

Supporting Information

Models of Surface Morphology and Electronic Structure of Indium Oxide and Indium Tin Oxide for Several Surface Hydroxylation Levels

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Input Files

The typical input files (atomic positions) used in the calculations are provided below for each model considered in this study.

1. Atomic positions for IO Models

Model IO_b

In	0.000000000	0.000000000	0.357542723
In	0.000000000	0.500000119	0.357542723
In	0.500000238	0.000000000	0.357542723
In	0.500000179	0.500000119	0.357542723
In	0.000000000	0.000000000	0.642457664
In	0.000000000	0.500000179	0.642457664
In	0.500000179	0.000000000	0.642457664
In	0.500000119	0.500000179	0.642457664
In	0.000000000	0.000000000	0.142457545
In	0.000000000	0.500000179	0.142457575
In	0.500000179	0.000000000	0.142457575
In	0.500000119	0.500000179	0.142457575
In	0.000000000	0.000000000	0.857542813
In	0.000000000	0.500000179	0.857542813
In	0.500000238	0.000000000	0.857542813
In	0.500000119	0.500000119	0.857542813
In	0.333333552	0.166666523	0.690876007
In	0.333333641	0.666666746	0.690876067
In	0.833333850	0.166666582	0.690876007
In	0.833333850	0.666666806	0.690876007
In	0.333333671	0.166666612	0.975791216
In	0.333333641	0.666666746	0.975791156

In	0.833333790	0.166666627	0.975791216
In	0.833333790	0.666666687	0.975791216
In	0.333333701	0.166666597	0.475790918
In	0.333333641	0.666666746	0.475790858
In	0.833333790	0.166666657	0.475790918
In	0.833333790	0.666666687	0.475790918
In	0.333333552	0.166666538	0.190875888
In	0.333333641	0.666666746	0.190875888
In	0.833333850	0.166666567	0.190875888
In	0.833333850	0.666666806	0.190875888
In	0.166666552	0.333333641	0.024209119
In	0.166666582	0.833333731	0.024209119
In	0.666666746	0.333333582	0.024209170
In	0.666666687	0.833333731	0.024209119
In	0.166666523	0.333333522	0.309124351
In	0.166666493	0.833333731	0.309124351
In	0.666666746	0.333333582	0.309124321
In	0.666666806	0.833333790	0.309124351
In	0.166666493	0.333333522	0.809124529
In	0.166666508	0.833333790	0.809124529
In	0.666666746	0.333333582	0.809124470
In	0.666666806	0.833333790	0.809124529
In	0.166666597	0.333333671	0.524209380
In	0.166666567	0.833333671	0.524209380
In	0.666666746	0.333333582	0.524209440
In	0.666666687	0.833333731	0.524209380
O	0.148190632	0.000000000	0.250000119
O	0.148190662	0.500000119	0.250000149
O	0.648190975	0.000000000	0.250000119
O	0.648190916	0.500000238	0.250000119
O	0.351809502	0.000000000	0.750000238
O	0.351809442	0.500000119	0.750000298
O	0.851809680	0.000000000	0.750000238
O	0.851809621	0.500000238	0.750000238
O	0.000000000	0.148190588	0.250000119
O	-0.000000000	0.648190856	0.250000119
O	0.500000119	0.148190632	0.250000119
O	0.500000238	0.648190796	0.250000149
O	0.000000000	0.351809502	0.750000238
O	0.000000000	0.851809740	0.750000238
O	0.500000179	0.351809531	0.750000238
O	0.500000179	0.851809680	0.750000298
O	0.351809531	0.351809412	0.250000119
O	0.351809502	0.851809621	0.250000149
O	0.851809680	0.351809412	0.250000119
O	0.851809740	0.851809621	0.250000119
O	0.148190603	0.148190707	0.750000238
O	0.148190603	0.648190916	0.750000298
O	0.648190856	0.148190707	0.750000238
O	0.648190856	0.648190916	0.750000238
O	0.481524199	0.166666403	0.583333492
O	0.481524199	0.666666746	0.583333492
O	0.981524348	0.166666463	0.583333492
O	0.981524467	0.666666746	0.583333492
O	0.185142860	0.166666567	0.083333321
O	0.185142875	0.666666746	0.083333299
O	0.685143173	0.166666582	0.083333321
O	0.685143113	0.666666746	0.083333313

O	0.333333671	0.314857215	0.583333492
O	0.333333641	0.814857304	0.583333492
O	0.833333850	0.314857215	0.583333492
O	0.833333790	0.814857364	0.583333492
O	0.333333671	0.018475870	0.083333313
O	0.333333641	0.518476009	0.083333299
O	0.833333790	0.018475881	0.083333321
O	0.833333790	0.518476069	0.083333321
O	0.185142875	0.018475870	0.583333492
O	0.185142949	0.518476129	0.583333492
O	0.685143054	0.018475860	0.583333492
O	0.685143113	0.518476129	0.583333492
O	0.481524259	0.314857274	0.083333321
O	0.481524289	0.814857364	0.083333299
O	0.981524408	0.314857274	0.083333313
O	0.981524467	0.814857364	0.083333321
O	0.314857274	0.333333582	0.916666985
O	0.314857304	0.833333731	0.916666985
O	0.814857423	0.333333582	0.916667044
O	0.814857423	0.833333790	0.916666985
O	0.018475950	0.333333701	0.416666895
O	0.018475849	0.833333790	0.416666895
O	0.518476129	0.333333701	0.416666895
O	0.518476129	0.833333850	0.416666865
O	0.166666538	0.481524259	0.916666985
O	0.166666523	0.981524587	0.916666985
O	0.666666746	0.481524318	0.916667044
O	0.666666865	0.981524587	0.916666985
O	0.166666493	0.185142860	0.416666895
O	0.166666433	0.685143113	0.416666865
O	0.666666687	0.185142905	0.416666895
O	0.666666687	0.685143113	0.416666895
O	0.018475840	0.185142860	0.916666985
O	0.018475920	0.685143173	0.916666985
O	0.518476009	0.185142845	0.916667044
O	0.518476129	0.685143173	0.916666985
O	0.314857244	0.481524229	0.416666865
O	0.314857304	0.981524467	0.416666895
O	0.814857423	0.481524229	0.416666895
O	0.814857483	0.981524467	0.416666895

Model IO_b-bcc

In	0.249999947	0.250000004	0.250000027
In	0.750000044	0.750000026	0.750000009
In	0.249999988	0.750000023	0.749999991
In	0.750000042	0.250000003	0.250000007
In	0.749999995	0.750000007	0.249999992
In	0.250000001	0.249999980	0.749999956
In	0.750000026	0.249999981	0.750000005
In	0.249999985	0.750000009	0.249999994
In	0.466283159	0.000000014	0.250000014
In	0.533716825	0.000000016	0.750000001
In	0.033716846	0.000000021	0.749999997
In	0.966283199	0.000000018	0.250000021
In	0.533716820	0.499999972	0.250000039
In	0.466283200	0.499999952	0.749999991

In	0.966283194	0.499999987	0.749999986
In	0.033716823	0.499999983	0.250000000
In	0.249999964	0.466283162	0.000000029
In	0.750000016	0.533716775	0.000000032
In	0.750000019	0.033716856	0.000000017
In	0.249999995	0.966283228	0.000000018
In	0.249999974	0.533716747	0.499999966
In	0.750000024	0.466283142	0.499999973
In	0.750000010	0.966283280	0.500000007
In	0.249999991	0.033716849	0.499999989
In	-0.000000005	0.249999999	0.466283142
In	0.000000008	0.750000005	0.533716815
In	-0.000000003	0.750000027	0.033716805
In	-0.000000005	0.249999990	0.966283212
In	0.499999984	0.249999998	0.533716824
In	0.500000000	0.750000003	0.466283158
In	0.499999992	0.750000002	0.966283188
In	0.500000009	0.249999991	0.033716801
O	0.391284646	0.154553780	0.381228618
O	0.608715360	0.845446241	0.618771379
O	0.108715349	0.845446247	0.881228609
O	0.891284700	0.154553769	0.118771394
O	0.608715326	0.654553758	0.118771400
O	0.391284654	0.345446209	0.881228614
O	0.891284676	0.345446217	0.618771393
O	0.108715323	0.654553771	0.381228621
O	0.381228612	0.391284672	0.154553779
O	0.618771404	0.608715329	0.845446235
O	0.881228625	0.108715325	0.845446251
O	0.118771401	0.891284683	0.154553765
O	0.118771391	0.608715336	0.654553755
O	0.881228614	0.391284661	0.345446209
O	0.618771391	0.891284700	0.345446239
O	0.381228607	0.108715320	0.654553769
O	0.154553783	0.381228597	0.391284653
O	0.845446220	0.618771408	0.608715363
O	0.845446215	0.881228609	0.108715364
O	0.154553801	0.118771413	0.891284646
O	0.654553799	0.118771407	0.608715350
O	0.345446205	0.881228596	0.391284636
O	0.345446206	0.618771393	0.891284640
O	0.654553786	0.381228593	0.108715357
O	0.891284673	0.654553755	0.881228611
O	0.108715316	0.345446229	0.118771386
O	0.608715360	0.345446203	0.381228614
O	0.391284674	0.654553751	0.618771376
O	0.108715332	0.154553776	0.618771389
O	0.891284658	0.845446241	0.381228633
O	0.391284661	0.845446234	0.118771378
O	0.608715341	0.154553776	0.881228626
O	0.881228611	0.891284689	0.654553759
O	0.118771380	0.108715325	0.345446228
O	0.381228602	0.608715322	0.345446225
O	0.618771380	0.391284670	0.654553783
O	0.618771373	0.108715327	0.154553774
O	0.381228602	0.891284675	0.845446242
O	0.118771381	0.391284661	0.845446224
O	0.881228581	0.608715360	0.154553766

O	0.654553793	0.881228595	0.891284661
O	0.345446208	0.118771407	0.108715357
O	0.345446201	0.381228586	0.608715352
O	0.654553795	0.618771397	0.391284643
O	0.154553778	0.618771405	0.108715330
O	0.845446214	0.381228596	0.891284653
O	0.845446196	0.118771403	0.391284649
O	0.154553788	0.881228594	0.608715358

Model IO₀

In	0.000000000	0.000000000	0.151330024	0	0	0
In	0.000000000	0.500000119	0.151330024	0	0	0
In	0.500000238	0.000000000	0.151330024	0	0	0
In	0.500000179	0.500000119	0.151330024	0	0	0
In	0.000000050	0.000000235	0.274381413			
In	0.000000047	0.500000304	0.274381616			
In	0.499999968	0.000000271	0.274381564			
In	0.500000164	0.500000455	0.274381539			
In	0.000000000	0.000000000	0.060295182	0	0	0
In	0.000000000	0.500000179	0.060295195	0	0	0
In	0.500000179	0.000000000	0.060295195	0	0	0
In	0.500000119	0.500000179	0.060295195	0	0	0
In	-0.000000085	-0.000000409	0.366920624			
In	0.000000516	0.500001497	0.366920864			
In	0.500000141	-0.000000519	0.366920549			
In	0.499999921	0.500000211	0.366920671			
In	0.333333664	0.166667035	0.295021859			
In	0.333333369	0.666667104	0.295021996			
In	0.833333224	0.166666911	0.295021851			
In	0.833333463	0.666666818	0.295021913			
In	0.333333989	0.166663617	0.418234493			
In	0.333333156	0.666667423	0.418234658			
In	0.833335699	0.166669983	0.418234422			
In	0.833331034	0.666666329	0.418234721			
In	0.333333317	0.166666945	0.203607429			
In	0.333333324	0.666667041	0.203607404			
In	0.833333411	0.166667054	0.203607443			
In	0.833333314	0.666666951	0.203607480			
In	0.333333552	0.166666538	0.080788255	0	0	0
In	0.333333641	0.666666746	0.080788255	0	0	0
In	0.833333850	0.166666567	0.080788255	0	0	0
In	0.833333850	0.666666806	0.080788255	0	0	0
In	0.166670017	0.333332561	0.439382944			
In	0.166660714	0.833328988	0.439383207			
In	0.666668344	0.333335183	0.439383787			
In	0.666668120	0.833337105	0.439382968			
In	0.166666523	0.333333522	0.130836939	0	0	0
In	0.166666493	0.833333731	0.130836939	0	0	0
In	0.666666746	0.333333582	0.130836927	0	0	0
In	0.666666806	0.833333790	0.130836939	0	0	0
In	0.166666507	0.333333164	0.345205032			
In	0.166666201	0.833333619	0.345205234			
In	0.666667088	0.333333843	0.345205499			
In	0.666667326	0.833333703	0.345205140			
In	0.166666816	0.333333843	0.223590704			
In	0.166666751	0.833333593	0.223590720			
In	0.666666703	0.333333594	0.223590772			

In	0.666666587	0.833333668	0.223590719			
O	0.148190632	0.000000000	0.105812597	0	0	0
O	0.148190662	0.500000119	0.105812610	0	0	0
O	0.648190975	0.000000000	0.105812597	0	0	0
O	0.648190916	0.500000238	0.105812597	0	0	0
O	0.350993064	-0.001477589	0.318260460			
O	0.350993166	0.498522229	0.318260314			
O	0.850993111	-0.001477837	0.318260241			
O	0.850993092	0.498522480	0.318260628			
O	0.000000000	0.148190588	0.105812597	0	0	0
O	-0.000000000	0.648190856	0.105812597	0	0	0
O	0.500000119	0.148190632	0.105812597	0	0	0
O	0.500000238	0.648190796	0.105812610	0	0	0
O	0.001477459	0.352471115	0.318260477			
O	0.001477985	0.852471258	0.318260270			
O	0.501478433	0.352471245	0.318260517			
O	0.501478475	0.852471502	0.318260338			
O	0.351809531	0.351809412	0.105812597	0	0	0
O	0.351809502	0.851809621	0.105812610	0	0	0
O	0.851809680	0.351809412	0.105812597	0	0	0
O	0.851809740	0.851809621	0.105812597	0	0	0
O	0.147529049	0.149007030	0.318260201			
O	0.147528790	0.649007355	0.318260400			
O	0.647529262	0.149007582	0.318260538			
O	0.647529337	0.649007017	0.318260469			
O	0.481239362	0.165662651	0.247311337			
O	0.481239223	0.665662631	0.247311232			
O	0.981239401	0.165662754	0.247311198			
O	0.981239300	0.665662557	0.247311262			
O	0.174702143	0.157496933	0.455569218			
O	0.174695045	0.657493297	0.455567992			
O	0.674702909	0.157500051	0.455569237			
O	0.674694695	0.657497890	0.455568286			
O	0.334337928	0.315577398	0.247311203			
O	0.334337797	0.815577236	0.247311254			
O	0.834337648	0.315577305	0.247311341			
O	0.834337512	0.815577197	0.247311232			
O	0.342500997	0.017194674	0.455568012			
O	0.342507191	0.517202454	0.455567948			
O	0.842503436	0.017205401	0.455569253			
O	0.842501916	0.517204522	0.455569439			
O	0.184423067	0.018760897	0.247311197			
O	0.184423135	0.518761244	0.247311250			
O	0.684422943	0.018761115	0.247311224			
O	0.684423184	0.518760938	0.247311355			
O	0.482797060	0.325297143	0.455569190			
O	0.482798624	0.825304902	0.455568127			
O	0.982803878	0.325305960	0.455568046			
O	0.982794360	0.825297972	0.455569527			
O	0.313815431	0.329694758	0.388066611			
O	0.313814751	0.829695272	0.388066196			
O	0.813815916	0.329698429	0.388067144			
O	0.813815106	0.829696318	0.388066810			
O	0.018475950	0.333333701	0.176354341	0	0	0
O	0.018475849	0.833333790	0.176354341	0	0	0
O	0.518476129	0.333333701	0.176354341	0	0	0
O	0.518476129	0.833333850	0.176354328	0	0	0
O	0.170304846	0.484120116	0.388066206			

