Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

First Principles Investigation of Dissociative Adsorption of H_2 during CO_2 Hydrogenation over Cubic and Hexagonal In_2O_3 Catalysts

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This supplementary information is divided into two sections, briefly summarized below.

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Table S6. Atomic Bader charges for the homolytic dissociative adsorption of H_2 on the defective *c*-In_2O_3(111) surface with θ = 1 ML.

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Table S13. Optimized fractional coordinates for bulk, perfect, and defective surfaces of the In_2O_3 catalysts.

Section 1.

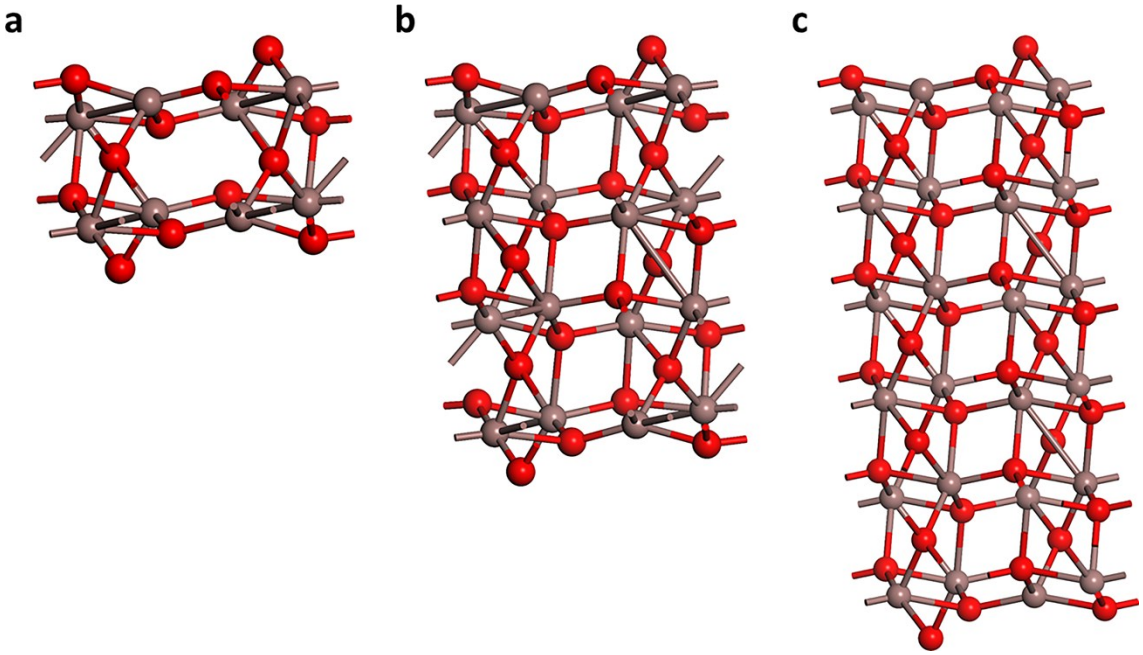

Figure S1. The slab models of the *h*-In_2O_3(104) surface with two, four and six layers.

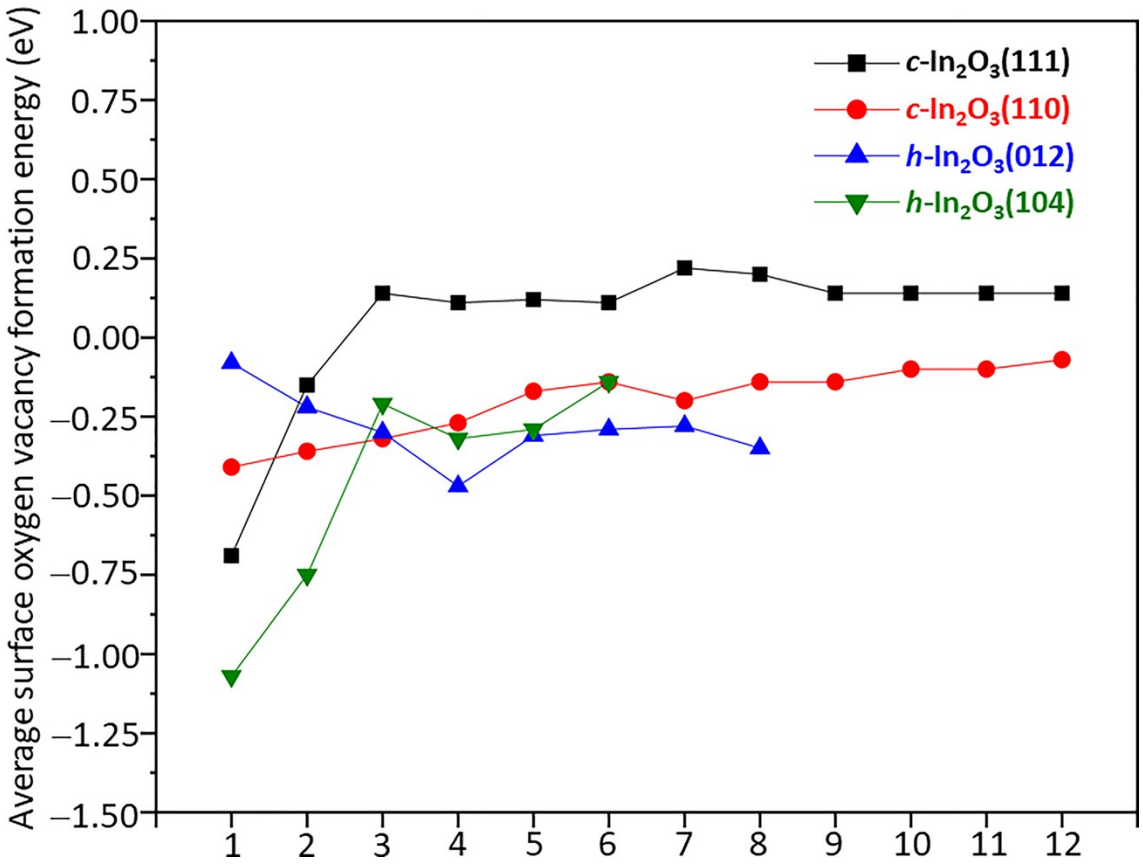

Figure S2. $E_{f,H2}$ (eV) for the In_2O_3 surfaces with different numbers of surface O_v.

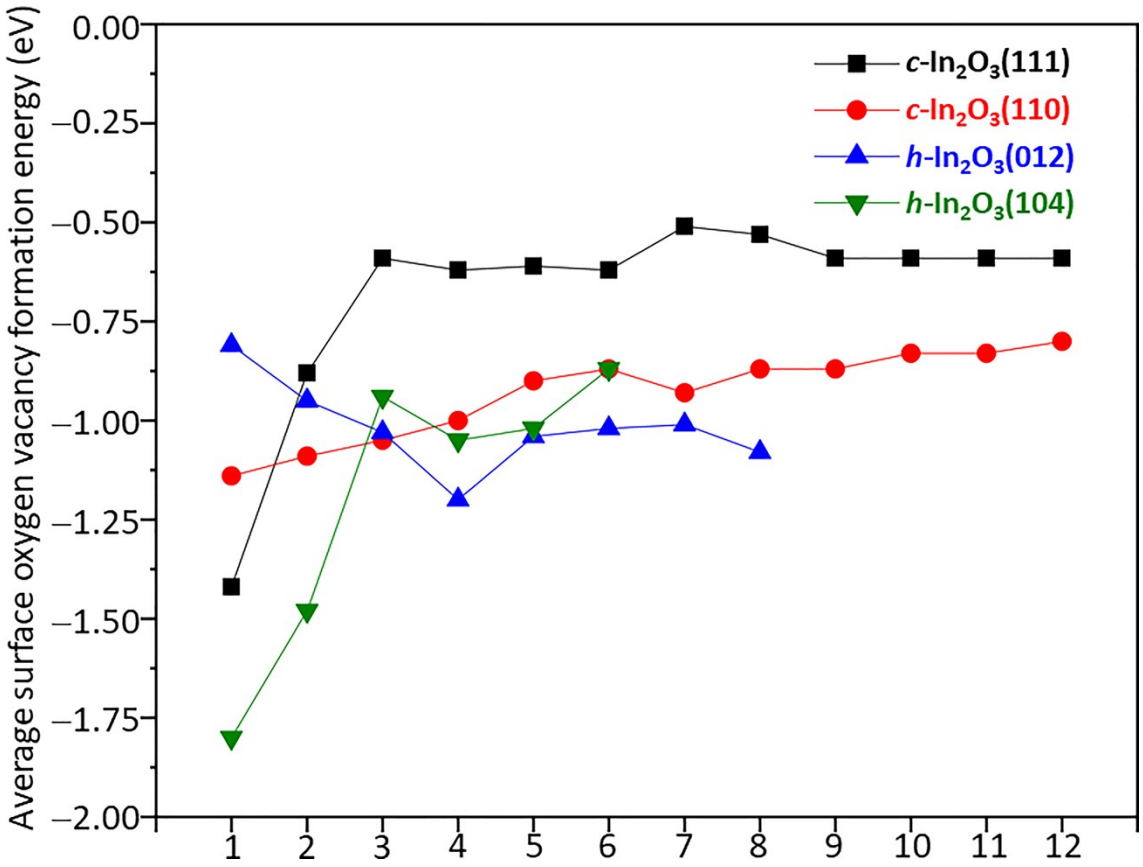

Figure S3. $E_{f,CO}$ (eV) for the In_2O_3 surfaces with different numbers of surface O_v.

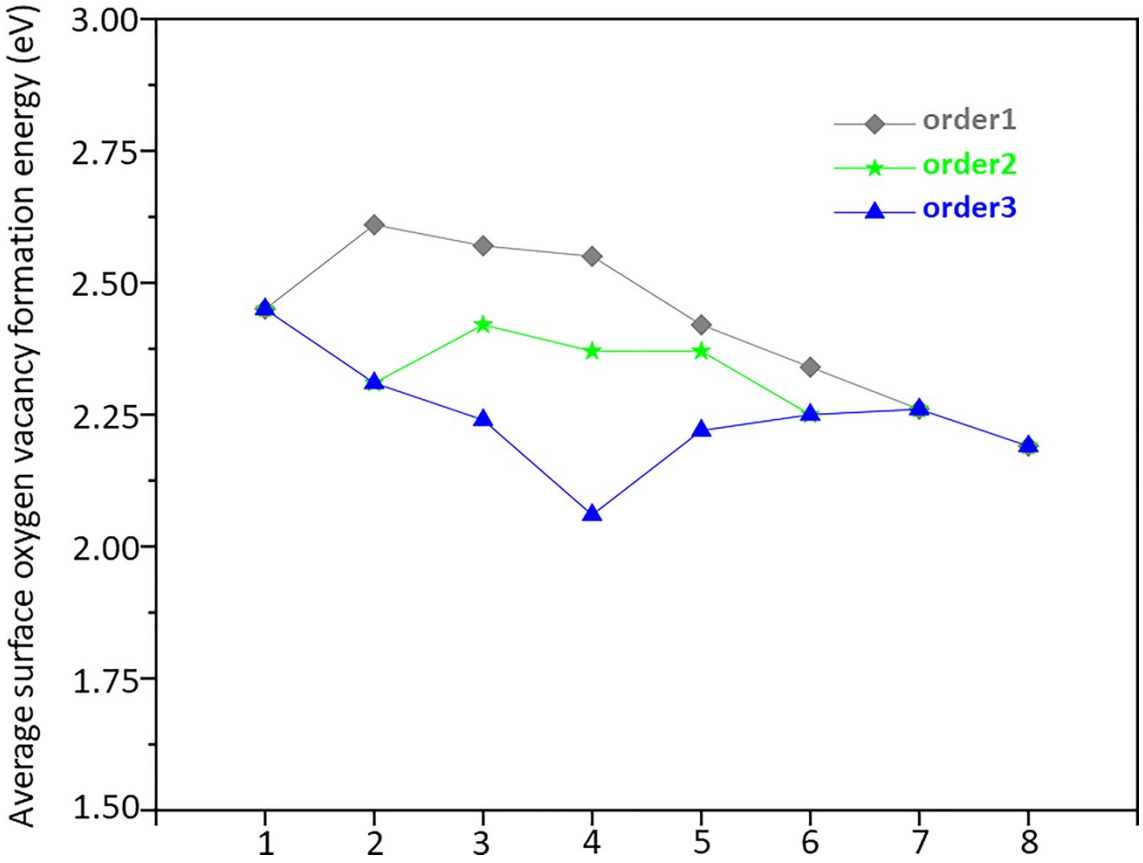

Figure S4. $E_{f,O2}$ (eV) for the *h*-In_2O_3(012) surface with different orders of removing the surface O atoms.

