T
0.4609137917154781	0.6993942074674304	0.3400331569125717	T	T	T
0.9701047157867743	0.4509491582392016	0.5667152197820592	T	T	T
0.4676714114533566	0.1990882835350900	0.3380281371240584	T	T	T
0.5265973279121081	0.6792613736644580	0.7372794197115839	T	T	T

Table S12 Optimized fractional coordinates of the $\text{In}_2\text{O}_3(110)$ -S4 surface.

O In H

1.0000000000000000		
10.2136999999999993	0.0000000000000000	0.0000000000000000
0.0000000000000000	14.4443000000000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	15.9873999999999992

O	In	H
47	32	1

Selective dynamics

Direct

0.6086157186081207	0.1847337515849393	0.4383476780325531	T	T	T
0.1099944229419230	0.6817260272170238	0.4363871751337154	T	T	T
0.1095121951051926	0.9663618553358275	0.4547548287242455	T	T	T
0.6155183799432066	0.4638613678334584	0.4517228810027190	T	T	T
0.3264824554165591	0.5827332176686219	0.3496338318895747	T	T	T
0.8262109065850830	0.0847973853281371	0.3483850393981373	T	T	T
0.8247949566440222	0.5638819115008145	0.5364198621790602	T	T	T
0.3270899062638569	0.0655460077143051	0.5347971320871996	T	T	T
0.1019113176229387	0.9664739401824464	0.6646908444388464	T	T	T
0.5828973816379139	0.4663798629332481	0.6736367429084120	T	T	T
0.3263637149461055	0.8180863406301504	0.3434189559785492	T	T	T
0.8318764315528867	0.3190891913269222	0.3425788981103930	T	T	T
0.6073514828520009	0.6817448318859453	0.6838419843614236	T	T	T
0.1027460723140906	0.1803001055092604	0.6831106204577795	T	T	T
0.8388785266089187	0.3270452607056533	0.5382692064832808	T	T	T
0.3371038224232549	0.8306633709425207	0.5350495465251602	T	T	T
0.5591668485749823	0.6928532243297144	0.4637764238096247	T	T	T
0.0628422787225230	0.1982329008811416	0.4611899567787910	T	T	T
0.3891276018888533	0.0667508513200070	0.3221850009040861	T	T	T
0.8895070495047980	0.5666267108853265	0.3219148724334480	T	T	T

0.8761817169238751	0.0851035784452449	0.5585598421450173	T	T	T
0.3750091198762864	0.5759611178965449	0.5668416526596787	T	T	T
0.0615437863268990	0.4573351943433783	0.4435413064595797	T	T	T
0.5615616594222951	0.9590329338861627	0.4428190424232619	T	T	T
0.8011173730771607	0.2124929087717128	0.6918241235227778	T	T	T
0.3018772110792859	0.7183316622763419	0.6811045072543422	T	T	T
0.8134315780804874	0.9361608946129421	0.6799876875798717	T	T	T
0.0991796110810852	0.3214064771096322	0.3149291127278935	T	T	T
0.5953355744171247	0.8190964986883207	0.3181899243172853	T	T	T
0.6056569616958034	0.8369310499683116	0.5769085240854169	T	T	T
0.1133047629189261	0.3417734734182389	0.5805612498237611	T	T	T
0.3346366427119599	0.4263675843037708	0.4553363843019484	T	T	T
0.8322936502312794	0.9269755995113584	0.4600945577800751	T	T	T
0.0915325702522950	0.0859951167111049	0.3117427467041051	T	T	T
0.5910754077780652	0.5861944903875765	0.3111368826152121	T	T	T
0.8298474964762407	0.7201252268723920	0.4372072528640341	T	T	T
0.3313179196140656	0.2216634828800338	0.4373679698166316	T	T	T
0.5978373458709685	0.0722243816184200	0.5840109605148869	T	T	T
0.0980893388332165	0.5695481375121345	0.5849876065605734	T	T	T
0.8778250094823282	0.6996216631875174	0.6684568965850052	T	T	T
0.3733293783936497	0.1992001933724023	0.6682927065587966	T	T	T
0.0299979746434628	0.8352367828419280	0.3250889350885416	T	T	T
0.5329651607937373	0.3346412392057875	0.3234460851172645	T	T	T
0.5616666025294896	0.3162844540203394	0.5656827559023618	T	T	T
0.0593232774745089	0.8128652746842410	0.5606508386740757	T	T	T
0.3710845952245559	0.9534646330921464	0.6841993572357159	T	T	T
0.8510619322423122	0.4511336015997642	0.6825232479903741	T	T	T
0.9727795529453181	0.2153011551457009	0.5832816072105734	T	T	T
0.4587264514791397	0.9295137157792847	0.3313204888603009	T	T	T
0.9638907286704563	0.4311513715892722	0.3292510094895935	T	T	T