O	0.170302966	0.984118073	0.388066827			
O	0.670303182	0.484118668	0.388067115			
O	0.670305385	0.984120534	0.388066716			
O	0.166666493	0.185142860	0.176354341	0	0	0
O	0.166666433	0.685143113	0.176354328	0	0	0
O	0.666666687	0.185142905	0.176354341	0	0	0
O	0.666666687	0.685143113	0.176354341	0	0	0
O	0.015881693	0.186184815	0.388066659			
O	0.015879580	0.686185454	0.388066857			
O	0.515882317	0.186184435	0.388067005			
O	0.515880359	0.686185422	0.388066282			
O	0.314857244	0.481524229	0.176354328	0	0	0
O	0.314857304	0.981524467	0.176354341	0	0	0
O	0.814857423	0.481524229	0.176354341	0	0	0
O	0.814857483	0.981524467	0.176354341	0	0	0

Model IO_0^m

In	0.000000084	0.000000170	0.151199028			
In	0.000000109	0.500000208	0.151198993			
In	0.499999986	0.000000122	0.151198991			
In	0.500000104	0.500000167	0.151198981			
In	0.000000134	0.000000170	0.273879613			
In	0.000000104	0.500000201	0.273879632			
In	0.500000081	0.000000179	0.273879616			
In	0.500000142	0.500000131	0.273879611			
In	0.000000000	0.000000000	0.060295182	0	0	0
In	0.000000000	0.500000179	0.060295195	0	0	0
In	0.500000179	0.000000000	0.060295195	0	0	0
In	0.500000119	0.500000179	0.060295195	0	0	0
In	0.000000151	0.000000241	0.363121028			
In	0.000000191	0.500000167	0.363121034			
In	0.500000090	0.000000224	0.363121031			
In	0.500000090	0.500000155	0.363121026			
In	0.333333436	0.166666865	0.291786674			
In	0.333333478	0.666666823	0.291786627			
In	0.833333459	0.166666811	0.291786667			
In	0.833333465	0.666666880	0.291786640			
In	0.333333391	0.166666809	0.393280819			
In	0.333333443	0.666666886	0.393280551			
In	0.833333525	0.166666913	0.393280819			
In	0.833333498	0.666666891	0.393280558			
In	0.333333474	0.166666922	0.201371168			
In	0.333333424	0.666666862	0.201371130			
In	0.833333340	0.166666820	0.201371161			
In	0.833333343	0.666666784	0.201371157			
In	0.333333552	0.166666538	0.080788255	0	0	0
In	0.333333641	0.666666746	0.080788255	0	0	0
In	0.833333850	0.166666567	0.080788255	0	0	0
In	0.833333850	0.666666806	0.080788255	0	0	0
In	0.166666552	0.333333641	0.010246514	0	0	0
In	0.166666582	0.833333731	0.010246514	0	0	0
In	0.666666746	0.333333582	0.010246536	0	0	0
In	0.666666687	0.833333731	0.010246514	0	0	0
In	0.166666523	0.333333522	0.130836939	0	0	0
In	0.166666493	0.833333731	0.130836939	0	0	0
In	0.666666746	0.333333582	0.130836927	0	0	0

In	0.666666806	0.833333790	0.130836939	0	0	0
In	0.166666719	0.333333479	0.350046519			
In	0.166666797	0.833333533	0.350046518			
In	0.666666798	0.333333505	0.350046515			
In	0.666666886	0.833333598	0.350046521			
In	0.166666769	0.333333532	0.222405656			
In	0.166666759	0.833333478	0.222405646			
In	0.666666795	0.333333496	0.222405655			
In	0.666666770	0.833333490	0.222405659			
O	0.148190632	0.000000000	0.105812597	0	0	0
O	0.148190662	0.500000119	0.105812610	0	0	0
O	0.648190975	0.000000000	0.105812597	0	0	0
O	0.648190916	0.500000238	0.105812597	0	0	0
O	0.347817703	0.000551434	0.319621124			
O	0.347817672	0.500551409	0.319621134			
O	0.847817805	0.000551444	0.319621123			
O	0.847817776	0.500551518	0.319621143			
O	0.000000000	0.148190588	0.105812597	0	0	0
O	-0.000000000	0.648190856	0.105812597	0	0	0
O	0.500000119	0.148190632	0.105812597	0	0	0
O	0.500000238	0.648190796	0.105812610	0	0	0
O	-0.000551148	0.347266540	0.319621127			
O	-0.000551169	0.847266489	0.319621151			
O	0.499448895	0.347266561	0.319621111			
O	0.499448823	0.847266473	0.319621146			
O	0.351809531	0.351809412	0.105812597	0	0	0
O	0.351809502	0.851809621	0.105812610	0	0	0
O	0.851809680	0.351809412	0.105812597	0	0	0
O	0.851809740	0.851809621	0.105812597	0	0	0
O	0.152733752	0.152182585	0.319621130			
O	0.152733875	0.652182594	0.319621147			
O	0.652733752	0.152182558	0.319621124			
O	0.652733840	0.652182596	0.319621141			
O	0.481567781	0.165179208	0.247419911			
O	0.481567763	0.665179111	0.247419897			
O	0.981567768	0.165179150	0.247419899			
O	0.981567745	0.665179155	0.247419902			
O	0.185142860	0.166666567	0.035270844	0	0	0
O	0.185142875	0.666666746	0.035270834	0	0	0
O	0.685143173	0.166666582	0.035270844	0	0	0
O	0.685143113	0.666666746	0.035270840	0	0	0
O	0.334821108	0.316388834	0.247419899			
O	0.334821123	0.816388827	0.247419890			
O	0.834821115	0.316388835	0.247419912			
O	0.834821105	0.816388833	0.247419910			
O	0.333333671	0.018475870	0.035270840	0	0	0
O	0.333333641	0.518476009	0.035270834	0	0	0
O	0.833333790	0.018475881	0.035270844	0	0	0
O	0.833333790	0.518476069	0.035270844	0	0	0
O	0.183611454	0.018432508	0.247419910			
O	0.183611426	0.518432555	0.247419896			
O	0.683611429	0.018432505	0.247419911			
O	0.683611473	0.518432511	0.247419902			
O	0.481524259	0.314857274	0.035270844	0	0	0
O	0.481524289	0.814857364	0.035270834	0	0	0
O	0.981524408	0.314857274	0.035270840	0	0	0
O	0.981524467	0.814857364	0.035270844	0	0	0
O	0.322753155	0.341568490	0.390993920			

O	0.322753163	0.841568597	0.390993934
O	0.822753233	0.341568553	0.390993918
O	0.822753245	0.841568621	0.390993934
O	0.018628080	0.333569027	0.176720917
O	0.018628071	0.833569020	0.176720936
O	0.518628189	0.333569073	0.176720902
O	0.518628152	0.833569096	0.176720916
O	0.158431774	0.481184837	0.390993937
O	0.158431741	0.981184889	0.390993928
O	0.658431773	0.481184903	0.390993916
O	0.658431829	0.981185025	0.390993905
O	0.166431246	0.185059399	0.176720890
O	0.166431232	0.685059431	0.176720875
O	0.666431170	0.185059331	0.176720883
O	0.666431228	0.685059407	0.176720895
O	0.018815424	0.177247127	0.390993937
O	0.018815455	0.677247107	0.390993907
O	0.518815357	0.177247142	0.390993930
O	0.518815431	0.677247156	0.390993903
O	0.314940894	0.481372141	0.176720888
O	0.314940839	0.981372182	0.176720897
O	0.814940936	0.481372126	0.176720896
O	0.814940917	0.981372144	0.176720921

Model IO₃₃

In	0.000000000	0.000000000	0.151330024	0	0	0
In	0.000000000	0.500000119	0.151330024	0	0	0
In	0.500000238	0.000000000	0.151330024	0	0	0
In	0.500000179	0.500000119	0.151330024	0	0	0
In	0.000902812	-0.000691410	0.275107199			
In	0.000903261	0.499308602	0.275106940			
In	0.500903868	-0.000691131	0.275106529			
In	0.500903166	0.499308356	0.275107280			
In	0.000000000	0.000000000	0.060295182	0	0	0
In	0.000000000	0.500000179	0.060295195	0	0	0
In	0.500000179	0.000000000	0.060295195	0	0	0
In	0.500000119	0.500000179	0.060295195	0	0	0
In	0.001825002	-0.000571467	0.367345559			
In	0.001823176	0.499428833	0.367345162			
In	0.501824135	-0.000574093	0.367344479			
In	0.501824456	0.499428844	0.367345535			
In	0.334513743	0.165918728	0.295815564			
In	0.334514596	0.665919185	0.295815740			
In	0.834513212	0.165918170	0.295815554			
In	0.834513117	0.665917788	0.295815712			
In	0.333257979	0.163664373	0.419416248			
In	0.333247224	0.663661163	0.419416995			
In	0.833255715	0.163663599	0.419418477			
In	0.833251243	0.663665740	0.419416393			
In	0.333852351	0.166582322	0.204219856			
In	0.333852355	0.666582060	0.204219829			
In	0.833852799	0.166582561	0.204219642			
In	0.833852198	0.666581970	0.204219823			
In	0.333333552	0.166666538	0.080788255	0	0	0
In	0.333333641	0.666666746	0.080788255	0	0	0
In	0.833333850	0.166666567	0.080788255	0	0	0
In	0.833333850	0.666666806	0.080788255	0	0	0

In	0.171411594	0.333457912	0.437703607			
In	0.171402760	0.833461017	0.437703296			
In	0.671412929	0.333464531	0.437704006			
In	0.671397375	0.833458247	0.437704391			
In	0.166666523	0.333333522	0.130836939	0	0	0
In	0.166666493	0.833333731	0.130836939	0	0	0
In	0.666666746	0.333333582	0.130836927	0	0	0
In	0.666666806	0.833333790	0.130836939	0	0	0
In	0.167816591	0.332243231	0.345942171			
In	0.167816939	0.832244500	0.345941689			
In	0.667817135	0.332242739	0.345942285			
In	0.667818853	0.832244625	0.345942454			
In	0.167275421	0.333104523	0.224285941			
In	0.167275352	0.833104608	0.224285765			
In	0.667275132	0.333104424	0.224285659			
In	0.667275360	0.833104098	0.224285783			
O	0.148190632	0.000000000	0.105812597	0	0	0
O	0.148190662	0.500000119	0.105812610	0	0	0
O	0.648190975	0.000000000	0.105812597	0	0	0
O	0.648190916	0.500000238	0.105812597	0	0	0
O	0.351786682	-0.002564129	0.318538558			
O	0.351787150	0.497437364	0.318539315			
O	0.851788002	-0.002561411	0.318539803			
O	0.851787024	0.497437009	0.318539634			
O	0.000000000	0.148190588	0.105812597	0	0	0
O	-0.000000000	0.648190856	0.105812597	0	0	0
O	0.500000119	0.148190632	0.105812597	0	0	0
O	0.500000238	0.648190796	0.105812610	0	0	0
O	0.002983685	0.351617633	0.318266973			
O	0.002982615	0.851617917	0.318267006			
O	0.502983382	0.351617422	0.318267444			
O	0.502985348	0.851618522	0.318266774			
O	0.351809531	0.351809412	0.105812597	0	0	0
O	0.351809502	0.851809621	0.105812610	0	0	0
O	0.851809680	0.351809412	0.105812597	0	0	0
O	0.851809740	0.851809621	0.105812597	0	0	0
O	0.148768620	0.148060446	0.318864253			
O	0.148769083	0.648060516	0.318864198			
O	0.648768478	0.148060503	0.318864217			
O	0.648768495	0.648059687	0.318864895			
O	0.482150338	0.164489280	0.247327351			
O	0.482150716	0.664489112	0.247327433			
O	0.982150026	0.164488894	0.247327437			
O	0.982149922	0.664488895	0.247327333			
O	0.178267333	0.159927035	0.457100320			
O	0.178258549	0.659933347	0.457100383			
O	0.678270717	0.159938074	0.457101884			
O	0.678251558	0.659926118	0.457098395			
O	0.335313105	0.315507060	0.247361963			
O	0.335312361	0.815506322	0.247361925			
O	0.835312680	0.315507011	0.247361737			
O	0.835312557	0.815506684	0.247361963			
O	0.329321546	0.017048771	0.460304024			
O	0.329342600	0.517047361	0.460299557			
O	0.829328531	0.017044130	0.460302776			
O	0.829349170	0.517054038	0.460299430			
O	0.185052558	0.018610291	0.247438566			
O	0.185053314	0.518610292	0.247438607			

O	0.685053279	0.018610325	0.247438468			
O	0.685052988	0.518610115	0.247438840			
O	0.485516826	0.310663268	0.461916085			
O	0.485501180	0.810678124	0.461913085			
O	0.985516327	0.310656911	0.461918284			
O	0.985506116	0.810670921	0.461914950			
O	0.317336387	0.328431374	0.389158070			
O	0.317333638	0.828431016	0.389157823			
O	0.817336992	0.328430448	0.389158249			
O	0.817336105	0.828433882	0.389158359			
O	0.018475950	0.333333701	0.176354341	0	0	0
O	0.018475849	0.833333790	0.176354341	0	0	0
O	0.518476129	0.333333701	0.176354341	0	0	0
O	0.518476129	0.833333850	0.176354328	0	0	0
O	0.168951783	0.479093644	0.389362014			
O	0.168957372	0.979099031	0.389361416			
O	0.668953563	0.479093924	0.389361955			
O	0.668954284	0.979095710	0.389362119			
O	0.166666493	0.185142860	0.176354341	0	0	0
O	0.166666433	0.685143113	0.176354328	0	0	0
O	0.666666687	0.185142905	0.176354341	0	0	0
O	0.666666687	0.685143113	0.176354341	0	0	0
O	0.016090403	0.184868081	0.389281954			
O	0.016087383	0.684871242	0.389280608			
O	0.516090841	0.184866875	0.389280918			
O	0.516086449	0.684868966	0.389281131			
O	0.314857244	0.481524229	0.176354328	0	0	0
O	0.314857304	0.981524467	0.176354341	0	0	0
O	0.814857423	0.481524229	0.176354341	0	0	0
O	0.814857483	0.981524467	0.176354341	0	0	0
H	0.459198316	0.253991127	0.485347962			
H	0.459184001	0.754040657	0.485349531			
H	0.959201487	0.253990823	0.485349760			
H	0.959191569	0.754016623	0.485348130			
I	0.185142860	0.166666567	0.035270844	0	0	0
I	0.185142875	0.666666746	0.035270834	0	0	0
I	0.685143173	0.166666582	0.035270844	0	0	0
I	0.685143113	0.666666746	0.035270840	0	0	0