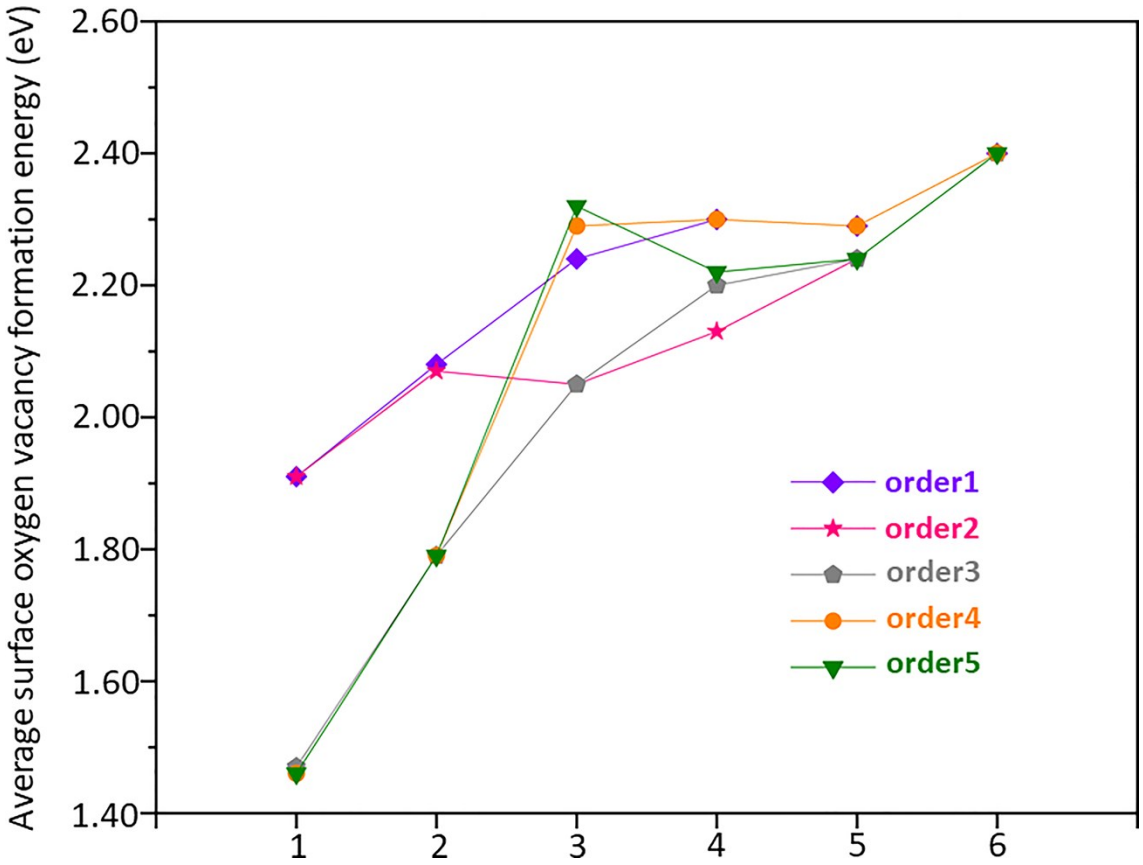

Figure S5. $E_{f,O2}$ (eV) for the *h*-In_2O_3(104) surface with different orders of removing the surface O atoms.

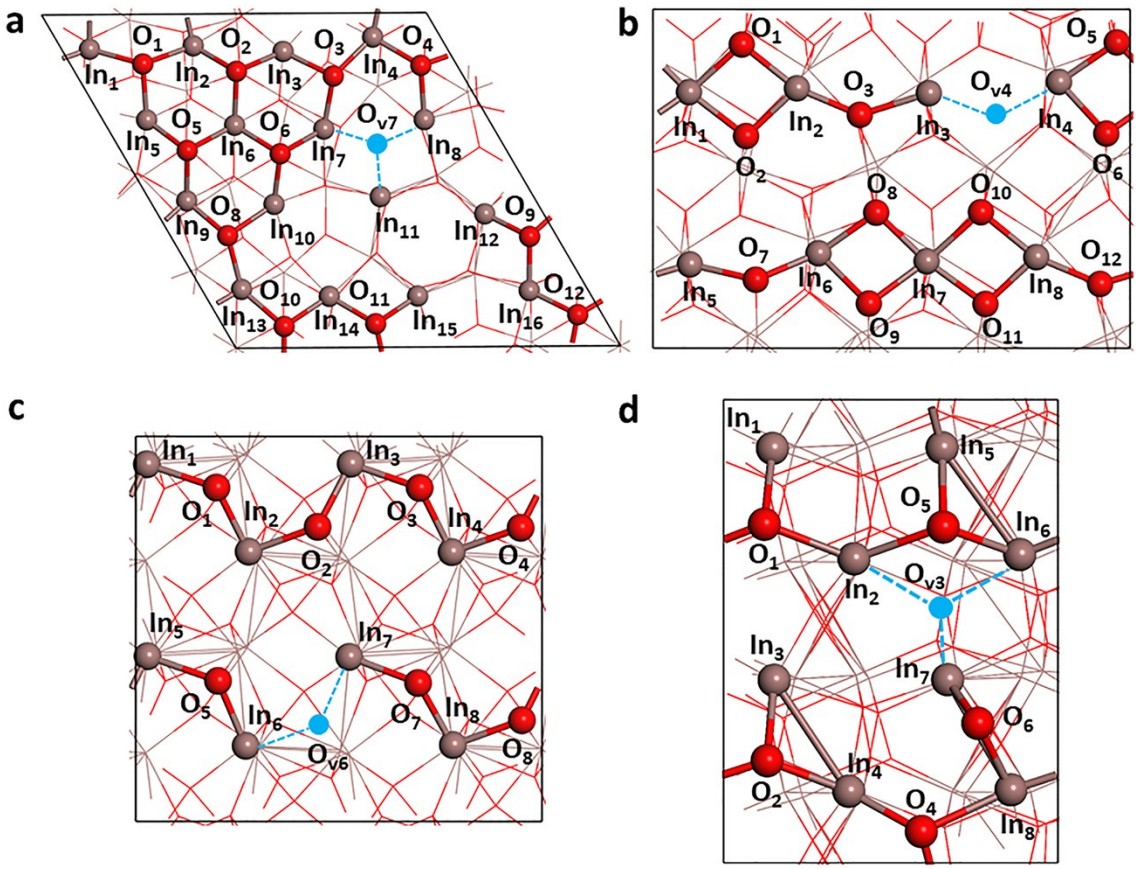

Figure S6. Optimized structures of the defective surfaces with an O_v for (a) *c*-In_2O_3(111), (b) *c*-In_2O_3(110), (c) *h*-In_2O_3(012), and (d) *h*-In_2O_3(104).

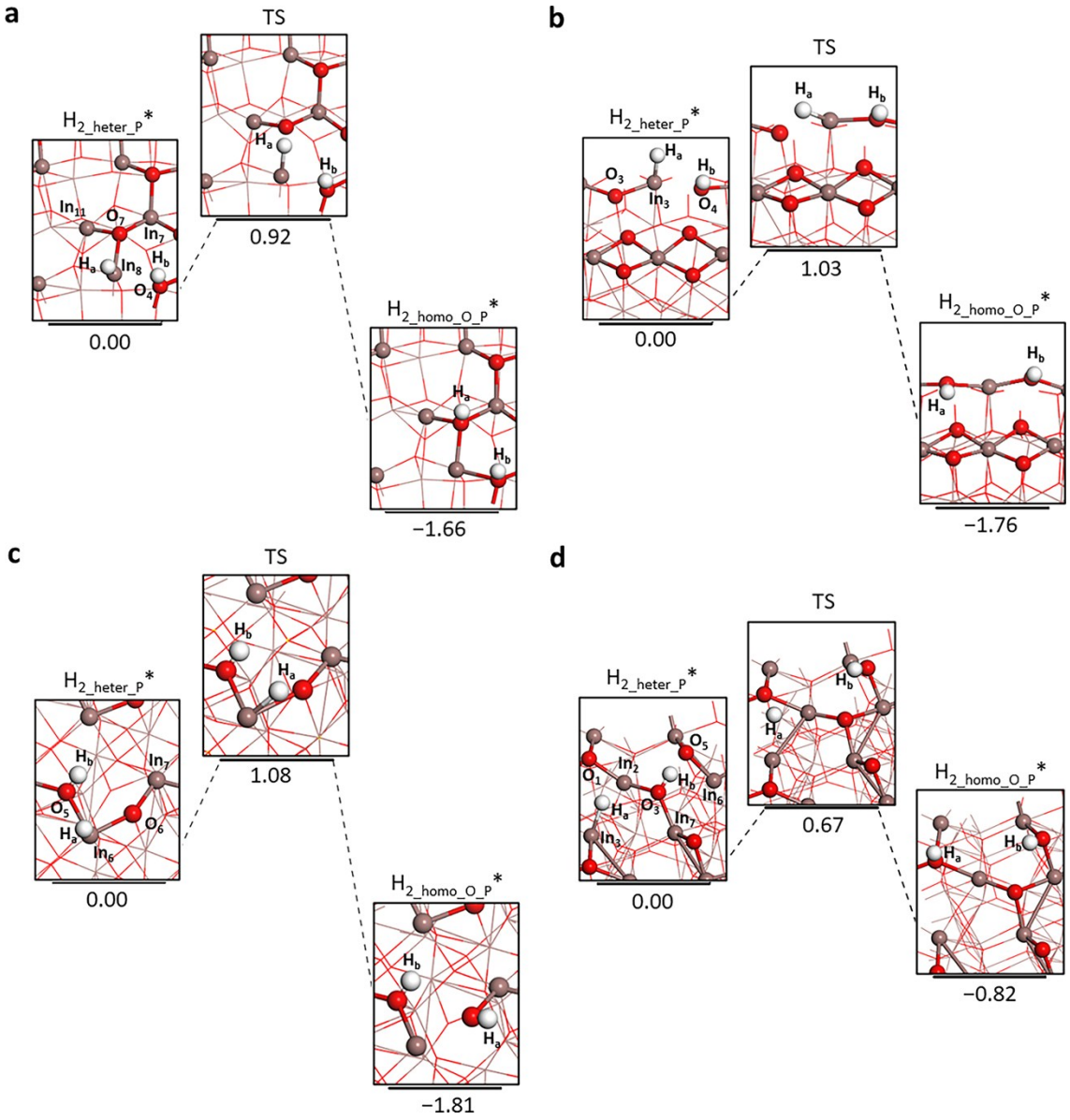

Figure S7. Potential energy profile (E_e: eV) for the hydride migration from an In site to an O site on the perfect In_2O_3 surfaces.

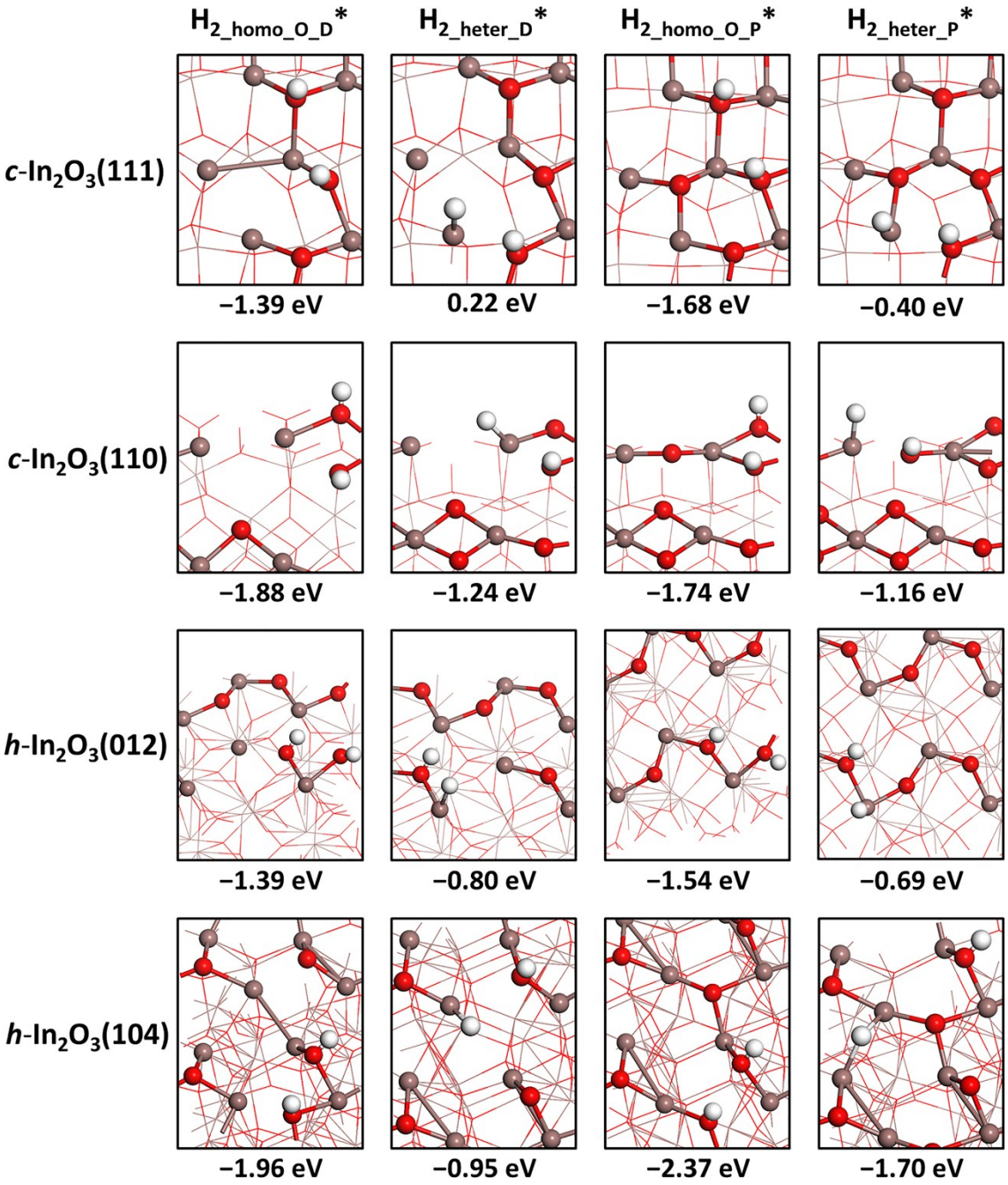

Figure S8. Homolytic and heterolytic dissociative adsorption energies (E_e: eV) of H_2 on the defective and perfect In_2O_3 surfaces.