0.4638039326670219	0.7158595912730358	0.5850572327398853	T	T	T
0.2204877310700450	0.5582397616395042	0.4635164326749179	T	T	T
0.2164028391269810	0.0912284885414804	0.4207660808513426	T	T	T
0.7168181111354908	0.5926766680208649	0.4195106673748374	T	T	T
0.7202495481066077	0.0591520511248115	0.4609587016270272	T	T	T
0.7509521885813898	0.5786964182687997	0.6647512369677213	T	T	T
0.1818229938905655	0.8260562375171052	0.4391605842594258	T	T	T
0.6879989240509278	0.3234366356605415	0.4362167388988189	T	T	T
0.2464262017022432	0.0730095563163333	0.6643305634601571	T	T	T
0.4629083925831503	0.1841145535284442	0.5480145225258500	T	T	T
0.9658997059958955	0.9722496026527221	0.3526690136378320	T	T	T
0.4674566063578049	0.4716601735035381	0.3466346323670447	T	T	T
0.9675679261472078	0.6828849876967906	0.5467003868403657	T	T	T
0.2221784132395706	0.8478653703779320	0.6521914127749108	T	T	T
0.2262809595953751	0.3005483409068659	0.6866667996297953	T	T	T
0.7336582944771319	0.8030134131177697	0.6747810468611890	T	T	T
0.7221253028974812	0.3380380055839489	0.6531017911124847	T	T	T
0.6778079447840630	0.8251147174865936	0.4451814759656056	T	T	T
0.2462139531302942	0.5756183140649010	0.6810863083263712	T	T	T
0.7539439276935221	0.0746936883545216	0.6686252932116534	T	T	T
0.1792223595918144	0.3254431907529164	0.4441401528395915	T	T	T
0.9646501478004201	0.2004441022405482	0.3390068156450444	T	T	T
0.4661805210181750	0.9519012259817232	0.5650577930754609	T	T	T
0.9681214928199395	0.7004314262584103	0.3388453854376672	T	T	T
0.4756666640844506	0.4491401801206141	0.5518131017004153	T	T	T
0.9672209035526578	0.9476588530856582	0.5661994768410756	T	T	T
0.4605874185195409	0.7002501862739420	0.3417936496136370	T	T	T
0.9660610388520732	0.4508536584091912	0.5659406577538885	T	T	T
0.4673475830906282	0.1999762998517632	0.3390194088571469	T	T	T
0.5211092300335424	0.4747883728899168	0.7199034918364299	T	T	T

Table S13 Optimized fractional coordinates of the $\text{In}_2\text{O}_3(111)$ surface.

In O

1.0000000000000000		
12.5091307398835667	-7.2221499999999965	0.0000000000000000
0.0000000000000000	14.4442999999999984	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.9854999999999947

In O

48 72

Selective dynamics

Direct

0.8500809444936821	0.4045036595857753	0.3542195540493439	T	T	T
0.5138229468809062	0.7386560570138637	0.5111613969919945	T	T	T
0.1806750317032665	0.0790187971616122	0.6824957380599512	T	T	T
0.8277571334974981	0.9294225228063953	0.3276317804376821	T	T	T
0.4945211786853351	0.2704020369207308	0.4977907120424756	T	T	T
0.1589169157445829	0.6040686346645308	0.6564527754039717	T	T	T
0.3218856569574425	0.4351411757060403	0.3323891963249714	T	T	T
0.9928486717518420	0.7633222602196992	0.4920480478395570	T	T	T
0.6579861199458635	0.0987169216582923	0.6697763540177918	T	T	T
0.8334094025559138	0.6774537827197109	0.3415637289879394	T	T	T
0.5037947590415874	0.0037682702683913	0.5051523731830985	T	T	T
0.1751808266568662	0.3314855617864802	0.6688044756341432	T	T	T
0.1172715502786135	0.6865156174885054	0.3324261345601571	T	T	T
0.7747533514681283	0.0155779366945361	0.4919923148036257	T	T	T
0.4451456159351783	0.3504750041297309	0.6694806222523451	T	T	T
0.6038474677536780	0.4497712236958051	0.3541237456909135	T	T	T
0.2697823720885056	0.7795366664217747	0.5112088596604204	T	T	T
0.9294611601282783	0.1055907195201917	0.6824724780580340	T	T	T
0.0987416371035029	0.4452744311243326	0.3397849351241166	T	T	T
0.7631727212586854	0.7748554452468859	0.5182333759960590	T	T	T

0.4353576618260422	0.1173978667271608	0.6769775254689681	T	T	T
0.0789917068407239	0.9027646744852916	0.3277050490583368	T	T	T
0.7380861014193039	0.2282664392259226	0.4979310332719822	T	T	T
0.4045200655230523	0.5589762670044928	0.6563016931414548	T	T	T
0.5632142886722653	0.6579312500427240	0.3396209389787797	T	T	T
0.2336680699950442	0.9925960000529829	0.5183713252875441	T	T	T
0.8911185108587395	0.3219261031264791	0.6770022516460161	T	T	T
0.8481624663802030	0.1750843956826564	0.3415413529516673	T	T	T
0.5042961920125884	0.5046974967263488	0.5048945985399252	T	T	T
0.1607248263460702	0.8332978337220264	0.6689981147948174	T	T	T
0.5586380962730252	0.1582967402247905	0.3542440868344681	T	T	T
0.2289008912735488	0.4944784586760028	0.5113388343844859	T	T	T
0.9027289626938524	0.8277337957613863	0.6823889933706863	T	T	T
0.1056611540934499	0.1806231102931692	0.3276541129266146	T	T	T
0.7801619702301138	0.5138836361434684	0.4977738819381910	T	T	T
0.4493454108581366	0.8495408061703416	0.6565882945580377	T	T	T
0.5732831146647486	0.8912540435376815	0.3323123527786032	T	T	T
0.2451198005687269	0.2336306212551799	0.4919704271201749	T	T	T
0.9096586931388304	0.5631651911287900	0.6696467749749881	T	T	T
0.3505810747116694	0.9097132124290693	0.3397978528350354	T	T	T
0.0158788327807891	0.2451505373570745	0.5182877111584386	T	T	T
0.6864235755278916	0.5731040141264720	0.6767238584363678	T	T	T
0.3310341492333717	0.1602567185484074	0.3415228041594024	T	T	T
0.0046885636529963	0.5041799275722890	0.5051149289931149	T	T	T
0.6768592643818356	0.8476617221951566	0.6688446635015910	T	T	T
0.3375097316283964	0.6709888279138871	0.3215634782825280	T	T	T
0.0042578701038490	0.0041622799461408	0.5051681487211593	T	T	T
0.6709531613504223	0.3374796525500871	0.6869935647246891	T	T	T
0.2644446002681504	0.7486402079214967	0.3952477224264732	T	T	T
0.9220462980075321	0.0781695507270408	0.5631041122953160	T	T	T