Model IO₆₆

In	0.000000000	0.000000000	0.151330024	0	0	0
In	0.000000000	0.500000119	0.151330024	0	0	0
In	0.500000238	0.000000000	0.151330024	0	0	0
In	0.500000179	0.500000119	0.151330024	0	0	0
In	0.000360710	-0.000236237	0.274327129			
In	-0.000535077	0.499311855	0.274471464			
In	0.499735282	-0.000348453	0.274241466			
In	0.500097006	0.500090500	0.274557536			
In	0.000000000	0.000000000	0.060295182	0	0	0
In	0.000000000	0.500000179	0.060295195	0	0	0
In	0.500000179	0.000000000	0.060295195	0	0	0
In	0.500000119	0.500000179	0.060295195	0	0	0
In	-0.000802043	-0.000004840	0.366228418			
In	0.000886588	0.500005696	0.366389186			
In	0.501380213	-0.001118633	0.365774809			
In	0.498098244	0.497680250	0.366736853			
In	0.333741793	0.166947368	0.295182188			

In	0.332870363	0.666158184	0.295335428			
In	0.832827487	0.165722610	0.295079419			
In	0.833542167	0.665904299	0.294998836			
In	0.325027193	0.164007382	0.419587070			
In	0.340307867	0.671185286	0.420404336			
In	0.836707835	0.171353701	0.418615074			
In	0.832765360	0.662502559	0.419872478			
In	0.333351991	0.166644178	0.203742209			
In	0.333352142	0.666629853	0.203781068			
In	0.833450911	0.166622035	0.203704688			
In	0.833304504	0.666628284	0.203669440			
In	0.333333552	0.166666538	0.080788255	0	0	0
In	0.333333641	0.666666746	0.080788255	0	0	0
In	0.833333850	0.166666567	0.080788255	0	0	0
In	0.833333850	0.666666806	0.080788255	0	0	0
In	0.173849922	0.343387844	0.436766156			
In	0.173207379	0.827362510	0.434777591			
In	0.651905168	0.320518582	0.435316815			
In	0.668236639	0.835916272	0.435004665			
In	0.166666523	0.333333522	0.130836939	0	0	0
In	0.166666493	0.833333731	0.130836939	0	0	0
In	0.666666746	0.333333582	0.130836927	0	0	0
In	0.666666806	0.833333790	0.130836939	0	0	0
In	0.165695894	0.332910875	0.345407487			
In	0.165988115	0.833358994	0.344836408			
In	0.666303644	0.333263916	0.345451797			
In	0.667682691	0.831720433	0.344861013			
In	0.166803227	0.333456977	0.223685470			
In	0.166622961	0.833142365	0.223598472			
In	0.666658218	0.333307551	0.223615683			
In	0.666648071	0.833072825	0.223595372			
O	0.148190632	0.000000000	0.105812597	0	0	0
O	0.148190662	0.500000119	0.105812610	0	0	0
O	0.648190975	0.000000000	0.105812597	0	0	0
O	0.648190916	0.500000238	0.105812597	0	0	0
O	0.349825628	-0.002322595	0.317817949			
O	0.351111400	0.498211003	0.318314723			
O	0.851265842	-0.002552274	0.318188539			
O	0.850674643	0.497984344	0.318598828			
O	0.000000000	0.148190588	0.105812597	0	0	0
O	-0.000000000	0.648190856	0.105812597	0	0	0
O	0.500000119	0.148190632	0.105812597	0	0	0
O	0.500000238	0.648190796	0.105812610	0	0	0
O	0.000012173	0.351431238	0.318426316			
O	0.000813941	0.852080475	0.318604849			
O	0.501636597	0.352724037	0.318463656			
O	0.502136782	0.852047153	0.318173322			
O	0.351809531	0.351809412	0.105812597	0	0	0
O	0.351809502	0.851809621	0.105812610	0	0	0
O	0.851809680	0.351809412	0.105812597	0	0	0
O	0.851809740	0.851809621	0.105812597	0	0	0
O	0.147465627	0.147774431	0.318693819			
O	0.146522046	0.648790084	0.318125384			
O	0.647636981	0.149229055	0.318143203			
O	0.648431640	0.648140388	0.318329321			
O	0.481358037	0.165798332	0.247306288			
O	0.481394241	0.665679051	0.247383167			
O	0.981490777	0.165773307	0.247458125			

O	0.981177164	0.665622617	0.247432957			
O	0.167948662	0.163910501	0.459687809			
O	0.173726406	0.651700890	0.455849584			
O	0.676942518	0.157437618	0.458765379			
O	0.709622595	0.694746158	0.465380430			
O	0.334124482	0.315338514	0.247486553			
O	0.334003877	0.815173233	0.247333078			
O	0.834156866	0.315434916	0.247262912			
O	0.834419812	0.815492089	0.247302096			
O	0.333990574	0.012885056	0.459901468			
O	0.347145858	0.520162620	0.456843102			
O	0.846236223	0.019272890	0.458677439			
O	0.814388250	0.500723854	0.462742259			
O	0.184229519	0.018442668	0.247276376			
O	0.184246526	0.518483682	0.247426051			
O	0.684495034	0.018462896	0.247334801			
O	0.684335518	0.518486986	0.247303683			
O	0.474724859	0.309746445	0.458245047			
O	0.496487572	0.846925056	0.452522563			
O	0.987861641	0.322991085	0.459505224			
O	0.993626412	0.797021139	0.465509355			
O	0.311861968	0.328207060	0.388729855			
O	0.314267045	0.829873836	0.387596395			
O	0.813122907	0.333617813	0.390432819			
O	0.816929397	0.829675903	0.390578543			
O	0.018475950	0.333333701	0.176354341	0	0	0
O	0.018475849	0.833333790	0.176354341	0	0	0
O	0.518476129	0.333333701	0.176354341	0	0	0
O	0.518476129	0.833333850	0.176354328	0	0	0
O	0.172341968	0.486557366	0.388020540			
O	0.164972237	0.978825445	0.390849288			
O	0.668094621	0.484248653	0.390066132			
O	0.676161440	0.988400111	0.387459751			
O	0.166666493	0.185142860	0.176354341	0	0	0
O	0.166666433	0.685143113	0.176354328	0	0	0
O	0.666666687	0.185142905	0.176354341	0	0	0
O	0.666666687	0.685143113	0.176354341	0	0	0
O	0.015604462	0.185699408	0.389178895			
O	0.012555406	0.683462912	0.389368102			
O	0.509902783	0.181342293	0.387812371			
O	0.520943377	0.686063526	0.388955945			
O	0.314857244	0.481524229	0.176354328	0	0	0
O	0.314857304	0.981524467	0.176354341	0	0	0
O	0.814857423	0.481524229	0.176354341	0	0	0
O	0.814857483	0.981524467	0.176354341	0	0	0
H	0.071132845	0.087941778	0.459535410			
H	0.590818853	0.066274354	0.458955169			
H	0.788318856	0.756590560	0.481820102			
H	0.310894931	0.035849130	0.484977859			
H	0.826042896	0.048678226	0.483208470			
H	0.767651004	0.515711400	0.484555393			
H	0.996624825	0.414902156	0.462010876			
H	0.981139864	0.724638630	0.483816048			
I	0.185142860	0.166666567	0.035270844	0	0	0
I	0.185142875	0.666666746	0.035270834	0	0	0
I	0.685143173	0.166666582	0.035270844	0	0	0
I	0.685143113	0.666666746	0.035270840	0	0	0
I	0.481524289	0.814857364	0.035270834	0	0	0

I	0.981524467	0.814857364	0.035270844	0	0	0
I	0.333333641	0.518476009	0.035270834	0	0	0
I	0.833333790	0.518476069	0.035270844	0	0	0

Model IO₁₀₀

In	0.000000000	0.000000000	0.151330024	0	0	0
In	0.000000000	0.500000119	0.151330024	0	0	0
In	0.500000238	0.000000000	0.151330024	0	0	0
In	0.500000179	0.500000119	0.151330024	0	0	0
In	-0.000001103	0.000000034	0.273644112			
In	0.000000334	0.500002893	0.273640331			
In	0.500000001	-0.000001193	0.273641342			
In	0.499996477	0.499999011	0.273641681			
In	0.000000000	0.000000000	0.060295182	0	0	0
In	0.000000000	0.500000179	0.060295195	0	0	0
In	0.500000179	0.000000000	0.060295195	0	0	0
In	0.500000119	0.500000179	0.060295195	0	0	0
In	0.000003479	-0.000000835	0.365055901			
In	0.000010383	0.500007620	0.365051694			
In	0.499993103	-0.000007540	0.365051913			
In	0.499993244	0.500003678	0.365052225			
In	0.333335032	0.166663622	0.294129034			
In	0.333333138	0.666666398	0.294129933			
In	0.833335212	0.166672413	0.294128573			
In	0.833325314	0.666664747	0.294128656			
In	0.333322828	0.166604537	0.419268209			
In	0.333334557	0.666662127	0.419263400			
In	0.833392812	0.166722549	0.419264980			
In	0.833292183	0.666682744	0.419266191			
In	0.333330951	0.166667568	0.202732257			
In	0.333332721	0.666667054	0.202732165			
In	0.833332871	0.166664382	0.202731805			
In	0.833335615	0.666669330	0.202731735			
In	0.333333552	0.166666538	0.080788255	0	0	0
In	0.333333641	0.666666746	0.080788255	0	0	0
In	0.833333850	0.166666567	0.080788255	0	0	0
In	0.833333850	0.666666806	0.080788255	0	0	0
In	0.166735252	0.333334132	0.433836291			
In	0.166611306	0.833256742	0.433836705			
In	0.666667732	0.333344084	0.433823612			
In	0.666656583	0.833399038	0.433837716			
In	0.166666523	0.333333522	0.130836939	0	0	0
In	0.166666493	0.833333731	0.130836939	0	0	0
In	0.666666746	0.333333582	0.130836927	0	0	0
In	0.666666806	0.833333790	0.130836939	0	0	0
In	0.166662493	0.333325507	0.344579389			
In	0.166662550	0.833335728	0.344580325			
In	0.666666676	0.333335079	0.344569926			
In	0.666671319	0.833337165	0.344579571			
In	0.166663107	0.333333416	0.222590536			
In	0.166669133	0.833337538	0.222590688			
In	0.666665751	0.333333119	0.222589472			
In	0.666666143	0.833330861	0.222590646			
O	0.148190632	0.000000000	0.105812597	0	0	0
O	0.148190662	0.500000119	0.105812610	0	0	0
O	0.648190975	0.000000000	0.105812597	0	0	0
O	0.648190916	0.500000238	0.105812597	0	0	0

O	0.351394174	-0.000633831	0.319113965			
O	0.351392052	0.499367550	0.319115562			
O	0.851402128	-0.000617298	0.319115195			
O	0.851398409	0.499370750	0.319108268			
O	0.000000000	0.148190588	0.105812597	0	0	0
O	-0.000000000	0.648190856	0.105812597	0	0	0
O	0.500000119	0.148190632	0.105812597	0	0	0
O	0.500000238	0.648190796	0.105812610	0	0	0
O	0.000634375	0.352030412	0.319113466			
O	0.000616169	0.852019461	0.319115687			
O	0.500628690	0.352028861	0.319109539			
O	0.500631131	0.852026571	0.319114802			
O	0.351809531	0.351809412	0.105812597	0	0	0
O	0.351809502	0.851809621	0.105812610	0	0	0
O	0.851809680	0.351809412	0.105812597	0	0	0
O	0.851809740	0.851809621	0.105812597	0	0	0
O	0.147978604	0.148595010	0.319115420			
O	0.147972969	0.648605872	0.319113901			
O	0.647970276	0.148602404	0.319109684			
O	0.647969383	0.648606325	0.319113921			
O	0.481659417	0.166563459	0.247848843			
O	0.481656958	0.666562253	0.247850402			
O	0.981661693	0.166565040	0.247851361			
O	0.981662333	0.666569850	0.247849712			
O	0.200813049	0.188321966	0.465158719			
O	0.200754358	0.688276147	0.465156083			
O	0.700821237	0.188390408	0.465149573			
O	0.700783552	0.688421695	0.465155840			
O	0.333430275	0.315094439	0.247850263			
O	0.333436557	0.815096106	0.247850513			
O	0.833436763	0.315097746	0.247848315			
O	0.833434756	0.815098457	0.247851228			
O	0.311596964	0.012364641	0.465157459			
O	0.311714551	0.512460210	0.465156873			
O	0.811667088	0.012486013	0.465156657			
O	0.811645056	0.512442316	0.465143391			
O	0.184901534	0.018338034	0.247851653			
O	0.184903816	0.518341810	0.247850395			
O	0.684904514	0.018337781	0.247849711			
O	0.684901516	0.518340707	0.247848291			
O	0.487556014	0.299199271	0.465148375			
O	0.487527156	0.799245393	0.465156150			
O	0.987639430	0.299215820	0.465154049			
O	0.987528815	0.799187052	0.465158819			
O	0.316575510	0.332247719	0.390601176			
O	0.316546467	0.832263765	0.390601777			
O	0.816564796	0.332287619	0.390594998			
O	0.816548464	0.832307572	0.390603648			
O	0.018475950	0.333333701	0.176354341	0	0	0
O	0.018475849	0.833333790	0.176354341	0	0	0
O	0.518476129	0.333333701	0.176354341	0	0	0
O	0.518476129	0.833333850	0.176354328	0	0	0
O	0.167729868	0.484275407	0.390602063			
O	0.167698653	0.984244170	0.390605218			
O	0.667721076	0.484288862	0.390594415			
O	0.667746633	0.984324504	0.390600554			
O	0.166666493	0.185142860	0.176354341	0	0	0
O	0.166666433	0.685143113	0.176354328	0	0	0