Section 2.

Table S1. Formation energies (eV) of single O_v on the *c*-In_2O_3 and *h*-In_2O_3 surfaces.

Surface	Reaction	O_{v1}	O_{v2}	O_{v3}	O_{v4}	O_{v5}	O_{v6}	O_{v7}	O_{v8}	O_{v9}	O_{v10}	O_{v11}	O_{v12}
	Thermal desorption	1.84	2.27	1.84	2.58	2.27	2.26	2.71	1.99	2.71	2.58	2.71	2.58
c-In_2O_3(111)	H_2 reduction	−0.69	−0.26	−0.69	0.05	−0.26	−0.27	0.17	−0.54	0.18	0.05	0.17	0.05
	CO reduction	−1.42	−0.99	−1.42	−0.68	−0.99	−1.00	−0.56	−1.27	−0.55	−0.68	−0.56	−0.68
	Thermal desorption	2.12	2.39	2.41	2.42	2.17	2.14	2.42	2.17	2.14	2.12	2.39	2.41
c-In_2O_3(110)	H_2 reduction	−0.41	−0.15	−0.12	−0.12	−0.37	−0.39	−0.12	−0.37	−0.39	−0.41	−0.15	−0.12
	CO reduction	−1.14	−0.87	−0.85	−0.85	−1.10	−1.12	−0.85	−1.10	−1.12	−1.14	−0.87	−0.85
	Thermal desorption	2.45	2.45	2.45	2.45	2.45	2.45	2.45	2.45				
h-In_2O_3(012)	H_2 reduction	−0.08	−0.08	−0.08	−0.08	−0.08	−0.08	−0.08	−0.08				
	CO reduction	−0.81	−0.81	−0.81	−0.81	−0.81	−0.81	−0.81	−0.81				
	Thermal desorption	1.46	1.46	1.91	1.91	1.47	1.47						
h-In_2O_3(104)	H_2 reduction	−1.07	−1.07	−0.63	−0.63	−1.07	−1.07						
	CO reduction	−1.80	−1.80	−1.36	−1.36	−1.80	−1.80						

Table S2. Formation energies of single O_v and dissociative adsorption energies of H_2 on the *h*-In_2O_3(104) surfaces with two, four and six layers.

h-In_2O_3(104)		O_v formation energy						Dissociative adsorption energy			
Layers	Atoms	O_{v1}	O_{v2}	O_{v3}	O_{v4}	O_{v5}	O_{v6}	$H_{2\_homo\_O\_P}$*	$H_{2\_heter\_P}$*	$H_{2\_homo\_O\_D}$*	$H_{2\_heter\_D}$*
2	40	1.57	1.57	2.14	2.14	1.57	1.57	−2.09	−1.50	−2.10	-0.91
4	80	1.46	1.46	1.91	1.91	1.47	1.47	−2.37	−1.70	−1.96	−0.95
6	120	1.39	1.39	1.84	1.84	1.39	1.39	−2.47	−1.72	−1.96	−0.97

Table S3. Oxygen vacancy distributions for the defective In_2O_3 surfaces at different O_v coverages corresponding to Figures 2, S2, and S3.

Number	Oxygen vacancies			
	c-In_2O_3(111)	*c*-In_2O_3(110)	*h*-In_2O_3(012)	*h*-In_2O_3(104)
1	O_{v1}	O_{v1}	O_{v5}	O_{v1}
2	O_{v1} O_{v3}	O_{v1} O_{v2}	O_{v5} O_{v6}	O_{v1} O_{v2}
3	O_{v1} O_{v3} O_{v8}	O_{v1} O_{v2} O_{v5}	O_{v5} O_{v6} O_{v7}	O_{v1} O_{v2} O_{v5}
4	O_{v1} O_{v3} O_{v8} O_{v2}	O_{v1} O_{v2} O_{v5} O_{v6}	O_{v5} O_{v6} O_{v7} O_{v8}	O_{v1} O_{v2} O_{v5} O_{v6}
5	O_{v1} O_{v3} O_{v8} O_{v2} O_{v5}	O_{v1} O_{v2} O_{v5} O_{v6} O_{v8}	O_{v5} O_{v6} O_{v7} O_{v8} O_{v1}	O_{v1} O_{v2} O_{v5} O_{v6} O_{v3}
6	O_{v1} O_{v3} O_{v8} O_{v2} O_{v5} O_{v6}	O_{v1} O_{v2} O_{v5} O_{v6} O_{v8} O_{v9}	O_{v5} O_{v6} O_{v7} O_{v8} O_{v1} O_{v2}	O_{v1} O_{v2} O_{v5} O_{v6} O_{v3} O_{v4}
7	O_{v1} O_{v3} O_{v8} O_{v2} O_{v5} O_{v6} O_{v4}	O_{v1} O_{v2} O_{v5} O_{v6} O_{v8} O_{v9} O_{v10}	O_{v5} O_{v6} O_{v7} O_{v8} O_{v1} O_{v2} O_{v3}	
8	O_{v1} O_{v3} O_{v8} O_{v2} O_{v5} O_{v6} O_{v4} O_{v10}	O_{v1} O_{v2} O_{v5} O_{v6} O_{v8} O_{v9} O_{v10} O_{v11}	O_{v5} O_{v6} O_{v7} O_{v8} O_{v1} O_{v2} O_{v3} O_{v4}	
9	O_{v1} O_{v3} O_{v8} O_{v2} O_{v5} O_{v6} O_{v4} O_{v10} O_{v12}	O_{v1} O_{v2} O_{v5} O_{v6} O_{v8} O_{v9} O_{v10} O_{v11} O_{v3}		
10	O_{v1} O_{v3} O_{v8} O_{v2} O_{v5} O_{v6} O_{v4} O_{v10} O_{v12} O_{v7}	O_{v1} O_{v2} O_{v5} O_{v6} O_{v8} O_{v9} O_{v10} O_{v11} O_{v3} O_{v4}		
11	O_{v1} O_{v3} O_{v8} O_{v2} O_{v5} O_{v6} O_{v4} O_{v10} O_{v12} O_{v7} O_{v9}	O_{v1} O_{v2} O_{v5} O_{v6} O_{v8} O_{v9} O_{v10} O_{v11} O_{v3} O_{v4} O_{v7}		
12	O_{v1} O_{v3} O_{v8} O_{v2} O_{v5} O_{v6} O_{v4} O_{v10} O_{v12} O_{v7} O_{v9} O_{v11}	O_{v1} O_{v2} O_{v5} O_{v6} O_{v8} O_{v9} O_{v10} O_{v11} O_{v3} O_{v4} O_{v7} O_{v12}		

Table S4. Oxygen vacancy distributions for the defective *h*-In_2O_3(012) surfaces with different orders of removing the surface O atoms corresponding to Figures S4.

Number	Oxygen vacancies		
	order1	order2	order3
1	O_{v5}	O_{v1}	O_{v2}
2	O_{v5} O_{v6}	O_{v1} O_{v3}	O_{v2} O_{v1}
3	O_{v5} O_{v6} O_{v7}	O_{v1} O_{v3} O_{v5}	O_{v2} O_{v1} O_{v6}
4	O_{v5} O_{v6} O_{v7} O_{v8}	O_{v1} O_{v3} O_{v5} O_{v7}	O_{v2} O_{v1} O_{v6} O_{v5}
5	O_{v5} O_{v6} O_{v7} O_{v8} O_{v1}	O_{v1} O_{v3} O_{v5} O_{v7} O_{v2}	O_{v2} O_{v1} O_{v6} O_{v5} O_{v3}
6	O_{v5} O_{v6} O_{v7} O_{v8} O_{v1} O_{v2}	O_{v1} O_{v3} O_{v5} O_{v7} O_{v2} O_{v4}	O_{v2} O_{v1} O_{v6} O_{v5} O_{v3} O_{v4}
7	O_{v5} O_{v6} O_{v7} O_{v8} O_{v1} O_{v2} O_{v3}	O_{v1} O_{v3} O_{v5} O_{v7} O_{v2} O_{v4} O_{v6}	O_{v2} O_{v1} O_{v6} O_{v5} O_{v3} O_{v4} O_{v7}
8	O_{v5} O_{v6} O_{v7} O_{v8} O_{v1} O_{v2} O_{v3} O_{v4}	O_{v1} O_{v3} O_{v5} O_{v7} O_{v2} O_{v4} O_{v6} O_{v8}	O_{v2} O_{v1} O_{v6} O_{v5} O_{v3} O_{v4} O_{v7} O_{v8}

Table S5. Oxygen vacancy distributions for the defective h-In_2O_3(104) surfaces with different orders of removing the surface O atoms corresponding to Figures S5.

Number	Oxygen vacancies				
	order1	order2	order3	order4	order5
1	O_{v1}	O_{v1}	O_{v6}	O_{v3}	O_{v3}
2	O_{v1} O_{v2}	O_{v1} O_{v2}	O_{v6} O_{v5}	O_{v3} O_{v4}	O_{v3} O_{v5}
3	O_{v1} O_{v2} O_{v5}	O_{v1} O_{v2} O_{v3}	O_{v6} O_{v5} O_{v4}	O_{v3} O_{v4} O_{v1}	O_{v3} O_{v5} O_{v6}
4	O_{v1} O_{v2} O_{v5} O_{v6}	O_{v1} O_{v2} O_{v3} O_{v4}	O_{v6} O_{v5} O_{v4} O_{v3}	O_{v3} O_{v4} O_{v1} O_{v2}	O_{v3} O_{v5} O_{v6} O_{v1}
5	O_{v1} O_{v2} O_{v5} O_{v6} O_{v3}	O_{v1} O_{v2} O_{v3} O_{v4} O_{v5}	O_{v6} O_{v5} O_{v4} O_{v3} O_{v2}	O_{v3} O_{v4} O_{v1} O_{v2} O_{v5}	O_{v3} O_{v5} O_{v6} O_{v1} O_{v2}
6	O_{v1} O_{v2} O_{v5} O_{v6} O_{v3} O_{v4}	O_{v1} O_{v2} O_{v3} O_{v4} O_{v5} O_{v6}	O_{v6} O_{v5} O_{v4} O_{v3} O_{v2} O_{v1}	O_{v3} O_{v4} O_{v1} O_{v2} O_{v5} O_{v6}	O_{v3} O_{v5} O_{v6} O_{v1} O_{v2} O_{v4}

Table S6. Atomic Bader charges (in |e|) for the homolytic dissociative adsorption of H_2 on the defective *c*-In_2O_3(111) surface with θ = 1 ML followed by further hydride migration.

Charge	In_7	In_8	In_{11}	H_a	H_b
*_D	+0.78	+0.85	+1.40		
TS1	+0.78	+1.13	+1.29	−0.14	−0.08
$H_{2\_homo\_In\_D\_1}$*	+0.76	+1.36	+1.46	−0.27	−0.23
TS2	+1.09	+0.99	+1.48	−0.27	−0.23
$H_{2\_homo\_In\_D\_2}$*	+1.38	+0.76	+1.49	−0.28	−0.27

Table S7. Atomic Bader charges (in |e|) for the *c*-In_2O_3(110) surface.

θ(ML)	Charge	In_1	In_2	In_3	In_4	O_4	O_5	O_6
0	Perfect	+1.74	+1.71	+1.71	+1.75	−1.13	−1.13	−1.15
1/12	O_{v4}	+1.72	+1.67	+1.04	+1.47		−1.12	−1.13
1	*_D	+0.29	+0.51	+0.61	+0.56			

Table S8. Atomic Bader charges (in |e|) for the *h*-In_2O_3(012) surface.

θ(ML)	Charge	In_5	In_6	In_7	In_8	O_5	O_6	O_7	O_8
0	Perfect	+1.75	+1.75	+1.75	+1.75	−1.14	−1.14	−1.14	−1.14
1/8	O_{v6}	+1.73	+1.50	+1.24	+1.73	−1.12		−1.13	−1.14
1	*_D	+0.74	+0.74	+0.74	+0.74				

Table S9. Atomic Bader charges (in |e|) for the *h*-In_2O_3(104) surface.

θ(ML)	Charge	In_2	In_6	In_7	O_1	O_3	O_5	O_6
0	Perfect	+1.70	+1.74	+1.76	−1.13	−1.14	−1.04	−1.04
1/6	O_{v3}	+1.23	+1.65	+1.63	−1.15		−1.11	−1.05
1	*_D	+0.69	+0.68	+1.24				

Table S10. E_f (eV) of the *c*-In_2O_3(110) and *c*-In_2O_3(111) surfaces with different surface O_v coverages by thermal desorption of molecular O_2, H_2 and CO reduction corresponding to Figures 2, S2, and S3.