0.5949157240385862	0.4232099250045144	0.7317735810170080	T	T	T
0.0134723656577871	0.5316858764644339	0.3845635171133607	T	T	T
0.6759408713589378	0.8629419479166539	0.5481466660996202	T	T	T
0.3414461364438285	0.1893953070831206	0.7119664664992702	T	T	T
0.9366635505952305	0.0973107868867479	0.3040279606620748	T	T	T
0.6124064999133844	0.4388479721967486	0.4746790285812690	T	T	T
0.2821169574903071	0.7761246936878315	0.6579346749168332	T	T	T
0.9110535083652704	0.8436970069908274	0.3040735289713766	T	T	T
0.5697132052780187	0.1778061563366523	0.4747967801341684	T	T	T
0.2323667398756993	0.5100879071397970	0.6569183555069200	T	T	T
0.5223353702474590	0.9949035048747900	0.3845768833335632	T	T	T
0.1911824005658833	0.3322607610345154	0.5481228381234706	T	T	T
0.8522202571513062	0.6669637981600006	0.7118554598568317	T	T	T
0.4234327776001178	0.8330078921728271	0.2769889489362580	T	T	T
0.0784625440669722	0.1605545252976714	0.4470699883260181	T	T	T
0.7488148627076161	0.4883415466633984	0.6137072455181877	T	T	T
0.4036215187507700	0.0725374473755653	0.3064124307298027	T	T	T
0.0638146304187964	0.3988522103795256	0.4712344544018158	T	T	T
0.7271726412433743	0.7340374485842457	0.6404959069924911	T	T	T
-0.0025846106960813	0.7271979195498840	0.3692966709361594	T	T	T
0.6685776256254956	0.0631501661444792	0.5383742960969593	T	T	T
0.3356093247619965	0.4034520653574431	0.7034070668899186	T	T	T
0.7263959024071964	0.2321054637142528	0.3547163469531908	T	T	T
0.3962557693595514	0.5707296234058867	0.5354340361617917	T	T	T
0.0717996262990050	0.9110512418945641	0.7060460654118271	T	T	T
0.6731602211913008	0.6048615986444243	0.3062430542277285	T	T	T
0.3393627181190814	0.9446657850271803	0.4712330584751764	T	T	T
0.0111773550129988	0.2811628799921789	0.6406104896212972	T	T	T
0.7338839081603730	0.0110902147819580	0.3692535549100626	T	T	T
0.3989570811821756	0.3398984436409397	0.5382725750135251	T	T	T

0.0720227090156067	0.6727729628815639	0.7034500129972681	T	T	T
0.4882872015263747	0.7440758117253294	0.3951643847025866	T	T	T
0.1604863991778245	0.0863507705799444	0.5631228913921225	T	T	T
0.8325995466686473	0.4133861947286176	0.7319826655531068	T	T	T
0.5099029521420717	0.2820571405974129	0.3547881166325734	T	T	T
0.1788381575626414	0.6123686024943191	0.5355974409729403	T	T	T
0.8435603022402220	0.9365472440168445	0.7059376292856946	T	T	T
0.1646723255801799	0.0716854571308834	0.3040362378220736	T	T	T
0.8307165270275606	0.3959651109598908	0.4747864958942796	T	T	T
0.4983006405544796	0.7263303898434154	0.6573715231515352	T	T	T
0.9358338445101493	0.3353497063118198	0.3063538407292991	T	T	T
0.6095419131346294	0.6692191296551877	0.4709928584853190	T	T	T
0.2744470362788321	0.9972392840663123	0.6406994350097471	T	T	T
0.6671920254284155	0.8191102803336361	0.2974605182081410	T	T	T
0.3318495587961717	0.1451360313528982	0.4620337859020366	T	T	T
0.9957050930576546	0.4768016567639731	0.6254222544579591	T	T	T
0.2597243650166178	0.5201018262114913	0.3952771971300745	T	T	T
0.9301699364646060	0.8479101768093456	0.5630331920199682	T	T	T
0.5852880812592931	0.1758460311909184	0.7319953984841103	T	T	T
0.4767843523725914	0.4860924547017849	0.3843375148164274	T	T	T
0.1455124958713108	0.8172629912177964	0.5482594595217233	T	T	T
0.8191602685714982	0.1560517536694075	0.7120855447672412	T	T	T
0.4135412343089528	0.5849804210051567	0.2769903065364335	T	T	T
0.0864242691618430	0.9299198983456117	0.4471159730549272	T	T	T
0.7441406276133824	0.2595971720296235	0.6138731134749126	T	T	T
0.2812533001335237	0.2745423447059086	0.3692494108288120	T	T	T
0.9452077849820055	0.6095124894476639	0.5383281095255459	T	T	T
0.6050330414450916	0.9362913142376252	0.7035640059649284	T	T	T
0.1755077584254578	0.5949379951062530	0.2770521005771936	T	T	T
0.8477388123891814	0.9220719637333299	0.4470573144668720	T	T	T

0.5199782518550790	0.2642586357589973	0.6137136445991790	T	T	T
0.1558490414071953	0.3412029686989609	0.2975711255836577	T	T	T
0.8175119588336982	0.6765962762185493	0.4620138337493547	T	T	T
0.4855482353718759	0.0127560113713220	0.6254660803669708	T	T	T
0.1894665188463235	0.8526337265709131	0.2976754350786479	T	T	T
0.8632759151580081	0.1908220307338539	0.4620436151155667	T	T	T
0.5316014412725071	0.5229205705705742	0.6252024979827161	T	T	T
0.7763234659357114	0.4985463140754134	0.3548300134583792	T	T	T
0.4374825360438042	0.8295094366822340	0.5357047018998514	T	T	T
0.0974520221217874	0.1648692009548510	0.7060193027034253	T	T	T

Table S14 Optimized fractional coordinates of the In₂O₃(111)-S1 surface.