O	0.666666687	0.185142905	0.176354341	0	0	0
O	0.666666687	0.685143113	0.176354341	0	0	0
O	0.015753387	0.183452059	0.390602136			
O	0.015679232	0.683427515	0.390600822			
O	0.515715293	0.183435729	0.390596260			
O	0.515725344	0.683455647	0.390602972			
O	0.314857244	0.481524229	0.176354328	0	0	0
O	0.314857304	0.981524467	0.176354341	0	0	0
O	0.814857423	0.481524229	0.176354341	0	0	0
O	0.814857483	0.981524467	0.176354341	0	0	0
H	0.278028182	0.249893346	0.482064756			
H	0.277981976	0.749909353	0.482051450			
H	0.777948811	0.249943248	0.482065026			
H	0.778007658	0.750034250	0.482051962			
H	0.249978973	0.027956962	0.482050926			
H	0.250072052	0.528044369	0.482051149			
H	0.750094853	0.028154048	0.482065351			
H	0.750047579	0.528037007	0.482071310			
H	0.471991550	0.222061381	0.482068447			
H	0.471939329	0.722026161	0.482053629			
H	0.972016682	0.221958907	0.482047866			
H	0.971875032	0.721973058	0.482063840			

Model IO₀-bcc

In	10.478190339	2.037609544	9.107076063
In	3.417978553	1.972314673	8.720389162
In	13.948190124	8.185655680	8.719973294
In	6.912582567	8.350347649	8.714699770
In	5.093219827	4.786877420	8.489884193
In	15.839518483	11.686562929	8.900953386
In	17.941369471	8.394372678	8.489967028
In	13.750017898	1.857986284	8.898679843
In	15.547906648	5.328372890	8.490077388
In	8.997526856	4.962145978	8.898992164
In	8.681139309	11.553937885	8.971931584
In	15.858468503	7.486986917	5.842370287
In	10.287441834	8.113939913	8.969908009
In	3.068643075	3.979258095	5.843377050
In	12.462704805	11.228852258	8.971557096
In	5.346610967	7.044314567	5.843620184
In	8.686314358	7.456352161	5.974384123
In	13.837095136	10.171853794	5.981287472
In	1.757497420	0.883780379	5.979913225
In	12.268277393	4.839985742	8.755820337
In	7.155134847	2.190614101	8.756548316
In	19.163817620	11.476017602	8.755386773
O	7.171042351	4.320713963	7.916907032
O	8.856130840	1.122233441	7.749673143
O	17.308181314	10.426291048	7.917283919
O	12.083364060	1.091895887	7.748358551
O	14.106226360	3.762194553	7.916436145
O	10.492480727	3.900631788	7.746963801
O	10.657425236	12.298989231	9.413168321
O	13.844261860	7.988702927	6.545964730
O	5.249341302	9.458250267	9.366782311
O	12.116661053	11.316682101	6.825406346
O	8.654954096	9.454770576	9.415401342

O	3.643696587	1.980498698	6.546865263			
O	13.816689402	6.190504489	9.368760706			
O	8.779909899	11.210334752	6.825384984			
O	12.117944162	9.143608798	9.408310728			
O	6.793653516	8.541363469	6.539842436			
O	5.211129130	2.856669684	9.369536325			
O	10.540104994	8.372518708	6.823369934			
O	2.975269884	4.176397675	8.524445094			
O	8.455563939	6.942829322	8.178418321			
O	5.224671312	6.865480616	8.512344860			
O	14.398263119	10.224557139	8.183328916			
O	16.077480369	7.468437338	8.529867425			
O	1.428364679	1.340116225	8.180474630			
O	17.896682635	8.146028313	6.305427909			
O	21.054751072	12.190258010	9.555695901			
O	12.437106857	5.420992758	6.388007576			
O	12.255592454	2.991452504	9.910234828			
O	15.785425436	5.415981154	6.306815820			
O	10.704197217	6.120466302	9.556647059			
O	6.569528205	2.046946299	6.389900479			
O	8.763666917	3.101061911	9.911504720			
O	4.901032854	4.946263135	6.305181981			
O	6.827206269	0.194758747	9.553107462			
O	19.579789745	11.039291826	6.386978409			
O	10.415442268	0.021405748	9.913165296			
In	17.652941548	10.320458087	5.747097776			
In	6.908062600	4.073707386	5.746969668			
In	14.023278646	4.114532491	5.746749344			
In	3.323655150	6.169764390	2.723682860	0	0	0
In	10.477454460	6.169764390	2.723682860	0	0	0
In	6.900554810	12.365136320	2.723682860	0	0	0
In	14.054354110	12.365136320	2.723682860	0	0	0
In	10.479093281	10.300823472	5.734436939			
In	12.248963227	0.727496453	5.663473054			
In	12.265904290	8.989071640	2.526839380	0	0	0
In	15.842803940	3.350457140	2.920526340	0	0	0
In	10.725860364	4.228574600	5.662738899			
In	3.564738190	0.113581810	2.526839380	0	0	0
In	6.659471770	6.030575030	2.920526340	0	0	0
In	8.457224667	1.159783301	5.665048751			
In	8.447921600	9.406639710	2.526839380	0	0	0
In	16.083886980	9.128261000	2.920526340	0	0	0
In	8.689004630	3.350457140	2.920526340	0	0	0
In	5.126350541	0.738296096	5.544124215			
In	17.390170730	12.225946970	2.920526340	0	0	0
In	7.129608802	10.448029449	5.541958680			
In	12.506987320	2.932889070	2.920526340	0	0	0
In	12.026754678	7.326770054	5.543724890			
In	5.112104980	8.989071640	2.526839380	0	0	0
In	14.295437150	6.308953750	2.526839380	0	0	0
In	4.871021940	3.211267780	2.526839380	0	0	0
O	10.216477942	0.053252803	5.164521706			
O	14.307598610	8.476920900	1.935140750	0	0	0
O	15.649550200	2.818280299	5.136480898			
O	16.030233480	5.149593150	1.692152960	0	0	0
O	12.327272395	2.804587571	5.163561949			
O	2.987426590	2.137816340	1.935140750	0	0	0
O	7.217250139	6.129577271	5.136156037			

O	5.007659510	5.293325770	1.692152960	0	0	0
O	8.889230397	3.257285894	5.162444563			
O	6.983538880	7.894555940	1.935140750	0	0	0
O	15.716361772	9.563650826	5.134394106			
O	17.548269690	8.066374250	1.692152960	0	0	0
O	10.730698960	4.079032880	3.206153810	0	0	0
O	5.299534520	1.286985260	3.341666230	0	0	0
O	8.584559160	1.239074380	3.206153810	0	0	0
O	6.564326240	10.322315680	3.341666230	0	0	0
O	12.117105260	0.800442050	3.206153810	0	0	0
O	12.414703310	6.899992230	3.341666230	0	0	0
O	10.224209960	8.260495900	2.241211910	0	0	0
O	-0.026417436	0.211560756	4.943925400			
O	15.655374400	11.052543520	2.105699490	0	0	0
O	8.817071242	9.289014831	4.698180884			
O	12.370349760	11.100454400	2.241211910	0	0	0
O	10.159904734	6.247849486	4.941142428			
O	14.390582680	2.017213100	2.105699490	0	0	0
O	12.189155464	9.367667541	4.699345335			
O	8.837803660	11.539086730	2.241211910	0	0	0
O	14.146380825	12.051766507	4.942629549			
O	8.540205610	5.439536550	2.105699490	0	0	0
O	10.431438588	12.247781940	4.700509565			
O	6.647310310	3.862607880	3.512224970	0	0	0
O	4.924675440	7.189935630	3.755212760	0	0	0
O	17.967482330	10.201712440	3.512224970	0	0	0
O	15.947249410	7.046203010	3.755212760	0	0	0
O	13.971370040	4.444972840	3.512224970	0	0	0
O	3.406639230	4.273154530	3.755212760	0	0	0

2. Atomic positions for ITO Models

Model ITO_b

In	-0.002380047	0.000480756	0.357612235
In	-0.000814642	0.497646358	0.358130648
In	0.502696274	0.000974917	0.357673202
In	0.500574471	0.500885982	0.357651727
In	-0.003156280	-0.001175051	0.642194146
In	-0.000050271	0.499325289	0.642392276
In	0.501888659	-0.000732150	0.642251599
In	0.501338940	0.502541574	0.641906856
In	-0.000802993	-0.000832221	0.141142996
In	0.000306403	0.499644952	0.141949811
In	0.501051691	0.001108925	0.141191885
In	0.499550482	0.500205196	0.142896314
In	-0.001289253	-0.001266971	0.857791768
In	0.000866919	0.500229645	0.857428409
In	0.500471070	0.000548908	0.857842259
In	0.500119212	0.500843154	0.858416527
Sn	0.332888216	0.166790989	0.686836875
In	0.333623766	0.666425083	0.691286256
In	0.832915370	0.167063555	0.691442220
In	0.834137985	0.666468555	0.691294820
Sn	0.333102237	0.165986604	0.979511936
In	0.333089888	0.667561184	0.975006685
Sn	0.833490508	0.166273794	0.979443150
In	0.833227814	0.666875808	0.975002115

In	0.332919476	0.166904300	0.471567227
In	0.333924135	0.666626545	0.475656112
In	0.833150359	0.166924667	0.476699464
In	0.833342810	0.666010937	0.475637814
In	0.333993452	0.166355164	0.194917916
In	0.332659021	0.666362827	0.190853083
In	0.833697321	0.166464426	0.195564339
In	0.833042323	0.667432980	0.190836040
In	0.168267675	0.335717855	0.024787739
In	0.165298432	0.830703054	0.024623545
In	0.668207040	0.336448659	0.024861658
In	0.664778013	0.830402243	0.024714351
In	0.167583541	0.334403682	0.309501396
Sn	0.166184078	0.832460943	0.313486833
In	0.667009789	0.334328309	0.309473945
In	0.665967457	0.832131942	0.308956655
In	0.166688022	0.334367727	0.807724976
In	0.166539022	0.832612030	0.808600064
In	0.666290598	0.333475106	0.807727466
In	0.667148105	0.832622061	0.807961916
In	0.166074669	0.333191667	0.524569841
In	0.167057944	0.833213796	0.528940277
In	0.666629703	0.333800523	0.524582722
In	0.666890307	0.833267484	0.523787225
O	0.149517677	-0.006414876	0.251645144
O	0.146388471	0.499236299	0.249330803
O	0.645812512	-0.001673307	0.249164868
O	0.647637250	0.499586297	0.249067362
O	0.349695249	0.005555449	0.747860458
O	0.353456651	0.499718717	0.750686812
O	0.853520956	0.001019135	0.750317309
O	0.852225626	0.499407241	0.750928074
O	0.003589867	0.147876486	0.247913810
O	0.005192570	0.655406264	0.251850522
O	0.502102021	0.147653018	0.248867461
O	0.498701540	0.647596179	0.250251438
O	0.000009188	0.351906630	0.750037138
O	0.001038271	0.853588646	0.750223938
O	0.493666095	0.344172437	0.748407661
O	0.499710798	0.853466150	0.751187177
O	0.351976634	0.351553951	0.250066975
O	0.344067261	0.851254887	0.250608331
O	0.852659015	0.354033934	0.249276012
O	0.852710093	0.853883157	0.249163642
O	0.154897688	0.150007058	0.749147952
O	0.148340513	0.648118622	0.749518343
O	0.646187946	0.147516673	0.750701882
O	0.647598602	0.645451925	0.750388391
O	0.477120893	0.165527973	0.584625151
O	0.481381075	0.667563966	0.583545425
O	0.981966389	0.167170443	0.583943685
O	0.980923386	0.666100569	0.583143503
O	0.187844890	0.165861976	0.081517577
O	0.185246486	0.665533075	0.083015746
O	0.688629494	0.167575713	0.080719473
O	0.685042920	0.665232130	0.082891368
O	0.333083622	0.311635544	0.585696559
O	0.334480188	0.815414626	0.583258747

O	0.832304149	0.314251231	0.583841248
O	0.834049707	0.813958868	0.582186821
O	0.333695027	0.021721066	0.080878825
O	0.334134154	0.519241423	0.082871812
O	0.832848743	0.021583645	0.080971961
O	0.834795287	0.519870288	0.083853609
O	0.187876062	0.022287360	0.585245665
O	0.185563582	0.519528474	0.582375467
O	0.686271335	0.018593264	0.583680411
O	0.685190553	0.518116858	0.583851571
O	0.477671353	0.311561107	0.080977838
O	0.480583482	0.815475236	0.083574295
O	0.977969004	0.310845848	0.081139360
O	0.981383194	0.815311997	0.082725958
O	0.314702474	0.326613445	0.917798954
O	0.314456288	0.835206067	0.915826675
O	0.814901542	0.326914202	0.917916033
O	0.813550244	0.833373189	0.916558698
O	0.018391388	0.332154060	0.416322018
O	0.022761740	0.834500513	0.415489525
O	0.518831712	0.333614527	0.416724898
O	0.517953355	0.832922490	0.416160065
O	0.167737908	0.479602143	0.916224897
O	0.171351111	0.988695287	0.918132006
O	0.666932516	0.478839651	0.915393038
O	0.672157875	0.988879129	0.918129481
O	0.165622575	0.184455493	0.416512741
O	0.167014161	0.688322575	0.414428314
O	0.666038524	0.185937730	0.417624880
O	0.667735165	0.685722639	0.416388834
O	0.012768204	0.184002525	0.917633210
O	0.019461768	0.686522720	0.916238534
O	0.512043856	0.184078794	0.918308717
O	0.519198793	0.687575049	0.916010084
O	0.314791295	0.480382502	0.417703328
O	0.311929055	0.978068973	0.414575854
O	0.815206092	0.481817630	0.416227179
O	0.813534244	0.981829281	0.416220673

Model ITO_b-bcc

In	0.249202578	0.249398088	0.250610052
In	0.750619689	0.749418704	0.751543675
In	0.249419146	0.749871181	0.750055097
In	0.750157564	0.249209319	0.249788590
In	0.750602391	0.750052054	0.248638785
Sn	0.250179110	0.249918289	0.750640209
In	0.751198947	0.249977932	0.750233711
In	0.250083093	0.750344664	0.248762205
In	0.467000770	0.000582932	0.249985602
In	0.533013869	-0.000367183	0.752314707
In	0.033125147	0.000049147	0.749695782
In	0.967853946	-0.000159811	0.249258909
Sn	0.532967701	0.499877511	0.249100574
In	0.467986519	0.500383486	0.750347494
In	0.966558712	0.500177477	0.749222458
In	0.032729108	0.499810103	0.249774200