θ (ML)	E_f (θ)					
	c-In_2O_3(111)			*c*-In_2O_3(110)		
	Thermal desorption	H_2 reduction	CO reduction	Thermal desorption	H_2 reduction	CO reduction
1/12	1.84	−0.69	−1.42	2.12	−0.41	−1.14
1/6	1.46	−0.15	−0.88	2.17	−0.36	−1.09
1/4	2.68	0.14	−0.59	2.21	−0.32	−1.05
1/3	2.65	0.11	−0.62	2.26	−0.27	−1.00
5/12	2.65	0.12	−0.61	2.36	−0.17	−0.90
1/2	2.65	0.11	−0.62	2.39	−0.14	−0.87
7/12	2.75	0.22	−0.51	2.33	−0.20	−0.93
2/3	2.74	0.20	−0.53	2.39	−0.14	−0.87
3/4	2.67	0.14	−0.59	2.40	−0.14	−0.87
5/6	2.67	0.14	−0.59	2.43	−0.10	−0.83
11/12	2.68	0.14	−0.59	2.43	−0.10	−0.83
1	2.67	0.14	−0.59	2.47	−0.07	−0.80

Table S11. E_f (eV) of *h*-In_2O_3(012) surface with different surface O_v coverages by thermal desorption of molecular O_2, H_2 and CO reduction corresponding to Figures 2, S2, and S3.

θ (ML)	E_f (θ)		
	Thermal desorption	H_2 reduction	CO reduction
1/8	2.45	−0.08	−0.81
1/4	2.31	−0.22	−0.95
3/8	2.24	−0.30	−1.03
1/2	2.06	−0.47	−1.20
5/8	2.22	−0.31	−1.04
3/4	2.25	−0.29	−1.02
7/8	2.26	−0.28	−1.01
1	2.19	−0.35	−1.08

Table S12. E_f (eV) of *h*-In_2O_3(104) surface with different surface O_v coverages by thermal desorption of molecular O_2, H_2 and CO reduction corresponding to Figures 2, S2, and S3.

θ (ML)	E_f (θ)		
	Thermal desorption	H_2 reduction	CO reduction
1/6	1.46	−1.07	−1.80
1/3	1.79	−0.75	−1.48
1/2	2.32	−0.21	−0.94
2/3	2.22	−0.32	−1.05
5/6	2.24	−0.29	−1.02
1	2.40	−0.14	−0.87

Table S13. Optimized fractional coordinates for bulk, perfect, and defective surfaces of the In_2O_3 catalysts.

Bulk lattice of *c*-In_2O_3

O In
1.00000000000000
−5.1068445150936430 5.1068445150936430 5.1068445150936430
5.1068445150936430 −5.1068445150936430 5.1068445150936430
5.1068445150936430 5.1068445150936430 −5.1068445150936430
O In
24 16
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0.2159434607377768 0.7500000000000000 0.9659434607377766
0.5340565392622233 0.2840565392622232 0.2500000000000000
0.9659434607377767 0.2159434607377768 0.7500000000000000
0.7500000000000000 0.4659434607377768 0.7159434607377766
0.2500000000000000 0.0340565392622232 0.7840565392622234
0.7159434607377767 0.7500000000000000 0.4659434607377768
0.7840565392622234 0.2500000000000000 0.0340565392622232

0.4659434607377768 0.7159434607377767 0.7500000000000000
0.0340565392622232 0.7840565392622233 0.2500000000000000
−0.0000000000000000 0.0000000000000000 −0.0000000000000000
0.5000000000000000 0.0000000000000000 0.5000000000000000
−0.0000000000000000 0.5000000000000000 0.5000000000000000
0.5000000000000000 0.5000000000000000 −0.0000000000000000

Bulk lattice of *h*-In_2O_3

O In
1.00000000000000
4.8039598245917281 −2.7735673314887164 −0.0000000000000000
0.0000000000000000 5.5471346629774327 0.0000000000000000
−0.0000000000000000 0.0000000000000000 14.5833847701357175
O In
18 12
Direct
0.7040602707237176 0.7040602707463151 0.2500000000000000
0.3707272707237215 0.0373932707463184 0.5833330000000032
0.0373932707237209 0.3707272707463193 0.9166669999999968
0.2959397292762824 0.0000000000225975 0.2500000000000000
0.9626067292762792 0.3333330000226007 0.5833330000000032
0.6292727292762785 0.6666670000226013 0.9166669999999968
0.0000000000000000 0.2959397292310730 0.2500000000000000
0.6666669999999968 0.6292727292310689 0.5833330000000032
0.3333330000000032 0.9626067292310697 0.9166669999999968
0.2959397292762824 0.2959397292536846 0.7500000000000000
0.9626067292762792 0.6292727292536811 0.0833330000000032
0.6292727292762785 0.9626067292536817 0.4166669999999968
0.7040602707237176 0.9999999999773955 0.7500000000000000
0.3707272707237215 0.3333329999774057 0.0833330000000032
0.0373932707237209 0.6666669999773923 0.4166669999999968
0.0000000000000000 0.7040602707689271 0.7500000000000000
0.6666669999999968 0.0373932707689302 0.0833330000000032
0.3333330000000032 0.3707272707689309 0.4166669999999968
0.6666669999999968 0.3333330000000032 0.4755713781864326
0.3333330000000032 0.6666669999999968 0.8089053781864333
0.0000000000000000 −0.0000000000000000 0.1422383781864365
0.3333330000000032 0.6666669999999968 0.0244286218135674
0.0000000000000000 −0.0000000000000000 0.3577616218135635
0.6666669999999968 0.3333330000000032 0.6910946218135667
0.3333330000000032 0.6666669999999968 0.5244286218135674
0.0000000000000000 −0.0000000000000000 0.8577616218135635
0.6666669999999968 0.3333330000000032 0.1910946218135667
0.6666669999999968 0.3333330000000032 0.9755713781864326
0.3333330000000032 0.6666669999999968 0.3089053781864333
0.0000000000000000 −0.0000000000000000 0.6422383781864365

Perfect *c*-In_2O_3(111) surface

O In
1.00000000000000
14.4443000000000001 0.0000000000000000 0.0000000000000000
−7.2221499999999965 12.5091307398835685 0.0000000000000000
0.0000000000000012 0.0000000000000021 15.0370999999999988
O In
48 32
Direct
0.1451191125797991 0.8150611844863780 0.3523893518322708
0.4745081607858450 0.4835909055908927 0.5445656780871995
0.7731649961060502 0.4907972508691523 0.5739323128811675
0.4270424208179376 0.8244213359467512 0.3559159556149969
0.2795475105821420 0.2718925628442799 0.5711498691509033
0.9343982605468356 0.5961663290441189 0.3631230384895437
0.4863633054828699 0.7401202402613152 0.5294537647649006
0.1610298684752062 0.0747591310127611 0.3288250643606457
0.1848408275339953 0.3300320612623339 0.3523609980944265
0.5164504550297209 0.9909366140020944 0.5445695470243517
0.5090858049985219 0.2823390678869893 0.5739462131221145
0.1756073048135539 0.6025952240770861 0.3558885554469269
0.7280871746855950 0.0076580886578169 0.5711994148708726
0.4038735441802321 0.3382205173510777 0.3630487854852434
0.2598822053380366 0.7461741799504441 0.5294385211410014
0.9251169737365404 0.0862464517577624 0.3288666041801958
0.6699615536784345 0.8548323119122059 0.3523548538195427
0.0091108224651091 0.5255405604516186 0.5446042871362627
0.7176643052387186 0.2267698345486424 0.5739506685467759
0.3973967415404153 0.5729666527559594 0.3559318618263451
0.9923917148194963 0.7205273738067028 0.5711869284641728
0.6617418617469267 0.0656421059189875 0.3630604444703220
0.2537207216141315 0.5136542467106934 0.5294810842064561
0.9137964939943020 0.8389527015043173 0.3288806525914126
0.1882144300108307 0.8516054568917677 0.6476090143045862
0.8588259307761310 0.1830752588721390 0.4554328640696589
0.5601679091403405 0.1758690386298670 0.4260654645360022
0.9062908927395539 0.8422448552269628 0.6440825792518169
0.0537859215261932 0.3947739375514592 0.4288491109453267
0.3989353443878660 0.0705002547399708 0.6368749296532140
0.8469701553306153 0.9265465074583574 0.4705448745027783
0.1723036574435091 0.5919075213819817 0.6711733350325196
0.1484925770040109 0.3366344144914056 0.6476375423973313
0.8168830513734139 0.6757296308176896 0.4554299252847627
0.8242481697729281 0.3843281255158060 0.4260513792834565
0.1577263815284151 0.0640712353123064 0.6441096172928715
0.6052461044817411 0.6590083188329272 0.4288000247944766
0.9294598648030115 0.3284461525184541 0.6369493372502862
0.0734515001319062 0.9204925863130324 0.4705597599720628

0.4082167724996504 0.5804201720037694 0.6711316214119617
0.6633717620740729 0.8118337754783047 0.6476438838017134
0.3242229664233381 0.1411263039265593 0.4553936786738689
0.6156693195810837 0.4398968642082740 0.4260478073640942
0.9359369615020480 0.0936998448943808 0.6440668253929895
0.3409410748791514 0.9461391507016341 0.4288115414490933
0.6715913203346564 0.6010229826157746 0.6369380489312075
0.0796128615656489 0.1530122870783333 0.4705174965900786
0.4195368317631099 0.8277138274413505 0.6711180359947670
0.1135268428242092 0.6840967059904850 0.6080323825819671
0.5494773824643627 0.1525980020713431 0.5757555821792084
0.2299847807024728 0.4909883742782011 0.3885313738383915
0.7745782340008217 0.0129384258572414 0.4012757643355346
0.3159618195813228 0.4294407622415121 0.6080097886301308
0.8474273917403311 0.3968882049052914 0.5757461204140754
0.5090119691600216 0.7389818481584263 0.3885146396380077
0.9870484885231411 0.7616731147062514 0.4013234579775883
0.5705476709803482 0.8865016168325196 0.6080319213654766
0.6031015508653850 0.4505171811058692 0.5757566488034462
0.2610125294899167 0.7699858748460880 0.3885058790213879
0.2383283052777964 0.2253621083253492 0.4012163307200562
0.2198066867426140 0.9825699265258531 0.3919659109661390
0.7838566733651974 0.5140688389704395 0.4242424329342478
0.1033486995890565 0.1756780603454133 0.6114672197053368
0.5587549984686750 0.6537277989193678 0.5987225785700546
0.0173717296289739 0.2372256715746610 0.3919889331705346
0.4859065283543559 0.2697783320401079 0.4242519095287691
0.8243213547276370 0.9276847346297245 0.6114840876655905
0.3462847545295096 0.9049933972650959 0.5986750492685645
0.7627858378117667 0.7801649424527631 0.3919670566774948
0.7302328239803815 0.2161494272931610 0.4242406867002162
0.0723208423386802 0.8966806475447578 0.6114923197410674
0.0950052178927374 0.4413045172122805 0.5987822126965801
0.0133189466501837 0.5134664098836342 0.4014524836026969
−0.0000134424194899 0.0000128047425126 0.3856068391987680
0.4865728541781378 0.4998348807500778 0.4014152223935677
0.5001452543589615 −0.0132919849319449 0.4014330177903410
0.8331865123529363 0.6799577136103208 0.5985672021555198
0.3200145814885574 0.1532001906961715 0.5985455920803422
0.3333469423009668 0.6666537255870266 0.6143917256905647
0.8467613361864128 0.1668323100570823 0.5985836424314855

Perfect *c*-In_2O_3(110) surface

O In
1.00000000000000
10.2136999999999993 0.0000000000000000 0.0000000000000000
0.0000000000000009 14.4443000000000001 0.0000000000000000
0.0000000000000010 0.0000000000000010 15.9873999999999992

O In
48 32
Direct
0.6089400700035356 0.1822731037628693 0.4373340599499958
0.1089400700035287 0.6822731037628628 0.4373340599499958
0.1098635696405312 0.9648202665210710 0.4557218489944125
0.6098635696405386 0.4648202665210777 0.4557218489944125
0.3260158848204119 0.5823517933990443 0.3464058512136479
0.8260158848204117 0.0823517933990442 0.3464058512136479
0.8260165533494214 0.5646986318546442 0.5356022490851571
0.3260165533494212 0.0646986318546517 0.5356022490851571
0.1000654455551523 0.9669355057171738 0.6658311982623719
0.6000654455551518 0.4669355057171738 0.6658311982623719
0.3277148308584424 0.8182065896043388 0.3470937678917306
0.8277148308584492 0.3182065896043391 0.3470937678917306
0.6039131611620581 0.6849929555452974 0.6821476541741593
0.1039131611620499 0.1849929555452977 0.6821476541741593
0.8347048508428668 0.3288992549281818 0.5391450544755959
0.3347048508428660 0.8288992549281817 0.5391450544755959
0.5602093538681556 0.6967361667741742 0.4608642755400719
0.0602093538681557 0.1967361667741740 0.4608642755400719
0.3885738083083067 0.0667711326965294 0.3219931242158511
0.8885738083083068 0.5667711326965224 0.3219931242158511
0.8755401135345799 0.0848799081835661 0.5578180759688367
0.3755401135345729 0.5848799081835589 0.5578180759688367
0.0603920963670669 0.4585366411994488 0.4420449490725661
0.5603920963670670 0.9585366411994491 0.4420449490725661
0.7970055770825339 0.2147458919860784 0.6879281351516956
0.2970055770825333 0.7147458919860715 0.6879281351516956
0.3112744133644468 0.4368428112910744 0.6787920119436518
0.8112744133644471 0.9368428112910744 0.6787920119436518
0.0940827905306655 0.3205982949537576 0.3142534981492986
0.5940827905306730 0.8205982949537579 0.3142534981492986
0.6064814723883095 0.8390647376946265 0.5749791398425733
0.1064814723883022 0.3390647376946265 0.5749791398425733
0.3327774280501923 0.4267686046114946 0.4593535329538815
0.8327774280501992 0.9267686046114880 0.4593535329538815
0.0917559926221567 0.0849302195868723 0.3124130972075024
0.5917559926221632 0.5849302195868651 0.3124130972075024
0.8287729051732498 0.7206812054799273 0.4374050979697712
0.3287729051732424 0.2206812054799348 0.4374050979697712
0.5963936058782431 0.0700315364852393 0.5836564198604666
0.0963936058782438 0.5700315364852387 0.5836564198604666
0.8731101025887897 0.6974153326215452 0.6693340976838412
0.3731101025887830 0.1974153326215447 0.6693340976838412
0.0298854843184856 0.8340073996245778 0.3248953608332189
0.5298854843184858 0.3340073996245854 0.3248953608332189
0.5571804560251611 0.3123130103186929 0.5633534149854514