In O H

1.0000000000000000		
12.5091307398836005	-7.2221500000000001	0.0000000000000000
0.0000000000000000	14.4443000000000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.9854999999999983

In	O	H
48	71	1

Selective dynamics

Direct

0.8508074533518069	0.4053437404659055	0.3551996836572180	T	T	T
0.5153179328140232	0.7407234097662920	0.5093467173603636	T	T	T
0.1682112991962083	0.0687924315772617	0.6811550697089387	T	T	T
0.8276119980561034	0.9290402106117480	0.3264451812333981	T	T	T
0.4937075651823361	0.2692265158391997	0.4952802093579837	T	T	T
0.1617162244959067	0.6016073736744773	0.6605652031539070	T	T	T
0.3222527387176852	0.4347928374036872	0.3280001756740565	T	T	T
0.9936519625563409	0.7630932968831882	0.4928903387168785	T	T	T
0.6606744848885944	0.0981539823587295	0.6688499393286247	T	T	T
0.8338847403954106	0.6774498177829482	0.3418292408873165	T	T	T
0.5050807586998249	0.0029316412283489	0.5033442871217175	T	T	T
0.1802530397325879	0.3314262432413476	0.6695865595293883	T	T	T
0.1170934462485321	0.6865623124312782	0.3319473931769273	T	T	T
0.7755822862107665	0.0156490928851585	0.4910867745650449	T	T	T
0.4466098321807734	0.3537212705947423	0.6619201465333479	T	T	T
0.6038792690931151	0.4503807474227833	0.3550595250482276	T	T	T
0.2700947150667196	0.7783618340693705	0.5109800586462169	T	T	T
0.9296068064480385	0.1048007121238153	0.6822325699404173	T	T	T
0.0978220437663379	0.4450365433179522	0.3357085989902141	T	T	T
0.7635684970453988	0.7744676049830385	0.5176713816642305	T	T	T

0.4381828483260747	0.1115883846527963	0.6758956454469562	T	T	T
0.0789162745185965	0.9024535240556196	0.3274561864964626	T	T	T
0.7388851980365309	0.2284575729404837	0.4975660625528444	T	T	T
0.4034763025253077	0.5648221503837469	0.6555642409427390	T	T	T
0.5632820844621573	0.6582588211105241	0.3364324678874167	T	T	T
0.2341124537270078	0.9931368124600092	0.5171474072115573	T	T	T
0.8932085350761834	0.3216892198184664	0.6769618756461968	T	T	T
0.8479927425090272	0.1751313993517740	0.3409618282009697	T	T	T
0.5021972446836994	0.5057929675766919	0.5032128321826439	T	T	T
0.1623852194072882	0.8310948367080921	0.6703511425418069	T	T	T
0.5591995900795181	0.1583756424427410	0.3539952137214892	T	T	T
0.2293461127971514	0.4938957101945551	0.5037215750756482	T	T	T
0.9001194502556278	0.8237349698792136	0.6822637100933688	T	T	T
0.1051161471749438	0.1806766302748234	0.3265316909859849	T	T	T
0.7799925986553208	0.5138247581345623	0.4982268678571971	T	T	T
0.4508209143864590	0.8498466009565185	0.6563015572662446	T	T	T
0.5735152605176033	0.8913943741718267	0.3304842097314056	T	T	T
0.2442193284503757	0.2345516844447925	0.4902925856416958	T	T	T
0.9107338896692331	0.5626349935920113	0.6702296143334929	T	T	T
0.3502216860518368	0.9096867077114450	0.3383682356173533	T	T	T
0.0160785658417167	0.2456690935490662	0.5184576414840266	T	T	T
0.6859540485796944	0.5727370148377114	0.6781251692769352	T	T	T
0.3303699091785542	0.1600731361253258	0.3403572581796062	T	T	T
0.0061571362001479	0.5045397198247069	0.5059669773957884	T	T	T
0.6783104294534837	0.8488654310430293	0.6682885820400477	T	T	T
0.3375898141766521	0.6713655151403839	0.3185797156363183	T	T	T
0.0035988612435836	0.0035463572689284	0.5038117619474395	T	T	T
0.6716131809201964	0.3367737477144615	0.6868018691172666	T	T	T
0.2642971178509714	0.7480896784928815	0.3951263791068780	T	T	T
0.9226899055081049	0.0777753592032699	0.5628508249746514	T	T	T

0.5899945899968351	0.4195973741269401	0.7296254609352352	T	T	T
0.0145891220768967	0.5322720844663614	0.3851759381662883	T	T	T
0.6775519475756183	0.8634489050789272	0.5476513933740160	T	T	T
0.3383272847964964	0.1944364445399256	0.7241018789141308	T	T	T
0.9364273617749018	0.0973737275928364	0.3037993690322678	T	T	T
0.6104793812563347	0.4392590510705343	0.4768742289310164	T	T	T
0.2833320949210544	0.7770981001759936	0.6590738279320590	T	T	T
0.9111149525872312	0.8431433567940178	0.3040497462174207	T	T	T
0.5698345547951782	0.1772477278606131	0.4754956850433250	T	T	T
0.2395671102784576	0.5108387424975699	0.6792316671699669	T	T	T
0.5221168515991219	0.9945715080589717	0.3833504582091265	T	T	T
0.1935839042515173	0.3360163883727628	0.5469934295149239	T	T	T
0.8504479389811940	0.6638521055983475	0.7140064776078947	T	T	T
0.4231211350512893	0.8332611166545326	0.2756573047025020	T	T	T
0.0788777828338756	0.1610838791938163	0.4468790730783127	T	T	T
0.7461743246003679	0.4867415309896250	0.6144509209457675	T	T	T
0.4043640288388093	0.0734090330335819	0.3057870590941870	T	T	T
0.0636978615820142	0.3986090577848246	0.4692535193901632	T	T	T
0.7254024681435030	0.7311321111430429	0.6402344977175164	T	T	T
-0.0019090896183959	0.7274010805692904	0.3704584234025686	T	T	T
0.6695912539496921	0.0632865223337920	0.5386180948510342	T	T	T
0.7268834652505268	0.2325899993722211	0.3564047198766725	T	T	T
0.3939461013611365	0.5717763639082030	0.5349662537676083	T	T	T
0.0692427712003768	0.9036716834781252	0.7070407107968454	T	T	T
0.6732382885264606	0.6045393739546848	0.3061983434919559	T	T	T
0.3397404575378940	0.9449920053409309	0.4716878770588299	T	T	T
0.0141953315509184	0.2800254681111025	0.6407643507639158	T	T	T
0.7335988893533631	0.0106664134348226	0.3689237267230120	T	T	T
0.3985102546896716	0.3409781976339489	0.5390039653073179	T	T	T
0.0727390846261977	0.6703967991547475	0.7046743588637115	T	T	T