In	0.249304050	0.468063614	0.000271684
In	0.751923100	0.533055694	-0.000860952
In	0.750598150	0.032494394	0.000015906
In	0.251227561	0.966452195	0.000249752
In	0.248710347	0.532971661	0.500190830
In	0.750975777	0.467170304	0.500645933
Sn	0.749806251	0.966734144	0.500182170
In	0.250525421	0.031719481	0.499141229
In	0.000573533	0.251226736	0.467276605
In	0.001251164	0.749041235	0.532980447
In	0.000546698	0.750510000	0.032894674
In	-0.000196743	0.249350152	0.967928344
In	0.499300430	0.250490390	0.532130497
In	0.499115135	0.749520789	0.467484909
In	0.498997068	0.749578421	0.966547692
In	0.500208354	0.247494298	0.032672382
O	0.390107568	0.153551044	0.382619398
O	0.612411592	0.847286657	0.616016431
O	0.108597003	0.847907631	0.880983804
O	0.891747266	0.154263257	0.120310450
O	0.603738122	0.651276177	0.122425498
O	0.387185644	0.340570857	0.879548459
O	0.891180925	0.345498376	0.619246568
O	0.109919219	0.655088543	0.380546815
O	0.384349344	0.393505302	0.154811885
O	0.619469539	0.608303413	0.847263940
O	0.883274106	0.108725001	0.846507036
O	0.119517952	0.891977632	0.154112946
O	0.118728527	0.609113118	0.655122051
O	0.880340019	0.389483398	0.345863209
O	0.622567190	0.894808489	0.349007966
O	0.379010007	0.112545041	0.659701636
O	0.154833958	0.381551384	0.390252451
O	0.845039488	0.620719736	0.608067151
O	0.845706583	0.880667548	0.109466662
O	0.160037975	0.121910394	0.887893961
O	0.654934688	0.115806968	0.606002413
O	0.347015974	0.879369232	0.390997787
O	0.345816575	0.617023842	0.890148928
O	0.651975725	0.384504017	0.111356773
O	0.892905369	0.654694087	0.880274498
O	0.110918875	0.346027130	0.116815147
O	0.603799804	0.349653978	0.376992025
O	0.390902972	0.652667446	0.617873880
O	0.113194984	0.159691965	0.622340502
O	0.887707138	0.847452087	0.384713915
O	0.392394635	0.846025624	0.119119263
O	0.610055825	0.155068538	0.879992591
O	0.877488611	0.896160231	0.651050158
O	0.116928982	0.108986254	0.348455031
O	0.383434389	0.605057912	0.342677220
O	0.617337610	0.389298497	0.652575043
O	0.619083331	0.109229530	0.154052420
O	0.380771006	0.890079707	0.844746255
O	0.121755764	0.387505653	0.840403786
O	0.880236986	0.608526293	0.154266209
O	0.654248359	0.880304197	0.891358641
O	0.344648129	0.119894656	0.109354277

O	0.339978940	0.378264500	0.613499490
O	0.652008137	0.616242131	0.387007263
O	0.153966757	0.619248224	0.108606921
O	0.847546522	0.380938619	0.891895153
O	0.842883478	0.116350421	0.394903376
O	0.152733881	0.882757925	0.609028628

Model ITO₀

In	0.000000000	0.000000000	0.151330024	0	0	0
In	0.000000000	0.500000119	0.151330024	0	0	0
In	0.500000238	0.000000000	0.151330024	0	0	0
In	0.500000179	0.500000119	0.151330024	0	0	0
In	-0.005001813	-0.002683763	0.279606611			
In	0.003690275	0.499863053	0.275045489			
In	0.501169155	-0.003852544	0.274472835			
In	0.500548519	0.503554925	0.274367698			
In	0.000000000	0.000000000	0.060295182	0	0	0
In	0.000000000	0.500000179	0.060295195	0	0	0
In	0.500000179	0.000000000	0.060295195	0	0	0
In	0.500000119	0.500000179	0.060295195	0	0	0
In	-0.000032729	0.005600601	0.420992580			
In	0.007733797	0.497805661	0.366183271			
In	0.492320301	0.010797850	0.363793418			
In	0.501353904	0.493562549	0.364820136			
Sn	0.337836275	0.169510352	0.290859126			
In	0.333936388	0.665605125	0.295646866			
In	0.832012799	0.169542450	0.294795499			
In	0.830135728	0.657558728	0.293619983			
Sn	0.341538597	0.167994942	0.423279904			
In	0.355428635	0.688863580	0.400570813			
Sn	0.851490542	0.198473571	0.429856567			
In	0.840268524	0.660651034	0.417451459			
In	0.333089873	0.168345031	0.201268897			
In	0.335959370	0.666544046	0.203617150			
In	0.834276679	0.166431244	0.203367454			
In	0.830909711	0.664733503	0.203246108			
In	0.333333552	0.166666538	0.080788255	0	0	0
In	0.333333641	0.666666746	0.080788255	0	0	0
In	0.833333850	0.166666567	0.080788255	0	0	0
In	0.833333850	0.666666806	0.080788255	0	0	0
In	0.173214196	0.337232474	0.435546788			
In	0.169752359	0.849104724	0.435410474			
In	0.662206137	0.341136763	0.448574052			
In	0.674123415	0.832394366	0.444340078			
In	0.166666523	0.333333522	0.130836939	0	0	0
Sn	0.166666493	0.833333731	0.130836939	0	0	0
In	0.666666746	0.333333582	0.130836927	0	0	0
In	0.666666806	0.833333790	0.130836939	0	0	0
In	0.161540016	0.314511515	0.346181281			
In	0.153363984	0.840427135	0.345579503			
In	0.673504110	0.335539925	0.348841525			
In	0.683638813	0.836434470	0.347339877			
In	0.164456198	0.330558597	0.223721691			
In	0.164934962	0.833463553	0.225720483			
In	0.667606920	0.332319783	0.223212258			
In	0.670714346	0.835401617	0.223546577			
O	0.148190632	0.000000000	0.105812597	0	0	0

O	0.148190662	0.500000119	0.105812610	0	0	0
O	0.648190975	0.000000000	0.105812597	0	0	0
O	0.648190916	0.500000238	0.105812597	0	0	0
O	0.344497268	0.002997078	0.315736436			
O	0.349810495	0.495083059	0.319393181			
O	0.839641738	-0.000784670	0.316238697			
O	0.854240115	0.494916000	0.318894877			
O	0.000000000	0.148190588	0.105812597	0	0	0
O	-0.000000000	0.648190856	0.105812597	0	0	0
O	0.500000119	0.148190632	0.105812597	0	0	0
O	0.500000238	0.648190796	0.105812610	0	0	0
O	0.007057740	0.351128462	0.319334689			
O	-0.005294413	0.839177688	0.314905967			
O	0.499615786	0.344144880	0.316140791			
O	0.499666382	0.850466663	0.322878056			
O	0.351809531	0.351809412	0.105812597	0	0	0
O	0.351809502	0.851809621	0.105812610	0	0	0
O	0.851809680	0.351809412	0.105812597	0	0	0
O	0.851809740	0.851809621	0.105812597	0	0	0
O	0.165378676	0.157055150	0.313542138			
O	0.150135166	0.652542000	0.319387541			
O	0.644280401	0.151572696	0.317958635			
O	0.649005927	0.647898113	0.318244259			
O	0.477883155	0.163154938	0.247320733			
O	0.482922973	0.669666829	0.248284945			
O	0.980763058	0.163873804	0.247832427			
O	0.980671303	0.659295259	0.245691824			
O	0.176896621	0.161003701	0.453755304			
O	0.404269281	0.706166929	0.463914857			
O	0.697855745	0.185186642	0.463030927			
O	0.571474109	0.655521268	0.482199495			
O	0.338812724	0.316001435	0.246698974			
O	0.333792922	0.814840123	0.247831561			
O	0.835102098	0.315643963	0.247817409			
O	0.836766496	0.815141035	0.246564391			
O	0.350393920	0.012489250	0.454115808			
O	0.430942486	0.602449480	0.476482052			
O	0.846317836	0.024906575	0.455445949			
O	0.782057730	0.540857648	0.466470207			
O	0.187812931	0.023388657	0.247466941			
O	0.187256103	0.518721718	0.247532949			
O	0.681053750	0.018752101	0.246385775			
O	0.682264855	0.515872530	0.247277731			
O	0.473983461	0.327071258	0.456785496			
O	0.570923392	0.931976790	0.420025488			
O	1.015267228	0.357475667	0.458140922			
O	0.985245239	0.831236876	0.453492063			
O	0.316329195	0.330144822	0.390094562			
O	0.307102920	0.838509782	0.386522384			
O	0.824915244	0.334545652	0.391569782			
O	0.805742200	0.826905199	0.396998228			
O	0.018475950	0.333333701	0.176354341	0	0	0
O	0.018475849	0.833333790	0.176354341	0	0	0
O	0.518476129	0.333333701	0.176354341	0	0	0
O	0.518476129	0.833333850	0.176354328	0	0	0
O	0.186830039	0.493619568	0.389826894			
O	0.174129917	0.998107675	0.390091983			
O	0.674629892	0.489031203	0.386791919			

O	0.674811950	1.010503910	0.389056038			
O	0.166666493	0.185142860	0.176354341	0	0	0
O	0.166666433	0.685143113	0.176354328	0	0	0
O	0.666666687	0.185142905	0.176354341	0	0	0
O	0.666666687	0.685143113	0.176354341	0	0	0
O	0.008297558	0.190253990	0.392781162			
O	0.027632882	0.681828570	0.392281307			
O	0.509077929	0.189758847	0.388190424			
O	0.532775720	0.682331543	0.390119132			
O	0.314857244	0.481524229	0.176354328	0	0	0
O	0.314857304	0.981524467	0.176354341	0	0	0
O	0.814857423	0.481524229	0.176354341	0	0	0
O	0.814857483	0.981524467	0.176354341	0	0	0

Model ITO₀^m

In	-0.002868039	0.001558099	0.150573437			
In	-0.000593806	0.495420785	0.150644266			
In	0.503401279	0.002359841	0.150691615			
In	0.500061227	0.500772970	0.150338568			
In	-0.000353774	0.001106881	0.272926710			
In	-0.000176820	0.500092156	0.274010272			
In	0.500617447	0.000496239	0.273250183			
In	0.500145367	0.499002724	0.273872653			
In	0.000000000	0.000000000	0.060295182	0	0	0
In	0.000000000	0.500000179	0.060295195	0	0	0
In	0.500000179	0.000000000	0.060295195	0	0	0
In	0.500000119	0.500000179	0.060295195	0	0	0
In	0.000501464	0.003077867	0.362181379			
In	-0.001090029	0.496809489	0.363377841			
In	0.501133170	0.003772500	0.362207608			
In	0.498421692	0.495656521	0.363210497			
In	0.331231848	0.166660753	0.293872690			
In	0.334028559	0.667052661	0.291590891			
In	0.831385675	0.163937250	0.294381529			
In	0.835903810	0.668489217	0.292139073			
Sn	0.333136319	0.166288608	0.411033016			
In	0.333935942	0.667686009	0.391359533			
Sn	0.832830216	0.166125693	0.411164047			
In	0.833794051	0.666996797	0.392528984			
In	0.329898540	0.165907158	0.201629183			
In	0.334170016	0.666982672	0.200612232			
In	0.834480256	0.165050542	0.202602353			
In	0.835093083	0.668718225	0.200761733			
In	0.333333552	0.166666538	0.080788255	0	0	0
In	0.333333641	0.666666746	0.080788255	0	0	0
In	0.833333850	0.166666567	0.080788255	0	0	0
In	0.833333850	0.666666806	0.080788255	0	0	0
In	0.166666552	0.333333641	0.010246514	0	0	0
In	0.166666582	0.833333731	0.010246514	0	0	0
In	0.666666746	0.333333582	0.010246536	0	0	0
In	0.666666687	0.833333731	0.010246514	0	0	0
In	0.166666523	0.333333522	0.130836939	0	0	0
Sn	0.166666493	0.833333731	0.130836939	0	0	0
In	0.666666746	0.333333582	0.130836927	0	0	0
In	0.666666806	0.833333790	0.130836939	0	0	0

In	0.163941721	0.332349408	0.348906230			
In	0.169235202	0.834835994	0.350110489			
In	0.664909726	0.332665495	0.349079740			
In	0.668143506	0.833257924	0.350150494			
In	0.167287065	0.334793321	0.222783010			
In	0.167503966	0.832970966	0.223185609			
Sn	0.666055687	0.333216478	0.221231170			
In	0.666178233	0.832433485	0.222654147			
O	0.148190632	0.000000000	0.105812597	0	0	0
O	0.148190662	0.500000119	0.105812610	0	0	0
O	0.648190975	0.000000000	0.105812597	0	0	0
O	0.648190916	0.500000238	0.105812597	0	0	0
O	0.348143318	-0.002785757	0.317180677			
O	0.347434898	0.500276595	0.320272459			
O	0.846516617	-0.006240048	0.317871464			
O	0.848520254	0.501579412	0.320236146			
O	0.000000000	0.148190588	0.105812597	0	0	0
O	-0.000000000	0.648190856	0.105812597	0	0	0
O	0.500000119	0.148190632	0.105812597	0	0	0
O	0.500000238	0.648190796	0.105812610	0	0	0
O	0.000775835	0.351070716	0.317549322			
O	0.002295899	0.848256466	0.320070008			
O	0.502202854	0.350381432	0.317936063			
O	0.499855498	0.846487969	0.320504288			
O	0.351809531	0.351809412	0.105812597	0	0	0
O	0.351809502	0.851809621	0.105812610	0	0	0
O	0.851809680	0.351809412	0.105812597	0	0	0
O	0.851809740	0.851809621	0.105812597	0	0	0
O	0.146183792	0.152232143	0.317740066			
O	0.154400418	0.652473711	0.320063895			
O	0.647368122	0.152683560	0.317882519			
O	0.654016085	0.650673130	0.319453367			
O	0.487310928	0.170409593	0.245851967			
O	0.481697891	0.663897117	0.247750911			
O	0.979915267	0.168382529	0.248036721			
O	0.981254223	0.664841877	0.247025516			
O	0.185142860	0.166666567	0.035270844	0	0	0
O	0.185142875	0.666666746	0.035270834	0	0	0
O	0.685143173	0.166666582	0.035270844	0	0	0
O	0.685143113	0.666666746	0.035270840	0	0	0
O	0.333749808	0.314618684	0.247948193			
O	0.336983034	0.816891661	0.246420348			
O	0.826268279	0.318041351	0.247418193			
O	0.836580042	0.813748867	0.246742462			
O	0.333333671	0.018475870	0.035270840	0	0	0
O	0.333333641	0.518476009	0.035270834	0	0	0
O	0.833333790	0.018475881	0.035270844	0	0	0
O	0.833333790	0.518476069	0.035270844	0	0	0
O	0.185677950	0.018648710	0.247258942			
O	0.183530853	0.522056873	0.246583594			
O	0.685013989	0.018461955	0.248080335			
O	0.683408979	0.511092734	0.246721568			
O	0.481524259	0.314857274	0.035270844	0	0	0
O	0.481524289	0.814857364	0.035270834	0	0	0
O	0.981524408	0.314857274	0.035270840	0	0	0
O	0.981524467	0.814857364	0.035270844	0	0	0
O	0.319404983	0.326405416	0.388421210			
O	0.325960562	0.844863321	0.390935294			