0.0571804560251609 0.8123130103186927 0.5633534149854514
0.3678607293832150 0.9522997565261115 0.6850439701993829
0.8678607293832221 0.4522997565261190 0.6850439701993829
0.9669944187367120 0.2175152471779577 0.5831012030206288
0.4579663335343470 0.9301089934475968 0.3305194108036675
0.9579663335343466 0.4301089934475968 0.3305194108036675
0.4669944187367122 0.7175152471779571 0.5831012030206288
0.2200544475411177 0.5582252778034510 0.4596151366245448
0.2140981051366947 0.0915099624226597 0.4221692712573185
0.7140981051366947 0.5915099624226525 0.4221692712573185
0.7200544475411172 0.0582252778034505 0.4596151366245448
0.7440892690756475 0.5736280578465590 0.6649820285570739
0.1813980352297797 0.8248176307504439 0.4413164522700388
0.6813980352297873 0.3248176307504439 0.4413164522700388
0.2440892690756476 0.0736280578465660 0.6649820285570739
0.4636250656510157 0.1824835023140427 0.5482354987665649
0.9673305840053595 0.9709875260250403 0.3525984050069902
0.4673305840053598 0.4709875260250473 0.3525984050069902
0.9636250656510159 0.6824835023140351 0.5482354987665649
0.2194153827914988 0.8461143241612678 0.6548512892962950
0.2323675336005972 0.3025238522875466 0.6735812777467310
0.7323675336005970 0.8025238522875389 0.6735812777467310
0.7194153827914986 0.3461143241612740 0.6548512892962950
0.6775052995244223 0.8258443854030988 0.4425157733845603
0.2524555817306386 0.5763144788864760 0.6673287432315885
0.7524555817306388 0.0763144788864832 0.6673287432315885
0.1775052995244156 0.3258443854030984 0.4425157733845603
0.9617236523507021 0.1995842117204985 0.3398512165075388
0.4644732185201267 0.9511647242863241 0.5655275274162157
0.9667210523741747 0.6996756450733584 0.3402700380548659
0.4658011453626771 0.4475628714937979 0.5668317735183414
0.9658011453626771 0.9475628714937983 0.5668317735183414
0.4617236523507021 0.6995842117204989 0.3398512165075388
0.9644732185201268 0.4511647242863314 0.5655275274162157
0.4667210523741745 0.1996756450733586 0.3402700380548659

Perfect *h*-In_2O_3(012) surface

O In
1.00000000000000
11.0386000000000006 0.0000000000000000 0.0000000000000000
0.0000000000000000 11.6846999999999994 0.0000000000000000
0.0000000000000000 0.0000000000000000 16.3939999999999984
O In
48 32
Direct
0.4868767525075243 0.1042788529057255 0.3040961329260812
0.2362100846927808 0.3201970221750027 0.5459615744852027
0.2093731324262444 0.1637996430641943 0.3673039546580407

0.4593731324262444 0.3884403569358105 0.6326960453419596
0.4862100846927808 0.2320429778250022 0.4540384255147979
0.2368767525075244 0.4479611470942720 0.6959038670739194
0.3853899153072200 0.4820429778250020 0.4540384255147979
0.1622268675737564 0.4137996430641942 0.3673039546580407
0.3847232474924765 0.3542788529057256 0.3040961329260812
0.1347232474924765 0.1979611470942721 0.6959038670739194
0.1353899153072200 0.0701970221750027 0.5459615744852027
0.4122268675737564 0.1384403569358104 0.6326960453419596
0.9868767525075239 0.1042788529057255 0.3040961329260812
0.7362100846927813 0.3201970221750027 0.5459615744852027
0.7093731324262442 0.1637996430641943 0.3673039546580407
0.9593731324262442 0.3884403569358105 0.6326960453419596
0.9862100846927813 0.2320429778250022 0.4540384255147979
0.7368767525075239 0.4479611470942720 0.6959038670739194
0.8853899153072196 0.4820429778250020 0.4540384255147979
0.6622268675737566 0.4137996430641942 0.3673039546580407
0.8847232474924769 0.3542788529057256 0.3040961329260812
0.6347232474924769 0.1979611470942721 0.6959038670739194
0.6353899153072196 0.0701970221750027 0.5459615744852027
0.9122268675737566 0.1384403569358104 0.6326960453419596
0.4868767525075243 0.6042788529057255 0.3040961329260812
0.2362100846927808 0.8201970221750028 0.5459615744852027
0.2093731324262444 0.6637996430641946 0.3673039546580407
0.4593731324262444 0.8884403569358101 0.6326960453419596
0.4862100846927808 0.7320429778250019 0.4540384255147979
0.2368767525075244 0.9479611470942721 0.6959038670739194
0.3853899153072200 0.9820429778250019 0.4540384255147979
0.1622268675737564 0.9137996430641946 0.3673039546580407
0.3847232474924765 0.8542788529057255 0.3040961329260812
0.1347232474924765 0.6979611470942721 0.6959038670739194
0.1353899153072200 0.5701970221750028 0.5459615744852027
0.4122268675737564 0.6384403569358101 0.6326960453419596
0.9868767525075239 0.6042788529057255 0.3040961329260812
0.7362100846927813 0.8201970221750028 0.5459615744852027
0.7093731324262442 0.6637996430641946 0.3673039546580407
0.9593731324262442 0.8884403569358101 0.6326960453419596
0.9862100846927813 0.7320429778250019 0.4540384255147979
0.7368767525075239 0.9479611470942721 0.6959038670739194
0.8853899153072196 0.9820429778250019 0.4540384255147979
0.6622268675737566 0.9137996430641946 0.3673039546580407
0.8847232474924769 0.8542788529057255 0.3040961329260812
0.6347232474924769 0.6979611470942721 0.6959038670739194
0.6353899153072196 0.5701970221750028 0.5459615744852027
0.9122268675737566 0.6384403569358101 0.6326960453419596
0.0498233563255517 0.2737866710379679 0.3271439600989097
0.3126651656019588 0.0008526936310043 0.5740191479030473
0.0626651656019588 0.0513873063689933 0.4259808520969530

0.2998233563255520 0.2784533289620297 0.6728560399010901
0.3089348343980420 0.3013873063689935 0.4259808520969530
0.0717766436744490 0.0284533289620298 0.6728560399010899
0.3217766436744488 0.0237866710379678 0.3271439600989097
0.0589348343980420 0.2508526936310042 0.5740191479030473
0.5498233563255519 0.2737866710379679 0.3271439600989097
0.8126651656019586 0.0008526936310043 0.5740191479030473
0.5626651656019586 0.0513873063689933 0.4259808520969530
0.7998233563255519 0.2784533289620297 0.6728560399010901
0.8089348343980423 0.3013873063689935 0.4259808520969530
0.5717766436744489 0.0284533289620298 0.6728560399010899
0.8217766436744489 0.0237866710379678 0.3271439600989097
0.5589348343980423 0.2508526936310042 0.5740191479030473
0.0498233563255517 0.7737866710379676 0.3271439600989097
0.3126651656019588 0.5008526936310042 0.5740191479030473
0.0626651656019588 0.5513873063689934 0.4259808520969530
0.2998233563255520 0.7784533289620300 0.6728560399010901
0.3089348343980420 0.8013873063689934 0.4259808520969530
0.0717766436744490 0.5284533289620300 0.6728560399010899
0.3217766436744488 0.5237866710379676 0.3271439600989097
0.0589348343980420 0.7508526936310043 0.5740191479030473
0.5498233563255519 0.7737866710379676 0.3271439600989097
0.8126651656019586 0.5008526936310042 0.5740191479030473
0.5626651656019586 0.5513873063689934 0.4259808520969530
0.7998233563255519 0.7784533289620300 0.6728560399010899
0.8089348343980423 0.8013873063689934 0.4259808520969530
0.5717766436744489 0.5284533289620300 0.6728560399010901
0.8217766436744489 0.5237866710379676 0.3271439600989097
0.5589348343980423 0.7508526936310043 0.5740191479030473

Perfect *h*-In_2O_3(104) surface

O In
1.00000000000000
8.0410003662000005 0.0000000000000000 0.0000000000000000
0.0000000000000000 11.0943002700999998 0.0000000000000000
0.0000000000000000 0.0000000000000000 21.6168003081999984
O In
48 32
Direct
0.1283164170000006 0.3258005380000029 0.5938591959999968
0.5948254469999981 0.0745844989999966 0.7318537829999983
0.9653918149999967 0.0844046919999997 0.2663239540000006
0.3172960280000012 0.0448215119999986 0.3652836979999989
0.7938935760000021 0.2980467980000014 0.4976985449999987
0.1767812969999980 0.3134430349999988 0.3167347910000018
0.6589541439999991 0.0765332579999978 0.4570353029999978
0.2663018699999995 0.0431170129999998 0.6379617449999984
0.7701285480000024 0.2991822660000025 0.7701174019999968

0.4606798590000025 0.3233882780000030 0.4030193689999990
0.9384331700000033 0.0745184499999993 0.5392086510000027
0.4109536710000015 0.3338520819999999 0.6802986860000004
0.5014763470000005 0.2254766229999987 0.2681212430000031
0.9680870769999999 0.4740811289999982 0.4061761199999978
0.1309160890000030 0.2155440900000016 0.7336639760000025
0.6854608060000018 0.4662223159999996 0.3197381199999967
0.1581590469999981 0.2254967539999981 0.4607896799999978
0.6358587149999977 0.4765140120000027 0.5969448090000000
0.3261708020000000 0.0009098129999998 0.2298903020000012
0.8301106689999997 0.2568841579999983 0.3620341720000013
0.4376529460000000 0.2235627769999979 0.5429322119999966
0.9195543530000023 0.4865541759999985 0.6832761169999984
0.3026185040000016 0.0019909700000014 0.5022993680000027
0.7789615989999987 0.2550958400000027 0.6347227689999997
0.1283164620000008 0.8258005380000029 0.5938587189999964
0.5948265789999994 0.5745854379999997 0.7318541409999995
0.9653923509999984 0.5844044090000011 0.2663238940000028
0.3172959090000020 0.5448212619999993 0.3652837870000027
0.7938938140000005 0.7980461719999994 0.4976982470000024
0.1767816249999967 0.8134424690000017 0.3167348500000031
0.6589540840000012 0.5765332579999978 0.4570353029999978
0.2663016019999986 0.5431171660000018 0.6379619240000025
0.7701286670000016 0.7991834879999971 0.7701178189999993
0.4606798590000025 0.8233881589999967 0.4030190710000028
0.9384332899999990 0.5745186810000007 0.5392084719999986
0.4109536109999965 0.8338512779999974 0.6802981499999987
0.5014771219999972 0.7254761459999983 0.2681213919999976
0.9680871959999990 0.9740812779999999 0.4061760599999999
0.1309168339999971 0.7155441640000006 0.7336636189999979
0.6854609849999989 0.9662225249999992 0.3197379710000021
0.1581589580000013 0.7254963520000004 0.4607895019999972
0.6358589530000032 0.9765135649999976 0.5969444509999988
0.3261720240000017 0.5009091499999982 0.2298899740000024
0.8301107289999976 0.7568840380000026 0.3620340530000021
0.4376533330000001 0.7235621809999984 0.5429317950000012
0.9195550080000032 0.9865532520000002 0.6832755800000001
0.3026186530000032 0.5019910339999996 0.5022996659999990
0.7789615390000009 0.7550955410000029 0.6347224120000021
0.4338561300000023 0.3986861710000014 0.2981556650000030
0.9178737399999974 0.1522970649999991 0.4409464299999968
0.3964857460000033 0.4006476100000000 0.5799881820000010
0.8597855570000021 0.1586339620000032 0.7205237749999966
0.7220935819999994 0.1469431670000034 0.2911994460000003
0.2129221109999975 0.4002518360000025 0.4241215879999984
0.6823042629999989 0.1512350889999965 0.5588049890000022
0.1407311560000011 0.3857647780000022 0.6899422999999985
0.1787492189999966 0.1476938129999965 0.5590384010000022

0.6624586579999985 0.4013288319999972 0.7018290760000028
0.2363370659999973 0.1413549040000035 0.2794872819999981
0.6999135610000025 0.3993158339999994 0.4200382530000013
0.3741849959999968 0.1531035450000005 0.7088085410000033
0.9556412100000031 0.4142625929999966 0.3100867570000005
0.4142554700000005 0.1486918479999986 0.4411550160000033
0.8835331800000006 0.3996851440000029 0.5758941169999972
0.4338558019999965 0.8986867070000031 0.2981555160000013
0.9178737399999974 0.6522967220000027 0.4409461919999984
0.3964861330000033 0.9006476400000025 0.5799877640000020
0.8597872260000017 0.6586313250000018 0.7205233569999976
0.7220924499999981 0.6469435099999998 0.2911992670000032
0.2129220070000031 0.9002521629999976 0.4241211710000030
0.6823039650000027 0.6512343879999989 0.5588048099999980
0.1407313790000018 0.8857644200000010 0.6899420620000001
0.1787492189999966 0.6476929780000020 0.5590383409999973
0.6624566910000027 0.9013304710000014 0.7018280630000007
0.2363367080000032 0.6413561700000017 0.2794876689999981
0.6999136210000003 0.8993163109999998 0.4200379549999980
0.3741835650000027 0.6531040070000032 0.7088083619999992
0.9556410309999990 0.9142631890000033 0.3100865780000035
0.4142557679999967 0.6486916539999967 0.4411549570000020
0.8835330610000014 0.8996855620000019 0.5758933420000005