0.4886627426719400	0.7435929713092841	0.3932889453505262	T	T	T
0.1610279847106719	0.0862286145440143	0.5633012708152682	T	T	T
0.8325616790988708	0.4125409747726430	0.7315723274104515	T	T	T
0.5096720884406152	0.2821629028244134	0.3577424630205113	T	T	T
0.1827903454960576	0.6100625622609469	0.5389013096755273	T	T	T
0.8439818668089968	0.9350696905442054	0.7056830657323803	T	T	T
0.1642090098537579	0.0715246622838425	0.3041228520863312	T	T	T
0.8317890750498346	0.3968154228313281	0.4762907866468614	T	T	T
0.5018624713500967	0.7303716323364801	0.6541891847561028	T	T	T
0.9348583952931573	0.3357952919695552	0.3049978732623503	T	T	T
0.6089020466461160	0.6686794476470070	0.4716194576254475	T	T	T
0.2755751308327156	0.0050395529148572	0.6465376140600840	T	T	T
0.6671474498711661	0.8195331658312712	0.2948859571433915	T	T	T
0.3305147852120602	0.1462412403473045	0.4615957290151727	T	T	T
0.9985976318954677	0.4756987975961244	0.6262418595680739	T	T	T
0.2599681649739310	0.5204347297111890	0.3900493537427308	T	T	T
0.9304979270064848	0.8477437103586145	0.5634474621275949	T	T	T
0.5848966530102149	0.1751064628206095	0.7320715009799278	T	T	T
0.4757547985151917	0.4865659183423310	0.3833778787607493	T	T	T
0.1481795112009031	0.8195605774313004	0.5500697478537603	T	T	T
0.8206573344592648	0.1566753775582697	0.7124249395377573	T	T	T
0.4141257472396161	0.5852667329837675	0.2738339079674996	T	T	T
0.0870266269228103	0.9297893151609991	0.4473949250327228	T	T	T
0.7436797185893944	0.2591306511040874	0.6144147964766973	T	T	T
0.2815052567807724	0.2754900765955813	0.3681192411994809	T	T	T
0.9457748452857109	0.6093463418230721	0.5407460213417603	T	T	T
0.6063103837227197	0.9372939573866788	0.7043904215685126	T	T	T
0.1748991967956015	0.5958263365961233	0.2750920317553965	T	T	T
0.8479199542326802	0.9212350407322519	0.4460887482062597	T	T	T
0.5088053851107665	0.2570146267797025	0.6141646469008416	T	T	T

0.1558216836559397	0.3409111285679322	0.2945229150230081	T	T	T
0.8180489044975020	0.6760810140940593	0.4626901567023251	T	T	T
0.4869533260194656	0.0110277668201908	0.6238624679576835	T	T	T
0.1893515427516556	0.8524020738173056	0.2967344846486240	T	T	T
0.8638855197273996	0.1909102962346161	0.4618157291841994	T	T	T
0.5238285174846590	0.5227323487783782	0.6289037215350344	T	T	T
0.7759695933287108	0.4985678476826974	0.3573287641315377	T	T	T
0.4377576567596724	0.8296740327237441	0.5348698206079908	T	T	T
0.0970739793238673	0.1608193273804745	0.7091672927750861	T	T	T
0.3412907279956475	0.2105820204171609	0.7772476113582458	T	T	T

Table S15 Optimized fractional coordinates of the In₂O₃(111)-S2 surface.

In O H

1.0000000000000000		
12.5091307398836005	-7.2221500000000001	0.0000000000000000
0.0000000000000000	14.4443000000000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.9854999999999983

In	O	H
48	71	1

Selective dynamics

Direct

0.8511526260876371	0.4058853892055009	0.3552831502090294	T	T	T
0.5144278084104660	0.7397229246986252	0.5115662822020711	T	T	T
0.1777192108349129	0.0764296405628012	0.6819430775801471	T	T	T
0.8277632496698907	0.9290100806350134	0.3262361905391851	T	T	T
0.4947670139959712	0.2702622389317283	0.4948189587340523	T	T	T
0.1619352553697199	0.6024234247162948	0.6611503326379837	T	T	T
0.3219866507986795	0.4344017282873824	0.3290015122967286	T	T	T
0.9930299444739668	0.7625128694260890	0.4929016166532458	T	T	T
0.6593504811877708	0.0982207371531012	0.6682075175724864	T	T	T
0.8338580798120144	0.6776624215010377	0.3416039133118386	T	T	T
0.5036708086783235	0.0032872548755673	0.5045311436408764	T	T	T
0.1781374605811900	0.3309399893361455	0.6695724742878513	T	T	T
0.1172078914347468	0.6863450815109947	0.3325537367899111	T	T	T
0.7752886604299332	0.0157504744211767	0.4907969055125044	T	T	T
0.4297976708634089	0.3420837801754416	0.6599181326320867	T	T	T
0.6037096850077119	0.4504478931748164	0.3543310730857656	T	T	T
0.2694272469805782	0.7776534287959574	0.5111965528003580	T	T	T
0.9297522171851108	0.1053185279738971	0.6820899665331288	T	T	T
0.0979551998606245	0.4449707852260275	0.3372637332075679	T	T	T
0.7640070859713907	0.7757766368331744	0.5171304088323058	T	T	T