O	0.819989422	0.326980793	0.388442273
O	0.825629852	0.843785615	0.391012042
O	0.017726030	0.332862052	0.177624675
O	0.022798683	0.833204933	0.174632855
O	0.521838805	0.333852885	0.178477276
O	0.519037039	0.835374052	0.176991280
O	0.159714370	0.479744664	0.390624574
O	0.169571621	0.995808157	0.388424859
O	0.659445748	0.479554662	0.390796939
O	0.669401031	0.995382307	0.388484597
O	0.164465580	0.183916693	0.177148548
O	0.166595110	0.689112951	0.174554221
O	0.666850649	0.188433415	0.178767987
O	0.666371794	0.684068280	0.177265483
O	0.006167691	0.177679633	0.388624928
O	0.019612335	0.676753367	0.390706948
O	0.506864648	0.177791098	0.388964500
O	0.519230337	0.675699236	0.390454183
O	0.315083021	0.480807086	0.177070450
O	0.311376291	0.979031749	0.174778198
O	0.813271395	0.478055817	0.178333772
O	0.813887442	0.980147666	0.177529775

Model ITO₃₃

In	0.000000000	0.000000000	0.151330020	0	0	0
In	0.000000000	0.500000120	0.151330020	0	0	0
In	0.500000240	0.000000000	0.151330020	0	0	0
In	0.500000180	0.500000120	0.151330020	0	0	0
In	-0.002247313	-0.001033001	0.275276165			
In	0.000350761	0.499353426	0.275470644			
In	0.502101478	-0.000923651	0.275413879			
In	0.501795430	0.502225773	0.275453231			
In	0.000000000	0.000000000	0.060295180	0	0	0
In	0.000000000	0.500000180	0.060295200	0	0	0
In	0.500000180	0.000000000	0.060295200	0	0	0
In	0.500000120	0.500000180	0.060295200	0	0	0
In	-0.005014906	-0.003538382	0.368944025			
In	0.001625963	0.498002752	0.368548774			
In	0.502994594	0.001466378	0.369067439			
In	0.500250795	0.500480110	0.369493358			
Sn	0.333425017	0.166948365	0.292961152			
In	0.333570818	0.665798775	0.296700027			
In	0.833798924	0.167576334	0.296802237			
In	0.834844985	0.665954098	0.296726630			
Sn	0.331052390	0.166107258	0.420225282			
In	0.345872488	0.675166175	0.420590571			
Sn	0.837141787	0.167428790	0.419698657			
In	0.841144363	0.665468870	0.420676856			
In	0.333731033	0.169021658	0.202445269			
In	0.335662540	0.666642738	0.204615366			
In	0.833674317	0.166832544	0.204381553			
In	0.830908166	0.664143712	0.204625303			
In	0.333333550	0.166666540	0.080788260	0	0	0
In	0.333333640	0.666666750	0.080788260	0	0	0
In	0.833333850	0.166666570	0.080788260	0	0	0
In	0.833333850	0.666666810	0.080788260	0	0	0
In	0.168237790	0.346885310	0.439447155			

In	0.171323561	0.835994600	0.437654128			
In	0.659879862	0.334488345	0.439146413			
In	0.676857696	0.836773534	0.437600780			
In	0.166666520	0.333333520	0.130836940	0	0	0
Sn	0.166666490	0.833333730	0.130836940	0	0	0
In	0.666666750	0.333333580	0.130836930	0	0	0
In	0.666666810	0.833333790	0.130836940	0	0	0
In	0.168915451	0.334182837	0.346321035			
In	0.167669467	0.834065459	0.345864850			
In	0.666413586	0.332627413	0.346361012			
In	0.667573284	0.832206522	0.345400656			
In	0.165618697	0.333302813	0.224370859			
In	0.167059658	0.832999327	0.226088480			
In	0.666673370	0.332491848	0.224349938			
In	0.667952924	0.834092415	0.224091634			
O	0.148190630	0.000000000	0.105812600	0	0	0
O	0.148190660	0.500000120	0.105812610	0	0	0
O	0.648190980	0.000000000	0.105812600	0	0	0
O	0.648190920	0.500000240	0.105812600	0	0	0
O	0.345998784	0.003083085	0.315613984			
O	0.353835660	0.498252205	0.319151390			
O	0.852182849	-0.002111083	0.318077981			
O	0.851184301	0.496798579	0.319104239			
O	0.000000000	0.148190590	0.105812600	0	0	0
O	0.000000000	0.648190860	0.105812600	0	0	0
O	0.500000120	0.148190630	0.105812600	0	0	0
O	0.500000240	0.648190800	0.105812610	0	0	0
O	0.005021192	0.353521650	0.317967709			
O	0.003398454	0.854054099	0.318452672			
O	0.496425351	0.342607526	0.316170998			
O	0.501163430	0.853309561	0.319064142			
O	0.351809530	0.351809410	0.105812600	0	0	0
O	0.351809500	0.851809620	0.105812610	0	0	0
O	0.851809680	0.351809410	0.105812600	0	0	0
O	0.851809740	0.851809620	0.105812600	0	0	0
O	0.157627384	0.154458679	0.315813067			
O	0.148319642	0.651192697	0.317481021			
O	0.645771701	0.149366385	0.318018792			
O	0.647726013	0.646236313	0.318315665			
O	0.476434070	0.163843339	0.247474470			
O	0.482352631	0.666403213	0.247803519			
O	0.981549049	0.164914127	0.247348775			
O	0.980887714	0.664891842	0.247394710			
O	0.172149370	0.163759308	0.455585956			
O	0.195395834	0.675507838	0.462167911			
O	0.675006399	0.157243729	0.455118373			
O	0.691089089	0.670642426	0.462007216			
O	0.334990780	0.313355238	0.247866410			
O	0.336566619	0.817305884	0.247111768			
O	0.834185599	0.315490932	0.247576937			
O	0.835499939	0.815094747	0.247170279			
O	0.346874414	0.021126201	0.452663588			
O	0.345630445	0.519819004	0.456826374			
O	0.857407406	0.021560404	0.450754193			
O	0.838298677	0.507861891	0.456226275			
O	0.186841015	0.022799064	0.247436855			
O	0.185375288	0.519343741	0.247250591			
O	0.684815155	0.018947591	0.247477579			

O	0.683421674	0.516845995	0.247574748			
O	0.473267717	0.315628563	0.455610052			
O	0.503343691	0.848167905	0.452610031			
O	0.977166147	0.317826952	0.455074911			
O	0.993355785	0.834596435	0.454468658			
O	0.314501415	0.322741002	0.388675306			
O	0.315256933	0.829668585	0.387316810			
O	0.814231455	0.320584775	0.388331140			
O	0.811924284	0.821183087	0.387823996			
O	0.018475950	0.333333700	0.176354340	0	0	0
O	0.018475850	0.833333790	0.176354340	0	0	0
O	0.518476130	0.333333700	0.176354340	0	0	0
O	0.518476130	0.833333850	0.176354330	0	0	0
O	0.177614092	0.490145688	0.388647147			
O	0.176976293	0.997433879	0.386839343			
O	0.672114028	0.484950267	0.388143863			
O	0.683151348	0.998304832	0.386328489			
O	0.166666490	0.185142860	0.176354340	0	0	0
O	0.166666430	0.685143110	0.176354330	0	0	0
O	0.666666690	0.185142910	0.176354340	0	0	0
O	0.666666690	0.685143110	0.176354340	0	0	0
O	0.010156813	0.185988094	0.385621239			
O	0.023860933	0.687310390	0.389146818			
O	0.507721904	0.185308767	0.387225942			
O	0.523892211	0.689872281	0.388997169			
O	0.314857240	0.481524230	0.176354330	0	0	0
O	0.314857300	0.981524470	0.176354340	0	0	0
O	0.814857420	0.481524230	0.176354340	0	0	0
O	0.814857480	0.981524470	0.176354340	0	0	0
H	0.079464650	0.079750397	0.457032311			
H	0.247003919	0.703239320	0.486413183			
H	0.588766458	0.066361989	0.457389020			
H	0.742328653	0.695936116	0.486323787			
I	0.185142860	0.166666567	0.035270844	0	0	0
I	0.185142875	0.666666746	0.035270834	0	0	0
I	0.685143173	0.166666582	0.035270844	0	0	0
I	0.685143113	0.666666746	0.035270840	0	0	0

Model ITO₆₆

In	0.000000000	0.000000000	0.151330020	0	0	0
In	0.000000000	0.500000120	0.151330020	0	0	0
In	0.500000240	0.000000000	0.151330020	0	0	0
In	0.500000180	0.500000120	0.151330020	0	0	0
In	-0.002933211	-0.001730678	0.273786587			
In	0.001079179	0.499268333	0.273841492			
In	0.502811390	-0.001170554	0.273910875			
In	0.502524780	0.502722445	0.273819698			
In	0.000000000	0.000000000	0.060295180	0	0	0
In	0.000000000	0.500000180	0.060295200	0	0	0
In	0.500000180	0.000000000	0.060295200	0	0	0
In	0.500000120	0.500000180	0.060295200	0	0	0
In	-0.000479906	-0.001728980	0.365862416			
In	0.002658659	0.499422364	0.365894140			
In	0.501778738	0.000635700	0.365984856			
In	0.501626099	0.499893788	0.366335866			
Sn	0.333645571	0.166309688	0.292308693			
In	0.334601420	0.666240691	0.294329024			

In	0.834103741	0.167149395	0.294119273			
In	0.835715946	0.666155962	0.294343467			
Sn	0.329826229	0.165824667	0.420511945			
In	0.339085997	0.667380076	0.420433731			
Sn	0.831946490	0.166082887	0.420006261			
In	0.837419043	0.663627074	0.420412908			
In	0.333741810	0.168369272	0.200940152			
In	0.335129085	0.666576298	0.202656964			
In	0.833765987	0.166811251	0.202242250			
In	0.831566797	0.664793314	0.202664278			
In	0.333333550	0.166666540	0.080788260	0	0	0
In	0.333333640	0.666666750	0.080788260	0	0	0
In	0.833333850	0.166666570	0.080788260	0	0	0
In	0.833333850	0.666666810	0.080788260	0	0	0
In	0.163599794	0.334297696	0.435792295			
In	0.171641490	0.830487017	0.435198458			
In	0.661327669	0.329980938	0.435790748			
In	0.673408852	0.830603289	0.435071300			
In	0.166666520	0.333333520	0.130836940	0	0	0
Sn	0.166666490	0.833333730	0.130836940	0	0	0
In	0.666666750	0.333333580	0.130836930	0	0	0
In	0.666666810	0.833333790	0.130836940	0	0	0
In	0.168626233	0.334933218	0.344565852			
In	0.167779182	0.831601276	0.344761005			
In	0.667631220	0.334383849	0.344535371			
In	0.667909847	0.831030104	0.344396470			
In	0.166064840	0.333329875	0.222129564			
In	0.167239860	0.832783821	0.223485583			
In	0.667460200	0.333002953	0.222161789			
In	0.667814834	0.833814004	0.221963053			
O	0.148190630	0.000000000	0.105812600	0	0	0
O	0.148190660	0.500000120	0.105812610	0	0	0
O	0.648190980	0.000000000	0.105812600	0	0	0
O	0.648190920	0.500000240	0.105812600	0	0	0
O	0.350394951	0.006100035	0.319501074			
O	0.355613823	0.500686243	0.320937270			
O	0.854506974	0.001165040	0.320683782			
O	0.854057314	0.499949493	0.320946931			
O	0.000000000	0.148190590	0.105812600	0	0	0
O	0.000000000	0.648190860	0.105812600	0	0	0
O	0.500000120	0.148190630	0.105812600	0	0	0
O	0.500000240	0.648190800	0.105812610	0	0	0
O	0.000653150	0.351146889	0.320644460			
O	0.002228853	0.853104990	0.320531374			
O	0.493482724	0.342670266	0.319659215			
O	0.500481906	0.852827205	0.320892665			
O	0.351809530	0.351809410	0.105812600	0	0	0
O	0.351809500	0.851809620	0.105812610	0	0	0
O	0.851809680	0.351809410	0.105812600	0	0	0
O	0.851809740	0.851809620	0.105812600	0	0	0
O	0.157228908	0.150037314	0.320095952			
O	0.149719303	0.647325471	0.320223378			
O	0.648106530	0.147469198	0.321174165			
O	0.649173616	0.644098521	0.320599284			
O	0.478731217	0.166030802	0.249643707			
O	0.483274889	0.668239118	0.248883487			
O	0.982958853	0.166872631	0.248796904			
O	0.982490873	0.666770017	0.248668322			

O	0.180940514	0.166492880	0.461524690			
O	0.200940952	0.680179414	0.466660699			
O	0.682462550	0.164235112	0.461347739			
O	0.700337373	0.679425944	0.466700806			
O	0.333290783	0.311900722	0.249830904			
O	0.334171417	0.815622883	0.248791108			
O	0.832915184	0.314160601	0.248822624			
O	0.832989137	0.813269181	0.248657951			
O	0.339947420	0.020482353	0.460593585			
O	0.333001386	0.505785760	0.464029531			
O	0.844380562	0.021122293	0.459814011			
O	0.828499387	0.502302760	0.464354730			
O	0.188218216	0.021535400	0.249613178			
O	0.186945434	0.518272503	0.248717448			
O	0.687057166	0.018689073	0.248748435			
O	0.685352289	0.516300107	0.248991693			
O	0.476566260	0.310186173	0.462257261			
O	0.499248604	0.816284386	0.465775467			
O	0.977411045	0.310142943	0.462250053			
O	0.996137221	0.809134438	0.466621689			
O	0.316148127	0.327472132	0.393078004			
O	0.318877725	0.832515124	0.391753730			
O	0.815939330	0.326974514	0.393140274			
O	0.818489961	0.829031429	0.392013883			
O	0.018475950	0.333333700	0.176354340	0	0	0
O	0.018475850	0.833333790	0.176354340	0	0	0
O	0.518476130	0.333333700	0.176354340	0	0	0
O	0.518476130	0.833333850	0.176354330	0	0	0
O	0.172111612	0.484525664	0.392330168			
O	0.171051988	0.988085140	0.393383255			
O	0.669337384	0.480994657	0.391912838			
O	0.673003279	0.988046707	0.393107317			
O	0.166666490	0.185142860	0.176354340	0	0	0
O	0.166666430	0.685143110	0.176354330	0	0	0
O	0.666666690	0.185142910	0.176354340	0	0	0
O	0.666666690	0.685143110	0.176354340	0	0	0
O	0.010159725	0.183179586	0.392155762			
O	0.020486082	0.683931402	0.392529405			
O	0.506873445	0.181498687	0.392779469			
O	0.520941514	0.685314678	0.392407280			
O	0.314857240	0.481524230	0.176354330	0	0	0
O	0.314857300	0.981524470	0.176354340	0	0	0
O	0.814857420	0.481524230	0.176354340	0	0	0
O	0.814857480	0.981524470	0.176354340	0	0	0
H	0.090026514	0.080976499	0.461867648			
H	0.593740861	0.076448864	0.462482534			
H	0.772839957	0.734188033	0.485595795			
H	0.319923679	0.046986773	0.485654517			
H	0.296610109	0.521452362	0.488001352			
H	0.827493810	0.049346330	0.485035272			
H	0.789634673	0.518468781	0.487771869			
H	0.488268850	0.755649479	0.487536679			
I	0.185142860	0.166666567	0.035270844	0	0	0
I	0.185142875	0.666666746	0.035270834	0	0	0
I	0.685143173	0.166666582	0.035270844	0	0	0
I	0.685143113	0.666666746	0.035270840	0	0	0
I	0.481524289	0.814857364	0.035270834	0	0	0
I	0.981524467	0.814857364	0.035270844	0	0	0