Defective *c*-In_2O_3(111) surface with the O_{v7} site

O In
1.00000000000000
14.4443000000000001 0.0000000000000000 0.0000000000000000
-7.2221499999999965 12.5091307398835685 0.0000000000000000
0.0000000000000009 0.0000000000000016 15.0371000000000006
O In
47 32
Direct
0.1429500432523283 0.8140900786647434 0.3534411575922925
0.4799391767210576 0.4861547614454031 0.5485647020521298
0.7742000094242808 0.4930516378986645 0.5787873178993702
0.4271036188871337 0.8256491853354423 0.3518143267381963
0.2844557806981188 0.2749593636713045 0.5807359983178838
0.9317010964305754 0.5958253637329484 0.3635512158345074
0.4824047567230941 0.7460790679775692 0.5259838203820516
0.1608866158299641 0.0735062662513210 0.3239406427539460
0.1855729602579074 0.3308647379799463 0.3506032855531481
0.5173978566052475 0.9879584788182465 0.5431209050079046
0.5084483276164431 0.2781689570214322 0.5730342584889847
0.1761679327257623 0.6041721240617457 0.3576373270629349
0.7276337381875151 0.0092929107617366 0.6212474286440104
0.4052791636487931 0.3374890252294221 0.3621410871155179
0.2612718554743751 0.7501749387151923 0.5291770611973348
0.9303836660421386 0.0893014865329739 0.3228757022041063
0.6688863342001232 0.8510947769850369 0.3452308872408419
0.0100632537650049 0.5255654034477628 0.5436001708575945
0.7191500633214722 0.2262079595630988 0.5738160133624707
0.3976176974887399 0.5718729107283015 0.3582958665200117
0.9935382240361638 0.7230128128012654 0.5627860165336203
0.6633642816747715 0.0657890816531014 0.3600271818088774
0.2513523802023362 0.5127121993218093 0.5295724956149584
0.9127277109934425 0.8398741553752642 0.3332015333405491
0.1864021362512073 0.8504472199654040 0.6488434525394526
0.8551758393367450 0.1726347418061937 0.4587109532522980
0.5616880987240400 0.1737965270853457 0.4258027000284623
0.9051565210941225 0.8411707281712950 0.6419492310666669
0.0504288766462775 0.3932233960813689 0.4222939646350373
0.4004678535061026 0.0685949670269685 0.6371626098181780
0.8401687020170154 0.9319589288134661 0.4699739724357325
0.1715630957565348 0.5945789687425856 0.6714182739029082
0.1479655025717915 0.3376283184250243 0.6488288381940722
0.8111486499465592 0.6734380940169632 0.4564422548780243
0.8234321967384787 0.3836976050750030 0.4272820526200046

0.1603927113849286 0.0637789124183891 0.6429652512895699
0.6022718898058784 0.6600090670908267 0.4339992700822202
0.9304832252234769 0.3292630340743727 0.6378137967996786
0.0745181204736341 0.9240534334399774 0.4696879585357434
0.4080810907051423 0.5839024815692394 0.6676721224624318
0.6626749151864830 0.7996982755265847 0.6379257879718907
0.3224023488838211 0.1417492423090973 0.4548074131748755
0.6137680041564214 0.4383420403511252 0.4283165031386158
0.9436466843539213 0.0956472246316231 0.6394137375981728
0.3423004970031649 0.9484773016603560 0.4216370982245343
0.0844175620352094 0.1548340694645367 0.4677336095682565
0.4181551751237144 0.8264869104259487 0.6748663977318060
0.1125364058440181 0.6852475061518418 0.6052202105234188
0.5511552657116385 0.1497604590460780 0.5758241398335419
0.2284690566639429 0.4905439695904235 0.3884466668783422
0.7769001123121340 0.0131081608149713 0.3837731007669470
0.3144945393599885 0.4301328237165519 0.6114929386190728
0.8480481608290871 0.3971206788674545 0.5770193522517026
0.5068186718999050 0.7400450598294129 0.3849779741357491
0.9861971261580198 0.7612127655316169 0.4048559999069324
0.5697238533070559 0.8857412341853609 0.6144853871141285
0.6036221733985413 0.4476073145888756 0.5805459586017181
0.2615740082397354 0.7722517576335819 0.3874635557116513
0.2388895563674879 0.2244256346328647 0.3928241599972963
0.2195499675755472 0.9826623907624480 0.3893623914482229
0.7815968671599954 0.5126372927378102 0.4244221712862061
0.1087350800460444 0.1777203301563253 0.6100022457595510
0.5502247334573229 0.6545779020650642 0.5842470233113526
0.0178952068161500 0.2371798952473324 0.3922141324584040
0.4858496045552436 0.2669565807259711 0.4244929673884501
0.8246116406706588 0.9295252655179730 0.6133446612880529
0.3464304101799367 0.9044311514738536 0.6029477007792530
0.7617481369946131 0.7813047301726134 0.3954590857903652
0.7328634704140629 0.2150282506555220 0.4257574664585930
0.0730876566636378 0.8978364499728584 0.6101687322394144
0.0950097550883838 0.4428715469546712 0.6021745839128513
0.0121873234463284 0.5140246379179655 0.4000124722345765
1.0014147667139284 0.0010941179487611 0.3856491448488317
0.4871849807225752 0.4980876159428567 0.4021074061165917
0.5010967777256502 0.9874096256634286 0.3998060620018989
0.8326228059413109 0.6770876192451220 0.5989539765842856
0.3228223590768849 0.1534539768496343 0.5988687041451902
0.3306641159792668 0.6679368377071244 0.6133275345567598
0.8485391695494285 0.1663372455481913 0.6040284409788307

Defective *c*-In_2O_3(110) surface with the O_{v4} site

O In
1.00000000000000
10.2136999999999993 0.0000000000000000 0.0000000000000000
0.0000000000000009 14.4443000000000001 0.0000000000000000
0.0000000000000010 0.0000000000000010 15.9873999999999992
O In
47 32
Direct
0.6084218486684768 0.1822501374974544 0.4374581600636654
0.1081909088695893 0.6833168846823289 0.4377185529532702
0.1106576976953376 0.9634146879957456 0.4561994035305076
0.6085810333659818 0.4660352298480476 0.4560545349246817
0.3255115139464317 0.5841392217340996 0.3494340908182055
0.8257780999900247 0.0824468657941126 0.3465540446668404
0.8252660413930910 0.5646640786214522 0.5350187649814300
0.3275780483165420 0.0621062665737263 0.5351625287468165
0.0975685404461004 0.9720786366038311 0.6643488001486142
0.6003744887172109 0.4679203299810920 0.6666118306328936
0.3294779198500688 0.8186139607375266 0.3494716370898528
0.8260055651799445 0.3179812038991357 0.3462635734253382
0.5986909512067462 0.6873169041431950 0.6824765842730047
0.1039450814799660 0.1860145908657360 0.6829212937896004
0.8348888502894938 0.3294954773232461 0.5383340306495578
0.3343971762313296 0.8204897518251761 0.5455331190733460
0.5655948420906810 0.6958489582853647 0.4554531368674156
0.0607207828655051 0.1953010290526456 0.4612781146573464
0.3880542108294686 0.0671336735287677 0.3207962354622166
0.8884856514524470 0.5663256490598569 0.3206151405901212
0.8741295067811767 0.0855465534390516 0.5576866999715618
0.3722129893657007 0.5892874037760342 0.5646691686325157
0.0605996785056713 0.4590926896698340 0.4416809326118019
0.5602935528585603 0.9578397071690122 0.4419553745781444
0.7980246971703485 0.2155191912326374 0.6876626109274925
0.3113374686049717 0.4335390670848682 0.6743085530325003
0.8104133476379979 0.9371783487207173 0.6791086065323088
0.0939469301058266 0.3193563617548422 0.3154591723304387
0.5935844779387309 0.8213586657340988 0.3122242170921703
0.6108511729495577 0.8383485151459170 0.5715580743798100
0.1061247537127750 0.3381216484182543 0.5742923038031541
0.3324237465157217 0.4284588115117405 0.4607792058782350
0.8337381813010803 0.9275550914994135 0.4582047405538859
0.0916755201186729 0.0845996612834145 0.3126075922756629

0.5905647102403868 0.5837409289855865 0.3100332410851925
0.8306457293349502 0.7203007435400798 0.4364335357698990
0.3290379508243630 0.2201537835942656 0.4380428532728306
0.5963588341066449 0.0685768409063997 0.5845004974118636
0.0990597845674154 0.5704296155158161 0.5832273333483837
0.8696067743875694 0.6968955102394349 0.6687262383460127
0.3740378718294731 0.1951182180500799 0.6684915131053887
0.0301692513925431 0.8340333857123707 0.3244132726745108
0.5286876570540059 0.3343752728875667 0.3256265767850671
0.5572919771641303 0.3127769357850910 0.5635043141998451
0.0563822028045383 0.8123950783560873 0.5662322605142870
0.3665746230964321 0.9501808364236957 0.6854476423637809
0.8683623916709775 0.4524422105094001 0.6845857612870799
0.9670640065680789 0.2182249183582003 0.5831506543154001
0.4579836360632488 0.9309592715423400 0.3301014914334712
0.9578702415155277 0.4291170180874238 0.3309774414011731
0.4804681207961288 0.7141540050034131 0.5742747197973802
0.2200334973282307 0.5593468368716569 0.4634497472918726
0.2142034880863134 0.0912361619810308 0.4222022854855890
0.7172241592442051 0.5893695302454782 0.4189556205666923
0.7196187139667506 0.0587007080092946 0.4596462559197354
0.7435074200364727 0.5734364598522159 0.6647559154422144
0.1808845861948662 0.8238981505748116 0.4412243199139458
0.6802794541597738 0.3259271201895134 0.4414915108307393
0.2444527208573279 0.0753917807302442 0.6641517371243537
0.4649547924639719 0.1821066076766003 0.5479129477957951
0.9680083871296699 0.9712083272127673 0.3518033205505200
0.4655571058481910 0.4715548873634629 0.3537081330294106
0.9638536534957747 0.6810396000597861 0.5484348834214392
0.2140656920982316 0.8510100061889511 0.6548320331474078
0.2331937277765523 0.3016746410133453 0.6735877691155266
0.7314415781971224 0.8033419968532454 0.6740451670700868
0.7198881833984673 0.3470098614028804 0.6540277167291699
0.6815378049610752 0.8263189037862612 0.4387146311463428
0.2476471569455164 0.5780308206480522 0.6787123419116932
0.7528579786222522 0.0773736228882311 0.6679618293664942
0.1779695186168622 0.3260359323062630 0.4432421571094133
0.9611047790996570 0.1995300875710893 0.3406191828141084
0.4662520975858055 0.9493551690582969 0.5659449809045219
0.9680617161822493 0.6991462079798051 0.3392527112314100
0.4614928078132207 0.4478000720577365 0.5702166025322059
0.9637023644259253 0.9486658174524225 0.5659552524112311
0.4620562422036104 0.6991340378733545 0.3368046905568473
0.9663613812402784 0.4516205409387868 0.5657942526192891

0.4663879521539637 0.1999362832248144 0.3400418269059625

Defective *h*-In_2O_3(012) surface with the O_{v6} site

O In
1.00000000000000
11.0386000000000006 0.0000000000000000 0.0000000000000000
0.0000000000000007 11.6846999999999994 0.0000000000000000
0.0000000000000010 0.0000000000000010 16.3939999999999984
O In
47 32
Direct
0.4873266408188704 0.1046917057208583 0.3035422918684430
0.2342643711547460 0.3203252330319687 0.5458712373885621
0.2093845877825430 0.1646135356885391 0.3671174875472549
0.4571949339156604 0.3858289232008560 0.6321415249647152
0.4865125082180083 0.2326769799805849 0.4536579517648177
0.2348696446952903 0.4475527503048012 0.6960222022427497
0.3844774792936445 0.4826189522689625 0.4537613435891603
0.1623897672835897 0.4143825794870095 0.3663501857913412
0.3846322198496959 0.3548757668532897 0.3034029855507142
0.1329075302042183 0.1986045979408707 0.6955940537004711
0.1360238428133414 0.0697919296486221 0.5459438557738616
0.4133087445489489 0.1371017654208055 0.6339833466245944
0.9869601342255281 0.1052333146945064 0.3041767765181090
0.7369889084190484 0.3256254321827692 0.5495522423047674
0.7094658882151538 0.1644281900158555 0.3676024416464309
0.9474292918177859 0.3902779253499554 0.6386611533354271
0.9853249604539106 0.2334937683761455 0.4546523404479492
0.8882284862476665 0.4813762099071405 0.4510788952093669
0.6624657530341468 0.4140829715501629 0.3679273182768187
0.8839337206014543 0.3543989440632013 0.3028850475469383
0.6349104324485555 0.2024661068874676 0.6975028539471743
0.6357596487301970 0.0726438125396713 0.5465803914786859
0.9141455600831709 0.1345298767273439 0.6304849321939510
0.4875309411319349 0.6049773051598611 0.3032524064020226
0.2365496429559348 0.8194427299263252 0.5458793618661589
0.2101509968354016 0.6647146872221595 0.3668379188878611
0.4601315932080874 0.8869843420259850 0.6333029602855629
0.4874339298043106 0.7319312051966566 0.4541920234520074
0.2371824868998298 0.9472272786676731 0.6962347027120229
0.3854378041607407 0.9824208966355903 0.4539010154852433
0.1620555236307105 0.9144774961063038 0.3670693079732819
0.3844897273061023 0.8548674311058196 0.3037296262368355
0.1337440333235720 0.6987246682569022 0.6956808807099630