0.4357162973171336	0.1179492842540523	0.6764357540922060	T	T	T
0.0790165178643137	0.9022462601094469	0.3278882760947091	T	T	T
0.7388848123118357	0.2274253660013386	0.4951748698775205	T	T	T
0.4037333365291275	0.5631726637109179	0.6581785428393371	T	T	T
0.5625489776384455	0.6577722777448053	0.3370774522902797	T	T	T
0.2337005077377461	0.9921951922589247	0.5179705759408491	T	T	T
0.8942025233372684	0.3218061932469378	0.6765822479409339	T	T	T
0.8485157391310403	0.1750284289684894	0.3401727153107088	T	T	T
0.5022267906919426	0.5047929047223618	0.5038265777882683	T	T	T
0.1617823795256284	0.8322744646866258	0.6697494428419852	T	T	T
0.5588079335445729	0.1577422827259869	0.3541932932221474	T	T	T
0.2296795888364194	0.4932237106879336	0.5053396919643552	T	T	T
0.9031631695650117	0.8280072550723743	0.6824776290375868	T	T	T
0.1049703887565174	0.1801652711207384	0.3260560758262975	T	T	T
0.7793467786578002	0.5137248857952066	0.4976272009856121	T	T	T
0.4496506543186892	0.8512266772797344	0.6566823109752116	T	T	T
0.5732897452551622	0.8908792212804637	0.3319503156614485	T	T	T
0.2427737341617336	0.2324664591579289	0.4897173863073845	T	T	T
0.9113535537878877	0.5639112275128134	0.6699646569996304	T	T	T
0.3503313657877767	0.9093792734143874	0.3395758194382923	T	T	T
0.0158405244600488	0.2451425184507826	0.5178990035586278	T	T	T
0.6880120386202021	0.5780288192003428	0.6746767719933179	T	T	T
0.3302682749616122	0.1593428850875972	0.3407292655240702	T	T	T
0.0059312668630801	0.5042959268398596	0.5066262986470770	T	T	T
0.6779540103145453	0.8505370664460481	0.6679692619759483	T	T	T
0.3374225616138147	0.6709111037771390	0.3196855373648117	T	T	T
0.0039937156877988	0.0037133984816854	0.5043799855145276	T	T	T
0.6745257397463730	0.3341283617525495	0.6794480601241408	T	T	T
0.2642861409035096	0.7470504093418734	0.3955675566658693	T	T	T
0.9220911234714897	0.0776348416031255	0.5626817437555339	T	T	T

0.5965038035217635	0.4226457372570743	0.7379557544365833	T	T	T
0.0145038637222137	0.5325240818021814	0.3862231803609349	T	T	T
0.6773929728783107	0.8641848914526475	0.5473729131161965	T	T	T
0.3402292937466753	0.1921875793527963	0.7129067584783673	T	T	T
0.9363855506655334	0.0971060614017957	0.3025946657832967	T	T	T
0.6108368266683095	0.4401100293589276	0.4761514187946341	T	T	T
0.2826536213363580	0.7762290761928818	0.6598401737511594	T	T	T
0.9112662147139067	0.8431109957865041	0.3037986543877568	T	T	T
0.5694053337080077	0.1773188157615472	0.4757490799821758	T	T	T
0.2381311511378787	0.5096812837185757	0.6790511359127807	T	T	T
0.5223290608155332	0.9946105291094589	0.3843525081216614	T	T	T
0.1930350731386574	0.3347081855358469	0.5471991903026795	T	T	T
0.8501244415966004	0.6655159794600053	0.7130863351917477	T	T	T
0.4233183903591022	0.8327863120486415	0.2768949674670953	T	T	T
0.0777412769715712	0.1604980722393209	0.4461328745287457	T	T	T
0.7419621532309965	0.4863012570330059	0.6151614432827940	T	T	T
0.4043452855981714	0.0729014319150496	0.3058749225467147	T	T	T
0.0637861871305776	0.3986258475906531	0.4697365077392745	T	T	T
0.7252212399142355	0.7337249449169353	0.6394638139661328	T	T	T
-0.0023078605202261	0.7269200734015320	0.3706892406219289	T	T	T
0.6687571439352593	0.0629162330338892	0.5382406305370647	T	T	T
0.7268835879710441	0.2324741360038904	0.3573509531000058	T	T	T
0.3947785569821555	0.5692862593216510	0.5373918977203190	T	T	T
0.0715413897715106	0.9087221028053151	0.7063572053730161	T	T	T
0.6730114341955316	0.6048590243560795	0.3062416566789469	T	T	T
0.3388062611628994	0.9438962628605242	0.4710673716661917	T	T	T
0.0132998588103071	0.2805999811065202	0.6397151940953446	T	T	T
0.7340112713023494	0.0108719463176593	0.3685424032394273	T	T	T
0.3973487223613271	0.3400761362226046	0.5370926446663191	T	T	T
0.0724587518577654	0.6717277144244845	0.7048421464775475	T	T	T

0.4887704614396265	0.7428610772651693	0.3950527205454996	T	T	T
0.1606387183026182	0.0866550848111183	0.5627923731889557	T	T	T
0.8316563602416440	0.4128666651214714	0.7297336691706342	T	T	T
0.5100152535798298	0.2822556459652611	0.3577537700286668	T	T	T
0.1828096484558704	0.6094088150122431	0.5393775009493502	T	T	T
0.8431661320115843	0.9358023901928285	0.7060430058289178	T	T	T
0.1642680001235632	0.0710831804949937	0.3041040062311811	T	T	T
0.8312520546717500	0.3970548187192278	0.4763859772291726	T	T	T
0.5014875533116033	0.7296930872849732	0.6533471012730282	T	T	T
0.9349780783381046	0.3361843427423777	0.3052607463647556	T	T	T
0.6083157136135234	0.6674627483025480	0.4742755801602746	T	T	T
0.2748428430930833	-0.0007609884002163	0.6419646842261687	T	T	T
0.6667929168132796	0.8189132037536505	0.2960518696417333	T	T	T
0.3313992307095981	0.1457471296445375	0.4619640498807437	T	T	T
0.9990251653662430	0.4767155626652308	0.6268071795690365	T	T	T
0.2605506933867944	0.5202437827602030	0.3916275910223312	T	T	T
0.9300101386654793	0.8474774328554371	0.5634358986054979	T	T	T
0.5865283069275358	0.1784004024869136	0.7299776996340243	T	T	T
0.4758273053670765	0.4865784777874398	0.3837925282345007	T	T	T
0.1461279714107384	0.8161200397044345	0.5490286236494727	T	T	T
0.8198868263179854	0.1565993666681503	0.7121215086310793	T	T	T
0.4135213430408057	0.5848542759392120	0.2745398586995045	T	T	T
0.0867433892259270	0.9294685990124913	0.4476799624331705	T	T	T
0.7472704118887648	0.2590584106761942	0.6117025645019378	T	T	T
0.2812406967470154	0.2745791899647781	0.3680216633061706	T	T	T
0.9430540108074982	0.6078830088518101	0.5420657718935731	T	T	T
0.6047828649675943	0.9373721567594679	0.7044951795507617	T	T	T
0.1746939642854034	0.5951024793038814	0.2761147542076574	T	T	T
0.8482586707952612	0.9215630433159110	0.4459002851328368	T	T	T
0.5194686242141857	0.2691924055808380	0.6142948943701896	T	T	T