I	0.333333641	0.518476009	0.035270834	0	0	0
I	0.833333790	0.518476069	0.035270844	0	0	0

Model ITO₁₀₀

In	0.000000000	0.000000000	0.151330020	0	0	0
In	0.000000000	0.500000120	0.151330020	0	0	0
In	0.500000240	0.000000000	0.151330020	0	0	0
In	0.500000180	0.500000120	0.151330020	0	0	0
In	-0.003746176	-0.001681473	0.273775007			
In	0.000031361	0.498755233	0.273736551			
In	0.502439995	-0.000785325	0.273962728			
In	0.501803752	0.502704627	0.273736475			
In	0.000000000	0.000000000	0.060295180	0	0	0
In	0.000000000	0.500000180	0.060295200	0	0	0
In	0.500000180	0.000000000	0.060295200	0	0	0
In	0.500000120	0.500000180	0.060295200	0	0	0
In	0.000469379	-0.001169895	0.366189271			
In	0.002227922	0.499514773	0.366002320			
In	0.502518139	0.000845263	0.366246257			
In	0.501015274	0.500024868	0.366457682			
Sn	0.332718718	0.166282790	0.292181875			
In	0.333935295	0.666192504	0.293922433			
In	0.833353941	0.167172169	0.293835235			
In	0.835455695	0.666109527	0.293950924			
Sn	0.331901191	0.165896096	0.421960705			
In	0.338826360	0.667958672	0.420671057			
Sn	0.834756617	0.167093249	0.421496487			
In	0.835968344	0.663091856	0.420610981			
In	0.333669673	0.169081548	0.200371656			
In	0.335112922	0.666467600	0.202089374			
In	0.833378556	0.166705494	0.201628282			
In	0.830911795	0.664426703	0.202035006			
In	0.333333550	0.166666540	0.080788260	0	0	0
In	0.333333640	0.666666750	0.080788260	0	0	0
In	0.833333850	0.166666570	0.080788260	0	0	0
In	0.833333850	0.666666810	0.080788260	0	0	0
In	0.167427566	0.335286103	0.436319193			
In	0.170617093	0.830619077	0.434756747			
In	0.664564602	0.329901872	0.436377392			
In	0.673492555	0.831554335	0.434683341			
In	0.166666520	0.333333520	0.130836940	0	0	0
Sn	0.166666490	0.833333730	0.130836940	0	0	0
In	0.666666750	0.333333580	0.130836930	0	0	0
In	0.666666810	0.833333790	0.130836940	0	0	0
In	0.167772224	0.335329852	0.344675808			
In	0.167471001	0.831524989	0.344346556			
In	0.666573291	0.334267429	0.344743012			
In	0.668163955	0.831318644	0.344087206			
In	0.165403821	0.333384736	0.221862076			
In	0.167044644	0.833050682	0.223383494			
In	0.666725783	0.332853619	0.221894763			
In	0.667612794	0.833964598	0.221645441			
O	0.148190630	0.000000000	0.105812600	0	0	0
O	0.148190660	0.500000120	0.105812610	0	0	0
O	0.648190980	0.000000000	0.105812600	0	0	0
O	0.648190920	0.500000240	0.105812600	0	0	0
O	0.350620401	0.006685204	0.319484533			

O	0.354800166	0.500563741	0.321009564			
O	0.855079447	0.001802564	0.320788627			
O	0.852868856	0.499837438	0.321064936			
O	0.000000000	0.148190590	0.105812600	0	0	0
O	0.000000000	0.648190860	0.105812600	0	0	0
O	0.500000120	0.148190630	0.105812600	0	0	0
O	0.500000240	0.648190800	0.105812610	0	0	0
O	-0.000959912	0.350662746	0.320910657			
O	0.002278678	0.853628584	0.320405135			
O	0.492143536	0.342369968	0.319782390			
O	0.500446895	0.853274576	0.320912482			
O	0.351809530	0.351809410	0.105812600	0	0	0
O	0.351809500	0.851809620	0.105812610	0	0	0
O	0.851809680	0.351809410	0.105812600	0	0	0
O	0.851809740	0.851809620	0.105812600	0	0	0
O	0.156879413	0.150339207	0.320596060			
O	0.149074477	0.646668634	0.320086570			
O	0.647354764	0.147696892	0.321462515			
O	0.648989507	0.643821165	0.320634802			
O	0.478070735	0.166247994	0.249620539			
O	0.482785054	0.668521193	0.248842947			
O	0.982530977	0.167201728	0.248788021			
O	0.982077028	0.666766568	0.248618341			
O	0.181425544	0.165522448	0.462427336			
O	0.197899159	0.679817177	0.466392476			
O	0.682596382	0.162541163	0.461986694			
O	0.697664310	0.679236357	0.466635276			
O	0.331894922	0.311831122	0.249932263			
O	0.333963994	0.815979947	0.248747225			
O	0.831603135	0.313959029	0.248888268			
O	0.832525182	0.813035735	0.248482181			
O	0.339823169	0.017333803	0.461133846			
O	0.332882195	0.507810628	0.464908788			
O	0.845118160	0.018471446	0.460326969			
O	0.827225346	0.503297836	0.465267580			
O	0.187493055	0.021536677	0.249627660			
O	0.186255235	0.518211184	0.248627846			
O	0.686541478	0.018657877	0.248757539			
O	0.684591159	0.516085427	0.248889648			
O	0.481138483	0.308297327	0.464101774			
O	0.498693862	0.816663047	0.465355894			
O	0.982326307	0.310565750	0.463877959			
O	0.994987673	0.809779766	0.465996151			
O	0.318425502	0.327222827	0.394393304			
O	0.317598121	0.832058111	0.391550612			
O	0.817499688	0.326596946	0.394143192			
O	0.817738936	0.828540710	0.391857042			
O	0.018475950	0.333333700	0.176354340	0	0	0
O	0.018475850	0.833333790	0.176354340	0	0	0
O	0.518476130	0.333333700	0.176354340	0	0	0
O	0.518476130	0.833333850	0.176354330	0	0	0
O	0.173111711	0.484664993	0.392485712			
O	0.173146546	0.990173215	0.393837589			
O	0.668397771	0.479966068	0.392363501			
O	0.675998754	0.990788952	0.393630201			
O	0.166666490	0.185142860	0.176354340	0	0	0
O	0.166666430	0.685143110	0.176354330	0	0	0
O	0.666666690	0.185142910	0.176354340	0	0	0

O	0.666666690	0.685143110	0.176354340	0	0	0
O	0.011343784	0.184294457	0.392964495			
O	0.018493260	0.684207786	0.392251613			
O	0.507416837	0.181364080	0.393553175			
O	0.519695535	0.686113288	0.392281243			
O	0.314857240	0.481524230	0.176354330	0	0	0
O	0.314857300	0.981524470	0.176354340	0	0	0
O	0.814857420	0.481524230	0.176354340	0	0	0
O	0.814857480	0.981524470	0.176354340	0	0	0
H	0.090945548	0.079912036	0.462115033			
H	0.266878265	0.734468133	0.486066346			
H	0.593847786	0.074934512	0.461620225			
H	0.768615834	0.733112062	0.485987224			
H	0.323131620	0.042422548	0.486794782			
H	0.294293098	0.522530318	0.488580775			
H	0.832555180	0.043937731	0.486427758			
H	0.786847962	0.519264576	0.488402239			
H	0.481325525	0.395931319	0.467582411			
H	0.488702615	0.755673692	0.486954732			
H	0.980619396	0.397434530	0.467036971			
H	0.985465671	0.746265277	0.486803010			

Model ITO₀-bcc

Sn	10.475331401	2.045177083	8.948291116
In	3.432216164	1.993567611	8.744985052
In	13.958705093	8.177634178	8.748874079
In	6.896347545	8.360005336	8.726425955
In	5.103594409	4.799804026	8.493313119
In	15.815467421	11.689153583	8.875386436
In	17.918589293	8.386787183	8.513952066
In	13.742099860	1.858528518	8.882133176
In	15.564098993	5.312755121	8.516391507
In	9.021958424	4.982639052	8.858522424
Sn	8.689690244	11.571630234	8.943797732
In	15.849547286	7.466532042	5.867057341
In	10.314730040	8.127372610	8.988902641
In	3.069928326	3.954371577	5.833174755
In	12.459634703	11.208700316	8.973877604
In	5.331916191	7.056731827	5.859222217
In	8.702217152	7.469575568	6.001644414
In	13.819575056	10.166016474	5.981303411
In	1.762723713	0.881787620	5.961099815
In	12.292714158	4.861242832	8.714163102
In	7.151155127	2.188970267	8.740888907
In	19.153228266	11.447168803	8.700083249
O	7.217917062	4.307695691	7.810799975
O	8.875560994	1.163477069	7.702692596
O	17.287215330	10.437184432	7.924579123
O	12.035820775	1.110385491	7.725078808
O	14.109325524	3.741824918	7.931840151
O	10.496157356	3.832410773	7.703714525
O	10.611309322	12.278552944	9.432047470
O	13.861990434	7.989101492	6.552963500
O	5.218572258	9.456044777	9.388268750
O	12.095866185	11.330610178	6.838064107
O	8.658516869	9.527777273	9.394913450
O	3.649761814	1.966824965	6.570410223

O	13.833286798	6.167575723	9.391474511			
O	8.770759099	11.203694368	6.888462631			
O	12.140875895	9.138281006	9.454497496			
O	6.792592193	8.532327147	6.537134835			
O	5.257748111	2.887425890	9.373506932			
O	10.559804825	8.380994051	6.846902503			
O	2.999916500	4.168404110	8.502852997			
O	8.459111188	6.968342626	8.215611000			
O	5.223614948	6.869738265	8.404130552			
O	14.394407448	10.227214140	8.154287797			
O	16.069146018	7.459127972	8.524882339			
O	1.429376080	1.286447097	8.207730854			
O	17.869017309	8.163181542	6.305803592			
O	21.074110717	12.152689655	9.485936819			
O	12.436679640	5.421677257	6.419198806			
O	12.141818855	2.942536279	9.838008362			
O	15.797879862	5.399710779	6.318633639			
O	10.726435136	6.100380449	9.505625216			
O	6.559850327	2.106839159	6.304837468			
O	8.847694949	3.057721701	9.822281191			
O	4.967692666	4.879424966	6.261942040			
O	6.826144489	0.210894159	9.513636105			
O	19.575935191	11.045428880	6.417405483			
O	10.416893319	0.144783762	9.819617021			
In	17.651761460	10.316667554	5.753942829			
Sn	6.899233425	4.071545445	5.705397377			
In	14.028320214	4.119407376	5.732478980			
In	3.323655150	6.169764390	2.723682860	0	0	0
In	10.477454460	6.169764390	2.723682860	0	0	0
In	6.900554810	12.365136320	2.723682860	0	0	0
In	14.054354110	12.365136320	2.723682860	0	0	0
In	10.486729270	10.289466206	5.730636852			
In	12.253481310	0.722509160	5.599068678			
In	12.265904290	8.989071640	2.526839380	0	0	0
In	15.842803940	3.350457140	2.920526340	0	0	0
In	10.745653757	4.244735749	5.597379184			
In	3.564738190	0.113581810	2.526839380	0	0	0
In	6.659471770	6.030575030	2.920526340	0	0	0
In	8.454874001	1.152676984	5.586698530			
In	8.447921600	9.406639710	2.526839380	0	0	0
Sn	16.083886980	9.128261000	2.920526340	0	0	0
In	8.689004630	3.350457140	2.920526340	0	0	0
In	5.101526090	0.727434508	5.516974872			
In	17.390170730	12.225946970	2.920526340	0	0	0
In	7.113379323	10.432055078	5.522299756			
In	12.506987320	2.932889070	2.920526340	0	0	0
In	12.036048373	7.327430280	5.539622610			
In	5.112104980	8.989071640	2.526839380	0	0	0
In	14.295437150	6.308953750	2.526839380	0	0	0
In	4.871021940	3.211267780	2.526839380	0	0	0
O	10.210960658	0.025232220	5.180414495			
O	14.307598610	8.476920900	1.935140750	0	0	0
O	15.648075606	2.809208612	5.151338254			
O	16.030233480	5.149593150	1.692152960	0	0	0
O	12.332284617	2.809331988	5.187524465			
O	2.987426590	2.137816340	1.935140750	0	0	0
O	7.221086366	6.072343737	5.187107473			
O	5.007659510	5.293325770	1.692152960	0	0	0

O	8.825351644	3.317532658	5.201868439			
O	6.983538880	7.894555940	1.935140750	0	0	0
O	15.704989510	9.545219025	5.022812267			
O	17.548269690	8.066374250	1.692152960	0	0	0
O	10.730698960	4.079032880	3.206153810	0	0	0
O	5.299534520	1.286985260	3.341666230	0	0	0
O	8.584559160	1.239074380	3.206153810	0	0	0
O	6.564326240	10.322315680	3.341666230	0	0	0
O	12.117105260	0.800442050	3.206153810	0	0	0
O	12.414703310	6.899992230	3.341666230	0	0	0
O	10.224209960	8.260495900	2.241211910	0	0	0
O	-0.015764181	0.186319467	4.973999584			
O	15.655374400	11.052543520	2.105699490	0	0	0
O	8.819197919	9.289351882	4.728081383			
O	12.370349760	11.100454400	2.241211910	0	0	0
O	10.155694750	6.261983164	4.967014552			
O	14.390582680	2.017213100	2.105699490	0	0	0
O	12.198999780	9.368557408	4.707906128			
O	8.837803660	11.539086730	2.241211910	0	0	0
O	14.138599873	12.044689280	4.974139347			
O	8.540205610	5.439536550	2.105699490	0	0	0
O	10.405905553	12.230178201	4.714741685			
O	6.647310310	3.862607880	3.512224970	0	0	0
O	4.924675440	7.189935630	3.755212760	0	0	0
O	17.967482330	10.201712440	3.512224970	0	0	0
O	15.947249410	7.046203010	3.755212760	0	0	0
O	13.971370040	4.444972840	3.512224970	0	0	0
O	3.406639230	4.273154530	3.755212760	0	0	0