0.1330715382963331 0.5683631874734700 0.5465576453762003
0.4138505974291750 0.6374377655531217 0.6333580538085101
0.9875941501959490 0.6057186376944872 0.3029444816658885
0.7366130103167235 0.8191321634648441 0.5462115856783845
0.7099831138207022 0.6636239015355219 0.3671542338570603
0.9591285131561652 0.8861318800860881 0.6329730652326491
0.9856905287074911 0.7313763580276620 0.4543316117786919
0.7369891797889488 0.9503738901295800 0.6958388159064888
0.8853611094175089 0.9820894277962748 0.4533765100376702
0.6620022425448856 0.9146385479350272 0.3671295803780875
0.8842154961084541 0.8548422739395547 0.3034464136228832
0.6404071706416629 0.6948832771855579 0.6971359523390133
0.6357479739025611 0.5677177252270833 0.5470926064168409
0.9084951933052718 0.6333023263131379 0.6359472378870222
0.0495295825912591 0.2747139736121327 0.3266359862661646
0.3132886316342071 -0.0001552414335185 0.5742302565476517
0.0629499264633266 0.0521774829643987 0.4258572817045577
0.2992655539995664 0.2777809499944856 0.6731617469070149
0.3087764516430660 0.3022675121608243 0.4257460745243148
0.0725587540306298 0.0270341228828004 0.6724605676097970
0.3219170785276616 0.0245943614355008 0.3265735953202325
0.0583122287390415 0.2509511287139565 0.5744495227679118
0.5495530194125127 0.2743924013155868 0.3263319921364589
0.8118250142716061 -0.0014300594475964 0.5729470893348855
0.5624528964278306 0.0522185344624085 0.4258585150877425
0.8034508621997539 0.2705118866010579 0.6732411426741913
0.8082963165219605 0.3017563694284608 0.4255022291823629
0.5709929407189696 0.0288846366928019 0.6739384733214216
0.8217860228701946 0.0244900021942519 0.3264744401145249
0.5583003544207018 0.2511979453419901 0.5737867191033594
0.0497363560460608 0.7751000680276657 0.3265245428706530
0.3124459024831166 0.5007482765569472 0.5743988413176239
0.0650143785343178 0.5528520990309684 0.4244940063397853
0.3004364732918110 0.7774284819716065 0.6729907748354884
0.3097304651328139 0.8021783823953361 0.4257549416088489
0.0710678983021447 0.5288732820942805 0.6746321543962294
0.3223384868453192 0.5243653800113136 0.3260328978751627
0.0595376854117313 0.7496604001417174 0.5739617371381505
0.5498392858145201 0.7745826337115408 0.3266243457888500
0.8144252645456549 0.5041858013743027 0.5671377037147511
0.5619565136365753 0.5521626625987153 0.4254595373499822
0.8014787292071348 0.7803981423084936 0.6742224099130556
0.8087114664249037 0.8020566062116364 0.4253043932915786
0.5726030122604038 0.5252779264996573 0.6772122258173162

0.8222793149374633 0.5244416668431918 0.3248806604983351
0.5595015809100456 0.7489215087970235 0.5752023369329387

Defective *h*-In_2O_3(104) surface with the O_{v3} site

O In
1.00000000000000
8.0410003662000005 0.0000000000000000 0.0000000000000000
0.0000000000000000 11.0943002700999998 0.0000000000000000
0.0000000000000000 0.0000000000000000 21.6168003081999984
O In
47 32
Direct
0.1332705619999999 0.3290569480000016 0.5966854099999992
0.5914500359999977 0.0679100979999987 0.7348390220000027
0.9655579920000008 0.0847392749999969 0.2657148239999998
0.3201001879999978 0.0453787220000024 0.3651039599999990
0.7960218190000035 0.2997946440000021 0.4990788400000028
0.1770348550000023 0.3127663429999998 0.3178848330000008
0.6607795359999997 0.0762775390000030 0.4580601159999986
0.2669119830000000 0.0488163380000017 0.6383628250000015
0.7603574990000013 0.3014116290000004 0.7717111709999998
0.4624277349999986 0.3234661520000017 0.4029273089999990
0.9404361249999980 0.0776278820000016 0.5409166219999975
0.4177922310000000 0.3349705039999975 0.6817356350000026
0.5011954309999993 0.2247633039999997 0.2671991590000005
0.9688162799999986 0.4741262200000023 0.4055815339999995
0.1307202280000013 0.2206771079999967 0.7351596950000001
0.6861234899999999 0.4657346309999966 0.3192653360000008
0.1586847900000024 0.2267961200000030 0.4613761009999990
0.6382377739999967 0.4801883399999980 0.6020764109999988
0.3218852580000018 0.9991661310000026 0.2296840850000024
0.8290343879999966 0.2559993859999992 0.3623923660000017
0.4404034909999979 0.2274323549999977 0.5432752370000031
0.9181609749999993 0.4864993690000006 0.6838291290000029
0.3024065199999981 0.0043621650000034 0.5016503929999985
0.7837733029999967 0.2532509859999976 0.6362294549999987
0.1285206530000025 0.8305659290000023 0.5927333830000023
0.9657285210000026 0.5838770869999976 0.2654054460000026
0.3200715779999967 0.5452396869999987 0.3651320040000030
0.7937814000000003 0.7977874879999973 0.4957582059999979
0.1768657419999968 0.8126211760000004 0.3174061480000034
0.6604547499999995 0.5752366780000031 0.4583308400000021
0.2738605139999990 0.5497861500000027 0.6406915780000020
0.6568734649999968 0.7249132990000007 0.7494442460000030
0.4614596959999986 0.8233596680000019 0.4021769759999998
0.9404602649999987 0.5763115290000016 0.5403591390000031
0.4037450849999971 0.8332408670000007 0.6763038639999976

0.5010982749999968 0.7245275969999980 0.2666787209999981
0.9683275220000027 0.9747025969999967 0.4055318529999994
0.1223768959999987 0.7309870119999999 0.7374446390000031
0.6855519409999999 0.9658477899999980 0.3185858730000035
0.1591297840000010 0.7265988589999992 0.4612844879999969
0.6389245989999992 0.9767519829999998 0.5971309540000007
0.3230192660000029 0.4985484179999986 0.2297940110000027
0.8296627400000034 0.7560410500000003 0.3613107500000012
0.4413434860000010 0.7251068950000032 0.5415471199999971
0.9110687379999973 0.9776554110000006 0.6994264719999990
0.3031353350000003 0.5029309990000002 0.5022691490000000
0.7895767690000000 0.7599322200000032 0.6323410870000004
0.4347513319999976 0.3980417849999967 0.2976438399999992
0.9189306500000001 0.1525932400000016 0.4410245119999985
0.3963851930000004 0.4047500189999980 0.5806686880000029
0.8594774009999995 0.1578347089999994 0.7250903249999965
0.7225277419999969 0.1470739390000020 0.2903800610000005
0.2144615799999983 0.4007345440000023 0.4233117400000026
0.6831104760000031 0.1529578419999993 0.5593103169999978
0.1515583400000011 0.3941571410000009 0.6932922599999998
0.1819743069999973 0.1523281480000023 0.5590582490000031
0.6702718140000030 0.3953856529999982 0.6978876590000027
0.2367387410000035 0.1410613660000024 0.2794286609999972
0.7017323370000028 0.3991560640000031 0.4198909699999973
0.3746628459999997 0.1548030670000031 0.7116047140000035
0.9559481140000017 0.4135223330000031 0.3091555829999990
0.4161795079999990 0.1492450240000025 0.4408516290000009
0.8905909059999999 0.4004875720000030 0.5763502120000012
0.4339448810000022 0.8977161649999985 0.2970501180000014
0.9203114510000034 0.6522079109999979 0.4401783050000034
0.3970578610000004 0.9024657009999970 0.5780136589999998
0.8857811689999977 0.6655325290000036 0.7142537240000024
0.7223792079999996 0.6464552280000007 0.2899418470000015
0.2138512129999981 0.9004273409999968 0.4228174089999968
0.6843690279999990 0.6520729659999986 0.5578458909999995
0.1464839880000000 0.8946042660000018 0.6881673930000005
0.1831551940000011 0.6498917340000006 0.5602320429999992
0.6533179279999999 0.8961298469999974 0.6988923549999981
0.2366162089999975 0.6405180690000023 0.2791832690000007
0.7001456619999971 0.8999575380000024 0.4182656999999992
0.3901391630000006 0.6563675399999980 0.7196100950000002
0.9561283589999974 0.9137319920000024 0.3088375629999973
0.4157718120000027 0.6491084099999966 0.4409333469999979
0.8860195880000035 0.9001523849999984 0.5711473229999982

Fully reduced *c*-In_2O_3(111) surface

O In
1.00000000000000
14.4443000000000001 0.0000000000000000 0.0000000000000000
-7.2221499999999965 12.5091307398835685 0.0000000000000000
0.0000000000000009 0.0000000000000016 15.0371000000000006
O In
36 32
Direct
0.1470242711994905 0.8185281539406876 0.3486813037978116
0.4886565496720825 0.5008967281795162 0.5534862176497292
0.7761462849620978 0.4925089963112808 0.5762523671053197
0.4258540163022493 0.8251250972846701 0.3584299776551845
0.2607052035307168 0.2781391284826574 0.5731962004781203
0.9375543394428771 0.5979079469480266 0.3682967003142437
0.4893682738855136 0.7419766009325944 0.5284907695922078
0.1629387053090069 0.0803601454947894 0.3230406748292889
0.1813861409192498 0.3284990118029703 0.3484701209296074
0.4990914894789056 0.9877751042456392 0.5535295719721214
0.5075314875173068 0.2836047831899411 0.5762868627891143
0.1749120042691424 0.6007468970269174 0.3583879862190105
0.7217926401800806 -0.0174264556186268 0.5728730833007545
0.4021630414552949 0.3396681815840483 0.3681689526362721
0.2580300488399371 0.7473572070383000 0.5285753105116054
0.9194719174020758 0.0824803887266478 0.3231750480303203
0.6715166682581762 0.8529146036300146 0.3485374648304249
0.0122761409254426 0.5113816313634479 0.5534945308220790
0.7164811418486984 0.2239818074189686 0.5762766669126288
0.3992718454651177 0.5741254546105530 0.3583716798450139
1.0172564189972535 0.7392021168256450 0.5726936363282492
0.6603287112386118 0.0624726412898628 0.3682676746535308
0.2526116106308461 0.5105933944608281 0.5284988596894563
0.9175510566912137 0.8370128342304900 0.3232161254937978
0.8559566099204249 0.1763763592664607 0.4598226148642351
0.5602859884577962 0.1754151833084385 0.4281350337830346
0.0499471862848985 0.3902054926632355 0.4228736750970095
0.8507744006502018 0.9252008307861737 0.4651284965038659
0.8234775552639069 0.6794769850494540 0.4598183101992409
0.8247153620202137 0.3848874555253253 0.4281027646899622
0.6097885854264388 0.6597220205211403 0.4228451524074395
0.0747797830542464 0.9256903406297974 0.4651637301003071
0.3204430756147494 0.1441443999860022 0.4597442165029267
0.6151163186021190 0.4397881140689728 0.4281402208303461
0.3402432823130309 0.9500357093346260 0.4228966442592545

0.0746042436967832 0.1492744560001067 0.4650427001992968
0.1115367631112663 0.6699105347173014 0.6257894296894916
0.5464357428765125 0.1546445164446049 0.5790335017452222
0.2307238748179262 0.4889930568967711 0.3849465466263665
0.7731826072439383 0.0089814773176780 0.4038596864065703
0.3301731278706960 0.4418168701234380 0.6257433192748374
0.8454691987820379 0.3918063540279710 0.5790323905615208
0.5110073513215200 0.7417107931738094 0.3849468572438841
0.9909787080258937 0.7641987350173117 0.4040392316577961
0.5582081880492092 0.8883533632920236 0.6257457477256648
0.6082724027729260 0.4536597744239370 0.5790764129864683
0.2582800630170026 0.7692747041548053 0.3850221267889954
0.2358002004375198 0.2267404824794047 0.4035574509531994
0.2200450845952336 0.9882374891645909 0.3859304485001662
0.7844093618781384 0.5164474611194244 0.4259889123179931
0.0823913980973919 0.1813548972806216 0.6074553932304034
0.5996439862122925 0.6809194383510494 0.5758997663648995
0.0117116968307955 0.2317903844732666 0.3859150509896827
0.4835663404138361 0.2679774154007146 0.4260027026497401
0.8185737306512281 0.9010020933213775 0.6075041895494653
0.3190525646354251 0.9186971684922492 0.5759852353811061
0.7682062440450798 0.7799064635872215 0.3858933287222613
0.7321041673623919 0.2156154764486334 0.4259967492357507
0.0988883303271941 0.9175716959599972 0.6075428983104317
0.0812659592660109 0.4003554484198730 0.5759175487761165
0.0127142849292723 0.5131485825747353 0.4055431382909803
0.9999845567607353 -0.0000133611946813 0.3774825827439104
0.4868977316104042 0.4995649773343374 0.4055310407974622
0.5004182909736322 0.9873168468661501 0.4055743337410669
0.8478537004132161 0.6783698682492489 0.6092930254031376
0.3215873115222072 0.1695060426330434 0.6092494742882322
0.3333595554545499 0.6666319648251841 0.5954030752150693
0.8304850759683142 0.1520292380842998 0.6093070580093057