0.1555983539760925	0.3408857336552922	0.2955682032109437	T	T	T
0.8177894215186914	0.6761348911663900	0.4625937347041004	T	T	T
0.4860587927685857	0.0143129783994530	0.6249692428492900	T	T	T
0.1895254145439798	0.8520902190762267	0.2976085176347621	T	T	T
0.8641328235998710	0.1904958798964686	0.4609358765658083	T	T	T
0.5230456312614887	0.5135410841872475	0.6343171558039821	T	T	T
0.7758924706410670	0.4986572640604913	0.3568643903054694	T	T	T
0.4372046495665776	0.8299315483200400	0.5357308199605169	T	T	T
0.0969018163064836	0.1626327936930012	0.7077442873214724	T	T	T
0.5964600657008317	0.4180987675756427	0.7921030553679790	T	T	T

Table S16 Optimized fractional coordinates of the $\text{In}_2\text{O}_3(111)$ -S3 surface.

In O H

1.0000000000000000		
12.5091307398836005	-7.2221500000000001	0.0000000000000000
0.0000000000000000	14.4443000000000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	17.9854999999999983

In O H
48 71 1

Selective dynamics

Direct

0.8506463464963628	0.4056261955878484	0.3546495922565455	T	T	T
0.5154601096529240	0.7420766380056438	0.5086733447650146	T	T	T
0.1830122766555197	0.0717250880895559	0.6804254053357925	T	T	T
0.8278648461882825	0.9291601764932231	0.3268750647021029	T	T	T
0.4950341643382848	0.2703721754564851	0.4948992888496196	T	T	T
0.1623099271744916	0.6047318203060418	0.6592732048350292	T	T	T
0.3222765449681435	0.4345478012024994	0.3276346703735301	T	T	T
0.9932190414364851	0.7625440465199798	0.4926143526960584	T	T	T
0.6586482873999649	0.1003472643514934	0.6690656032239291	T	T	T
0.8338487355333678	0.6774573761259161	0.3418336815778998	T	T	T
0.5048283761193506	0.0047478296085211	0.5031612420022166	T	T	T
0.1869921599363675	0.3440108631739235	0.6710086451940787	T	T	T
0.1171293978629840	0.6867049833187581	0.3312763965686009	T	T	T
0.7748998006277945	0.0156062634811208	0.4906001411096493	T	T	T
0.4457934742692691	0.3461924352770312	0.6643044077866992	T	T	T
0.6034065526201543	0.4512365193665731	0.3558172944875280	T	T	T
0.2704440899774249	0.7785729584100015	0.5093859282180329	T	T	T
0.9187998054682275	0.1004380534402989	0.6811787044923054	T	T	T
0.0976095726580455	0.4451497438830387	0.3338367473422164	T	T	T
0.7631046829879460	0.7738950259540566	0.5182460623309646	T	T	T
0.4372379219438200	0.1178959588243282	0.6762797191530350	T	T	T
0.0789605394101329	0.9026211371062000	0.3279089310271517	T	T	T
0.7394714373007536	0.2287648870438695	0.4974544651703384	T	T	T
0.4033116102196605	0.5695920608527266	0.6549270914674670	T	T	T
0.5626370166749723	0.6581492682598172	0.3361965686849178	T	T	T
0.2340849257078298	0.9923319835210277	0.5166729593535491	T	T	T
0.8949066380734796	0.3230636610698260	0.6773892809099975	T	T	T
0.8487360133604991	0.1755153963158840	0.3410702909679468	T	T	T
0.5000231099987255	0.5046640702381436	0.5049729852870638	T	T	T
0.1619846734679824	0.8309425075010990	0.6683357386752721	T	T	T
0.5598233784726274	0.1588733905817076	0.3534245360001504	T	T	T
0.2290657013191128	0.4949019950118201	0.5014535457494482	T	T	T
0.9019233288767350	0.8253361183724358	0.6827196036432095	T	T	T
0.1054575276384459	0.1808235329157981	0.3275289030338984	T	T	T