Fully reduced *c*-In_2O_3(110) surface

O In
1.00000000000000
10.2136999999999993 0.0000000000000000 0.0000000000000000
0.0000000000000009 14.4443000000000001 0.0000000000000000
0.0000000000000010 0.0000000000000010 15.9873999999999992
O In
36 32
Direct
0.6099180865428737 0.1814693987649224 0.4343533994114800

0.1099180865428735 0.6814693987649220 0.4343533994114800
0.1151486573149182 0.9643582394744072 0.4531460562212499
0.6151486573149165 0.4643582394744064 0.4531460562212499
0.3285531456179464 0.5828642527263890 0.3459254562333135
0.8285531456179456 0.0828642527263894 0.3459254562333135
0.8215839682638524 0.5650830156282652 0.5410855499417635
0.3215839682638540 0.0650830156282648 0.5410855499417635
0.3343640014991947 0.8174453474300259 0.3513122857704455
0.8343640014991918 0.3174453474300267 0.3513122857704455
0.8332453072256399 0.3311414618917654 0.5498876400991022
0.3332453072256409 0.8311414618917647 0.5498876400991022
0.5678247194386138 0.6985096832195850 0.4576968131038111
0.0678247194386131 0.1985096832195849 0.4576968131038111
0.3910119396473039 0.0643589473137824 0.3213583788708584
0.8910119396473052 0.5643589473137837 0.3213583788708584
0.8548049451538066 0.0956532036638685 0.5615325039009077
0.3548049451538086 0.5956532036638689 0.5615325039009077
0.0658629992689302 0.4582752942100279 0.4388051070263616
0.5658629992689309 0.9582752942100277 0.4388051070263616
0.1002357313443741 0.3193509627656804 0.3126935700145120
0.6002357313443754 0.8193509627656813 0.3126935700145120
0.6124207005493864 0.8432337452678126 0.5799853397713345
0.1124207005493872 0.3432337452678119 0.5799853397713345
0.3388929289531302 0.4285313041879100 0.4595009683633161
0.8388929289531276 0.9285313041879113 0.4595009683633161
0.0928545659635969 0.0841189211345583 0.3092248543497280
0.5928545659635969 0.5841189211345580 0.3092248543497280
0.8333376600189414 0.7174945408164034 0.4320970608889583
0.3333376600189403 0.2174945408164040 0.4320970608889583
0.5841455228739557 0.0665661865190679 0.5894696694693677
0.0841455228739564 0.5665661865190682 0.5894696694693677
0.0355033448423015 0.8346934296522245 0.3253088324297176
0.5355033448423019 0.3346934296522248 0.3253088324297176
0.5451282403316405 0.3053321370087468 0.5670628449408578
0.0451282403316423 0.8053321370087474 0.5670628449408578
0.9806127352517985 0.2172098953331751 0.5779300149123623
0.4640236228125053 0.9283649357674358 0.3256918361117506
0.9640236228125053 0.4283649357674376 0.3256918361117506
0.4806127352517992 0.7172098953331748 0.5779300149123623
0.2242657977935148 0.5596194941933030 0.4604421968997628
0.2198607519532195 0.0896983502716752 0.4156995617229581
0.7198607519532207 0.5896983502716751 0.4156995617229581
0.7242657977935162 0.0596194941933020 0.4604421968997628
0.6825025107722853 0.5718393446335800 0.6590030209233392

0.1835678258587592 0.8233544774523565 0.4413742446014151
0.6835678258587667 0.3233544774523572 0.4413742446014151
0.1825025107722868 0.0718393446335799 0.6590030209233392
0.4649260780742773 0.1765799108580136 0.5378990729340432
0.9682130264706170 0.9709553055902810 0.3486460626953858
0.4682130264706159 0.4709553055902824 0.3486460626953858
0.9649260780742763 0.6765799108580113 0.5378990729340432
0.2005409336801786 0.8263042416701241 0.6697390964137716
0.2500149002623693 0.3268048773388904 0.6869560076027854
0.7500149002623714 0.8268048773388897 0.6869560076027854
0.7005409336801794 0.3263042416701240 0.6697390964137716
0.6864243828371055 0.8264078771673510 0.4411199036305015
0.2424663038593333 0.5755608153389195 0.6849229487104956
0.7424663038593331 0.0755608153389206 0.6849229487104956
0.1864243828371064 0.3264078771673491 0.4411199036305015
0.9652004405177891 0.1990850446607704 0.3372811500507324
0.4635684082820640 0.9501034742724892 0.5552861642753537
0.9718641155124108 0.6991197824446802 0.3322796471505577
0.4784317012113599 0.4551321013315194 0.5629127405577142
0.9784317012113584 0.9551321013315185 0.5629127405577142
0.4652004405177894 0.6990850446607716 0.3372811500507324
0.9635684082820635 0.4501034742724874 0.5552861642753537
0.4718641155124110 0.1991197824446808 0.3322796471505577

Fully reduced *h*-In_2O_3(012) surface

O In
1.00000000000000
11.0386000000000006 0.0000000000000000 0.0000000000000000
0.0000000000000007 11.6846999999999994 0.0000000000000000
0.0000000000000010 0.0000000000000010 16.3939999999999984
O In
40 32
Direct
0.4893092590946070 0.1043235986129083 0.3017427657549470
0.2296991785164958 0.3283170232483621 0.5494200301412906
0.2099003380249634 0.1639419883430852 0.3668096408663888
0.4514631536622241 0.3852064368139475 0.6313455211483351
0.4823579874695001 0.2307931547240781 0.4504155494789314
0.3892420125305007 0.4807931547240783 0.4504155494789314
0.1616996619750374 0.4139419883430853 0.3668096408663888
0.3822907409053938 0.3543235986129085 0.3017427657549470
0.1419008214835050 0.0783170232483619 0.5494200301412906
0.4201368463377767 0.1352064368139475 0.6313455211483351
0.9893092590946068 0.1043235986129083 0.3017427657549470

0.7296991785164957 0.3283170232483621 0.5494200301412906
0.7099003380249634 0.1639419883430852 0.3668096408663888
0.9514631536622243 0.3852064368139475 0.6313455211483351
0.9823579874694999 0.2307931547240781 0.4504155494789314
0.8892420125305009 0.4807931547240783 0.4504155494789314
0.6616996619750374 0.4139419883430853 0.3668096408663888
0.8822907409053941 0.3543235986129085 0.3017427657549470
0.6419008214835051 0.0783170232483619 0.5494200301412906
0.9201368463377765 0.1352064368139475 0.6313455211483351
0.4893092590946070 0.6043235986129082 0.3017427657549470
0.2296991785164958 0.8283170232483623 0.5494200301412906
0.2099003380249634 0.6639419883430852 0.3668096408663888
0.4514631536622241 0.8852064368139474 0.6313455211483351
0.4823579874695001 0.7307931547240785 0.4504155494789314
0.3892420125305007 0.9807931547240785 0.4504155494789314
0.1616996619750374 0.9139419883430852 0.3668096408663888
0.3822907409053938 0.8543235986129082 0.3017427657549470
0.1419008214835050 0.5783170232483623 0.5494200301412906
0.4201368463377767 0.6352064368139474 0.6313455211483351
0.9893092590946068 0.6043235986129082 0.3017427657549470
0.7296991785164957 0.8283170232483623 0.5494200301412906
0.7099003380249634 0.6639419883430852 0.3668096408663888
0.9514631536622243 0.8852064368139474 0.6313455211483351
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0.8822907409053941 0.8543235986129082 0.3017427657549470
0.6419008214835051 0.5783170232483623 0.5494200301412906
0.9201368463377765 0.6352064368139474 0.6313455211483351
0.0480338438857624 0.2748099143698680 0.3236306004801970
0.3180682146959202 0.0023081668295105 0.5681049207372389
0.0663345361750255 0.0530900618247081 0.4253240180030588
0.3015133954788238 0.2704496552335330 0.6873069533896103
0.3052654638249679 0.3030900618247082 0.4253240180030588
0.0700866045211702 0.0204496552335328 0.6873069533896103
0.3235661561142315 0.0248099143698680 0.3236306004801970
0.0535317853040735 0.2523081668295105 0.5681049207372389
0.5480338438857626 0.2748099143698680 0.3236306004801970
0.8180682146959201 0.0023081668295105 0.5681049207372389
0.5663345361750256 0.0530900618247081 0.4253240180030588
0.8015133954788238 0.2704496552335330 0.6873069533896103
0.8052654638249681 0.3030900618247082 0.4253240180030588
0.5700866045211699 0.0204496552335328 0.6873069533896103
0.8235661561142311 0.0248099143698680 0.3236306004801970

0.5535317853040808 0.2523081668295105 0.5681049207372389
0.0480338438857624 0.7748099143698676 0.3236306004801970
0.3180682146959202 0.5023081668295107 0.5681049207372389
0.0663345361750255 0.5530900618247080 0.4253240180030588
0.3015133954788238 0.7704496552335323 0.6873069533896103
0.3052654638249679 0.8030900618247080 0.4253240180030588
0.0700866045211702 0.5204496552335323 0.6873069533896103
0.3235661561142315 0.5248099143698676 0.3236306004801970
0.0535317853040735 0.7523081668295107 0.5681049207372389
0.5480338438857626 0.7748099143698676 0.3236306004801970
0.8180682146959201 0.5023081668295107 0.5681049207372389
0.5663345361750256 0.5530900618247080 0.4253240180030588
0.8015133954788238 0.7704496552335323 0.6873069533896103
0.8052654638249752 0.8030900618247080 0.4253240180030588
0.5700866045211699 0.5204496552335323 0.6873069533896103
0.8235661561142311 0.5248099143698676 0.3236306004801970
0.5535317853040808 0.7523081668295107 0.5681049207372389

Fully reduced *h*-In_2O_3(104) surface

O In
1.00000000000000
8.0410003662000005 0.0000000000000000 0.0000000000000000
0.0000000000000000 11.0943002700999998 0.0000000000000000
0.0000000000000000 0.0000000000000000 21.6168003081999984
O In
42 32
Direct
0.1275605459999980 0.3217763840000032 0.5976085879999999
0.9650851560000007 0.0848582070000035 0.2654838179999999
0.3185827129999979 0.0453016669999968 0.3647954870000021
0.7961190050000013 0.3011125600000000 0.4992916969999968
0.1761960070000015 0.3131985759999978 0.3175287239999989
0.6586667420000012 0.0776111839999984 0.4575956669999997
0.2630360490000001 0.0441511790000035 0.6400397880000028
0.4616472259999966 0.3237567050000010 0.4025285729999979
0.9362949499999971 0.0773702420000006 0.5406868919999965
0.4165956049999977 0.3244813749999977 0.6800421570000026
0.5009432969999992 0.2250418989999972 0.2665919559999992
0.9670856070000013 0.4748811099999983 0.4054695190000004
0.6851468289999971 0.4662477279999990 0.3190871669999993
0.1574653240000004 0.2262672049999992 0.4612156660000011
0.6275898410000025 0.4806960960000026 0.5961547030000034
0.3227719530000002 0.9991201059999995 0.2293204030000027
0.8285444639999966 0.2567172729999996 0.3624999330000023

0.4359206729999983 0.2249382310000030 0.5412286520000009
0.9105969209999998 0.4797072040000003 0.6796532190000022
0.2981231620000031 0.0010460490000028 0.5018328519999997
0.7668261070000000 0.2578373630000002 0.6370580339999989
0.1275413179999987 0.8217878170000006 0.5976353229999987
0.9650839700000020 0.5848533129999964 0.2654820309999977
0.3185691919999982 0.5452913840000022 0.3647968100000014
0.7960964700000019 0.8011130539999982 0.4992984029999974
0.1762039970000018 0.8131940629999974 0.3175336649999991
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0.2630790119999986 0.5441406280000010 0.6400327300000015
0.4616470779999986 0.8237524500000006 0.4025323230000026
0.9363063950000026 0.5773953579999969 0.5406681420000012
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0.9670802099999989 0.9748827000000020 0.4054715480000013
0.6851537069999978 0.9662457940000024 0.3190879610000010
0.1574710610000025 0.7262700420000030 0.4612246659999997
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0.4359026159999999 0.7249518340000023 0.5412476220000002
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0.1479428729999981 0.3826606169999991 0.6955487609999977
0.1809614869999976 0.1466878530000031 0.5596838789999978
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0.8862037450000031 0.6647317329999964 0.7189627690000009
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0.6802688100000012 0.6551279410000035 0.5576106310000029
0.1479235549999984 0.8827192859999968 0.6955644669999970
0.1809742069999984 0.6466703489999972 0.5596926139999994
0.6535793919999975 0.9141920929999969 0.6919952470000013
0.2362686499999995 0.6408610359999969 0.2790091600000011
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0.8887820819999988 0.9017357800000028 0.5771672019999983