0.7797503530294088	0.5140251683221735	0.4985514092691717	T	T	T
0.4509906579593838	0.8540453246000822	0.6554245074571963	T	T	T
0.5737652627933505	0.8918891943078027	0.3301054314575941	T	T	T
0.2443459126320454	0.2351760327877881	0.4919491895143429	T	T	T
0.9106872987525664	0.5641433213243281	0.6698970727223880	T	T	T
0.3507024374283477	0.9103597669866453	0.3381328177380504	T	T	T
0.0171543901472253	0.2462380038746732	0.5192556313472644	T	T	T
0.6844826779862851	0.5725770229142749	0.6796727061288220	T	T	T
0.3302109817060986	0.1602509468591977	0.3415838856014830	T	T	T
0.0058908301725933	0.5042202964597867	0.5053515515663121	T	T	T
0.6758039216344734	0.8474420644170072	0.6679648773796171	T	T	T
0.3375292521451185	0.6716758473367963	0.3168065832436483	T	T	T
0.0034974539775247	0.0033872274260669	0.5048858214046587	T	T	T
0.6733367038682712	0.3382500822722022	0.6862300231801627	T	T	T
0.2646672887966252	0.7474779964033144	0.3937293330765953	T	T	T
0.9220136569566445	0.0775476133154695	0.5636612148602730	T	T	T
0.5919907773436309	0.4203723663283506	0.7304324997263762	T	T	T
0.0147539554527588	0.5322190592628495	0.3842439119388231	T	T	T
0.6778154350967414	0.8637138590333520	0.5473809170287056	T	T	T
0.3402887691933370	0.1925170287036762	0.7116076212719837	T	T	T
0.9370180606752226	0.0974608992810578	0.3043556533132380	T	T	T
0.6106870771703675	0.4414783576734604	0.4772542968118894	T	T	T
0.2834442506427463	0.7778899737180948	0.6573088279317452	T	T	T
0.9111728246525594	0.8431469484017905	0.3042947776553719	T	T	T
0.5706868870775949	0.1777492962551381	0.4743044768200050	T	T	T
0.2433383493120098	0.5202914709548961	0.6823186162462697	T	T	T
0.5227293600788322	0.9950337554025008	0.3827881771536988	T	T	T
0.1939806870069778	0.3391417461635722	0.5467204386208786	T	T	T
0.8506888550953697	0.6657345912927186	0.7145242787873713	T	T	T
0.4234545439298196	0.8338237097858904	0.2748533065619999	T	T	T
0.0788053426587964	0.1612413284910732	0.4480538406438795	T	T	T
0.7472406031118258	0.4896699911971989	0.6148415349705112	T	T	T
0.4046670404856851	0.0745290687894664	0.3057580046715333	T	T	T
0.0626693888393887	0.3980462510227564	0.4688605212663370	T	T	T
0.7227594587624618	0.7290909876514943	0.6404326397932688	T	T	T
-0.0017234451111047	0.7275194118715800	0.3704657567002254	T	T	T
0.6694140551788668	0.0636593263653199	0.5382889517576194	T	T	T
0.7275471553716916	0.2329373349231393	0.3557805878407493	T	T	T
0.3933236090257481	0.5731630283921381	0.5345909766171333	T	T	T
0.0724508434408183	0.9067755812732190	0.7059143442681814	T	T	T
0.6729135449590704	0.6050066253320859	0.3065626661885164	T	T	T
0.3396052527581990	0.9447536824180762	0.4693621661330029	T	T	T
0.0158987988664434	0.2747530918455366	0.6445374858975730	T	T	T
0.7339785384211058	0.0109958604008441	0.3687119972342376	T	T	T

0.3988327823996370	0.3402521639223540	0.5397854541470184	T	T	T
0.0722663374663902	0.6712668774279485	0.7038127782648518	T	T	T
0.4887926327893160	0.7436457950178335	0.3927070222367797	T	T	T
0.1588979471240894	0.0881699866552698	0.5653577908793428	T	T	T
0.8346191205560725	0.4146781915388627	0.7310345524433883	T	T	T
0.5096541601125741	0.2828672139676429	0.3591665041003263	T	T	T
0.1827502350465498	0.6103579582917822	0.5375626595930239	T	T	T
0.8404771746460727	0.9329276454551642	0.7062960536806338	T	T	T
0.1642923665098603	0.0716095188912458	0.3050258864064641	T	T	T
0.8316302600197699	0.3971646591986345	0.4756885855834783	T	T	T
0.5018820035084748	0.7335689810961712	0.6535647758924419	T	T	T
0.9346997421729842	0.3357737549116670	0.3041672034652014	T	T	T
0.6076349295268958	0.6673451484081782	0.4738951145443625	T	T	T
0.2770059433878046	0.9978859632084509	0.6401368484582306	T	T	T
0.6674102369469134	0.8197157190325025	0.2950899386453725	T	T	T
0.3299094358835775	0.1460506756924582	0.4628284842593886	T	T	T
0.0011995480200717	0.4749428792844502	0.6258573023129543	T	T	T
0.2593211875378088	0.5208173606768561	0.3881982365097655	T	T	T
0.9296442850854910	0.8472306775117894	0.5639942563362373	T	T	T
0.5859134021089480	0.1775588999278927	0.7318899527869338	T	T	T
0.4748826021279380	0.4872639656490699	0.3841703818767869	T	T	T
0.1470009696082895	0.8170306083941160	0.5476924369925554	T	T	T
0.8185208353973177	0.1586288128525813	0.7148469812504786	T	T	T
0.4141422868719816	0.5852090443911707	0.2730129047718791	T	T	T
0.0868278185840115	0.9305089375467255	0.4480694018912832	T	T	T
0.7470281853217716	0.2606988734953061	0.6139745657970082	T	T	T
0.2812454713180582	0.2756878859971647	0.3691946240467083	T	T	T
0.9457142614084995	0.6085572961406980	0.5408718466445496	T	T	T
0.6067788863909008	0.9393750417528085	0.7032981831249140	T	T	T
0.1745687598920098	0.5959998947801376	0.2734000529365297	T	T	T
0.8481686443994945	0.9215136046428882	0.4466523815774541	T	T	T
0.5202773104855908	0.2627747241978764	0.6115587062216976	T	T	T
0.1559531604372238	0.3405489109894948	0.2939354842774698	T	T	T
0.8183646206423624	0.6764563251207929	0.4627249335828132	T	T	T
0.4869756551269244	0.0151748154314521	0.6237303346403630	T	T	T
0.1894378672350988	0.8528680285503877	0.2967633988818524	T	T	T
0.8647349799322457	0.1908989422249250	0.4621442281424719	T	T	T
0.5137248582808958	0.5158676971474713	0.6344766373264205	T	T	T
0.7756729078359276	0.4988223611813391	0.3570833705253798	T	T	T
0.4383894762968892	0.8316204577619195	0.5341178868929196	T	T	T
0.0807831431424992	0.1358578373538771	0.7233083106483099	T	T	T
0.0846470625804093	0.1386171160537455	0.7776426310088430	T	T	T