Model for ITO_{bv}

In	-0.002766336	0.000309602	0.355062789
In	0.000953273	0.497766753	0.358233776
In	0.501250447	-0.000585179	0.358111171
In	0.501089733	0.502821772	0.358290409
In	-0.003764834	-0.001124821	0.641872811
In	-0.000242098	0.497764646	0.643034059
In	0.500749673	-0.000422280	0.643283686
In	0.502895334	0.503482227	0.642815110
In	-0.001244818	-0.001141376	0.135148473
In	-0.004353954	0.496069003	0.144047096
In	0.503272680	0.006361417	0.143743230
In	0.502862914	0.498477988	0.145736580
In	-0.001565397	-0.001239472	0.857809780
In	0.006003372	0.501828134	0.859444336
In	0.498796298	-0.003582857	0.860566817
In	0.497698985	0.504435778	0.861289790
Sn	0.333048295	0.168665752	0.684998013
In	0.334094157	0.666549465	0.695269628
In	0.830053202	0.165264289	0.691410508
In	0.836038817	0.665574166	0.691412941
Sn	0.330604184	0.164463206	0.980911519
Sn	0.835223698	0.165239003	0.980875622
In	0.834092015	0.669919309	0.975579841
In	0.332474736	0.167982973	0.470102686
In	0.334309921	0.666659096	0.477336051
In	0.831922956	0.165938771	0.476173985
In	0.834642022	0.666126874	0.475241402

In	0.330434016	0.163974607	0.193818077
In	0.332169880	0.665427423	0.175836620
In	0.835985527	0.165007881	0.194583243
In	0.835583588	0.670942200	0.189079129
In	0.176814622	0.353511500	0.020577070
In	0.174507385	0.821793409	0.020675801
In	0.668022558	0.336197894	0.023277979
In	0.646123271	0.820873377	0.021272367
In	0.170371641	0.337206324	0.307431015
Sn	0.166609166	0.830905904	0.313512840
In	0.667319133	0.334675916	0.309653835
In	0.663285692	0.831339332	0.306747330
In	0.164430556	0.333829171	0.807345017
In	0.168532890	0.835101103	0.808559674
In	0.665472504	0.333636759	0.808997722
In	0.667644878	0.829889991	0.808554917
In	0.164894725	0.332826208	0.523927226
In	0.167601027	0.833891531	0.529238941
In	0.666301446	0.333692660	0.524308585
In	0.667424527	0.833155708	0.523205386
O	0.148747049	-0.009175258	0.252087508
O	0.146976857	0.500518263	0.251118828
O	0.650642399	0.005121269	0.254130937
O	0.651484982	0.501968669	0.250143063
O	0.348470628	0.008858966	0.743413405
O	0.353709315	0.497301115	0.748680796
O	0.852102251	-0.000606517	0.749443288
O	0.852155400	0.497909695	0.751756373
O	0.007018713	0.148301235	0.245971313
O	0.000146282	0.655392721	0.257711954
O	0.500551511	0.148760902	0.249780017
O	0.496352645	0.646454327	0.252072533
O	-0.002628866	0.348929012	0.746547736
O	0.002972013	0.854544795	0.749055066
O	0.493081867	0.342718284	0.747429774
O	0.502079965	0.855818098	0.749530744
O	0.354574713	0.346360987	0.255661022
O	0.343355167	0.850956690	0.253062848
O	0.851767780	0.351344527	0.249950221
O	0.852414623	0.856075696	0.247349290
O	0.155532636	0.151947302	0.747108318
O	0.146695833	0.648444667	0.747222774
O	0.644504755	0.147341051	0.752089316
O	0.650324435	0.644007001	0.748081588
O	0.476403830	0.165564268	0.583224361
O	0.482556538	0.668622295	0.584476921
O	0.981031223	0.166189045	0.583111208
O	0.981535080	0.665889055	0.582962221
O	0.188578218	0.170422530	0.081126826
O	0.172288668	0.661933770	0.092874717
O	0.691143710	0.170873197	0.081682169
O	0.685433555	0.666446274	0.083069335
O	0.333720655	0.312354033	0.584784594
O	0.333955028	0.815492370	0.583853742
O	0.830935780	0.313523335	0.583317322
O	0.834838652	0.814042859	0.581685535
O	0.332528823	0.021389019	0.081366921
O	0.336252141	0.507954139	0.093603688

O	0.827920989	0.017598728	0.080544515
O	0.831760446	0.518373224	0.084578798
O	0.187226875	0.023503433	0.583938589
O	0.185985876	0.519046544	0.582787296
O	0.685080255	0.018339122	0.583440699
O	0.685655900	0.517830924	0.583075273
O	0.478508291	0.309134163	0.081795070
O	0.490216869	0.827938234	0.094677118
O	0.978602589	0.309418865	0.081134720
O	0.987499221	0.815605842	0.082150444
O	0.316846137	0.324703364	0.917396546
O	0.310141713	0.845387412	0.909740782
O	0.814980821	0.324704047	0.918673600
O	0.817989927	0.836300704	0.917497033
O	0.017308430	0.330589360	0.415994265
O	0.024067749	0.836171388	0.415798532
O	0.519649461	0.334802721	0.417231055
O	0.517999677	0.832846565	0.417408670
O	0.160543633	0.467322677	0.909732555
O	0.169635240	0.993794594	0.918693155
O	0.666812474	0.479317861	0.915247755
O	0.674150641	0.992764149	0.918487560
O	0.164273799	0.183775517	0.416089014
O	0.167165495	0.689041289	0.416086504
O	0.664316121	0.185270212	0.417967100
O	0.669719468	0.686719125	0.416233159
O	0.008916208	0.178552238	0.918378523
O	0.016093007	0.684971351	0.914792495
O	0.510003506	0.184066726	0.919037749
O	0.529131800	0.692379283	0.910028522
O	0.314617875	0.480136060	0.419163895
O	0.311601711	0.978687150	0.415124852
O	0.816382159	0.481139381	0.416792704
O	0.813977898	0.981646204	0.415568669

Model ITO_{0v}

In	0.000000000	0.000000000	0.151330024	0	0	0
In	0.000000000	0.500000119	0.151330024	0	0	0
In	0.500000238	0.000000000	0.151330024	0	0	0
In	0.500000179	0.500000119	0.151330024	0	0	0
In	-0.004842587	-0.002090600	0.274883692			
In	-0.001071658	0.498901650	0.273808601			
In	0.501309637	-0.001882447	0.273143688			
In	0.502434334	0.504171885	0.276113908			
In	0.000000000	0.000000000	0.060295182	0	0	0
In	0.000000000	0.500000179	0.060295195	0	0	0
In	0.500000179	0.000000000	0.060295195	0	0	0
In	0.500000119	0.500000179	0.060295195	0	0	0
In	0.004805813	0.011335875	0.367945216			
In	0.002914289	0.491399339	0.365219268			
In	0.493608536	-0.001919871	0.364786585			
In	0.497547483	0.499105975	0.370845367			
Sn	0.332889238	0.168138002	0.292095504			
In	0.332613559	0.667527708	0.296564072			
In	0.831250423	0.164975539	0.295162455			
In	0.832890414	0.665082541	0.294905781			
Sn	0.310635593	0.151502056	0.428318747			

Sn	0.811667101	0.148116604	0.418830936			
In	0.838090871	0.661367148	0.408719497			
In	0.333258262	0.169662995	0.201573611			
In	0.335989162	0.666251583	0.203904176			
In	0.833590367	0.166526288	0.203002561			
In	0.829909936	0.663535415	0.203426712			
In	0.333333552	0.166666538	0.080788255	0	0	0
In	0.333333641	0.666666746	0.080788255	0	0	0
In	0.833333850	0.166666567	0.080788255	0	0	0
In	0.833333850	0.666666806	0.080788255	0	0	0
In	0.176138091	0.347992417	0.432520744			
In	0.203325213	0.817303272	0.432195709			
In	0.637561425	0.309094120	0.436673179			
In	0.689047418	0.802165191	0.442537081			
In	0.166666523	0.333333522	0.130836939	0	0	0
Sn	0.166666493	0.833333731	0.130836939	0	0	0
In	0.666666746	0.333333582	0.130836927	0	0	0
In	0.666666806	0.833333790	0.130836939	0	0	0
In	0.169899466	0.337360925	0.344532374			
In	0.165280809	0.835599038	0.344353136			
In	0.664018133	0.326965197	0.345312795			
In	0.666571790	0.831883864	0.348144597			
In	0.165015038	0.333507711	0.223266571			
In	0.166036756	0.833566066	0.224726538			
In	0.666096957	0.332631623	0.223081687			
In	0.667189000	0.833010038	0.222991427			
O	0.148190632	0.000000000	0.105812597	0	0	0
O	0.148190662	0.500000119	0.105812610	0	0	0
O	0.648190975	0.000000000	0.105812597	0	0	0
O	0.648190916	0.500000238	0.105812597	0	0	0
O	0.345289990	0.004256627	0.314597592			
O	0.356447196	0.503169275	0.319945210			
O	0.853466902	0.000255691	0.319179030			
O	0.851185223	0.498434175	0.319456675			
O	0.000000000	0.148190588	0.105812597	0	0	0
O	-0.000000000	0.648190856	0.105812597	0	0	0
O	0.500000119	0.148190632	0.105812597	0	0	0
O	0.500000238	0.648190796	0.105812610	0	0	0
O	0.005156168	0.350534990	0.316102911			
O	0.001883185	0.851075068	0.318099118			
O	0.493988037	0.341407333	0.317081414			
O	0.503431850	0.853241760	0.317763454			
O	0.351809531	0.351809412	0.105812597	0	0	0
O	0.351809502	0.851809621	0.105812610	0	0	0
O	0.851809680	0.351809412	0.105812597	0	0	0
O	0.851809740	0.851809621	0.105812597	0	0	0
O	0.155145837	0.152345738	0.317341246			
O	0.142974868	0.646789067	0.317802344			
O	0.642872626	0.148172661	0.315953667			
O	0.648770927	0.644515972	0.320405089			
O	0.475330467	0.164721530	0.247033908			
O	0.482533174	0.666726252	0.248030288			
O	0.981447678	0.164595348	0.247210690			
O	0.980386385	0.665279979	0.246874598			
O	0.165086655	0.177762198	0.456892923			
O	0.392285835	0.621217959	0.480476351			
O	0.753663560	0.236363160	0.460258221			
O	0.769701044	0.679557286	0.461067239			

O	0.333474782	0.313639985	0.248898737			
O	0.333269486	0.815501729	0.247214808			
O	0.832823085	0.314844389	0.247254895			
O	0.833954051	0.813805428	0.247376058			
O	0.315498034	-0.000859883	0.459340415			
O	0.403058713	0.535925982	0.456113629			
O	0.801048684	0.006234046	0.457317913			
O	1.054226447	0.523995261	0.464119227			
O	0.185559827	0.023119445	0.247804527			
O	0.186221248	0.519801119	0.247449081			
O	0.685688643	0.018612714	0.246921221			
O	0.682985337	0.516634388	0.247935914			
O	0.470364120	0.317217992	0.455307921			
O	0.510070192	0.736086354	0.488295315			
O	1.075948310	0.423003224	0.476538355			
O	1.160196446	0.654550767	0.475083254			
O	0.310128717	0.321622206	0.388226390			
O	0.311059090	0.824781342	0.382083525			
O	0.815674305	0.318063496	0.385439419			
O	0.828016537	0.833952584	0.386890890			
O	0.018475950	0.333333701	0.176354341	0	0	0
O	0.018475849	0.833333790	0.176354341	0	0	0
O	0.518476129	0.333333701	0.176354341	0	0	0
O	0.518476129	0.833333850	0.176354328	0	0	0
O	0.167164847	0.475413062	0.389293216			
O	0.167471726	0.987259250	0.390065025			
O	0.669379586	0.471431264	0.389285006			
O	0.665790875	0.991991787	0.385665860			
O	0.166666493	0.185142860	0.176354341	0	0	0
O	0.166666433	0.685143113	0.176354328	0	0	0
O	0.666666687	0.185142905	0.176354341	0	0	0
O	0.666666687	0.685143113	0.176354341	0	0	0
O	-0.003239915	0.185824771	0.390980391			
O	0.026030836	0.677722442	0.394122862			
O	0.501709484	0.176279613	0.389347404			
O	0.547070585	0.690731959	0.394969598			
O	0.314857244	0.481524229	0.176354328	0	0	0
O	0.314857304	0.981524467	0.176354341	0	0	0
O	0.814857423	0.481524229	0.176354341	0	0	0
O	0.814857483	0.981524467	0.176354341	0	0	0

Model ITO_{0v}^m

In	-0.004309612	0.000751822	0.151208968			
In	-0.000808836	0.496572412	0.151347944			
In	0.504644581	0.002355043	0.151143260			
In	0.500933753	0.501012594	0.151055266			
In	-0.002967113	-0.004589945	0.273197974			
In	-0.002103722	0.502215187	0.274053255			
In	0.503165726	-0.003309584	0.285962016			
In	0.507298420	0.506583351	0.274012085			
In	0.000000000	0.000000000	0.060295182	0	0	0
In	0.000000000	0.500000179	0.060295195	0	0	0
In	0.500000179	0.000000000	0.060295195	0	0	0
In	0.500000119	0.500000179	0.060295195	0	0	0
In	-0.003749136	0.011095529	0.363425509			
In	0.014100336	0.498205349	0.364559846			

In	0.482587608	0.484676002	0.365481453			
Sn	0.332539851	0.176196456	0.289455075			
In	0.327116540	0.656526349	0.291807980			
In	0.846232133	0.170971659	0.290616292			
In	0.833243009	0.666129960	0.292140945			
Sn	0.352239555	0.105936130	0.383568513			
In	0.374264664	0.737027708	0.385106722			
Sn	0.772482649	0.146570718	0.382160450			
In	0.830984339	0.663912439	0.394372672			
In	0.331945574	0.164758656	0.199307539			
In	0.336190610	0.668807087	0.201707075			
In	0.831655471	0.167701569	0.201906134			
In	0.834015407	0.666031747	0.200865729			
In	0.333333552	0.166666538	0.080788255	0	0	0
In	0.333333641	0.666666746	0.080788255	0	0	0
In	0.833333850	0.166666567	0.080788255	0	0	0
In	0.833333850	0.666666806	0.080788255	0	0	0
In	0.166666552	0.333333641	0.010246514	0	0	0
In	0.166666582	0.833333731	0.010246514	0	0	0
In	0.666666746	0.333333582	0.010246536	0	0	0
In	0.666666687	0.833333731	0.010246514	0	0	0
In	0.166666523	0.333333522	0.130836939	0	0	0
Sn	0.166666493	0.833333731	0.130836939	0	0	0
In	0.666666746	0.333333582	0.130836927	0	0	0
In	0.666666806	0.833333790	0.130836939	0	0	0
In	0.169239546	0.334491749	0.350495540			
In	0.151032561	0.824325410	0.349958324			
In	0.669422375	0.340903358	0.350154513			
In	0.665660330	0.825622934	0.350532856			
In	0.167167121	0.334662320	0.222048237			
In	0.173404052	0.834220565	0.224224549			
In	0.662423892	0.328930493	0.223707935			
In	0.666242706	0.837247539	0.223341848			
O	0.148190632	0.000000000	0.105812597	0	0	0
O	0.148190662	0.500000119	0.105812610	0	0	0
O	0.648190975	0.000000000	0.105812597	0	0	0
O	0.648190916	0.500000238	0.105812597	0	0	0
O	0.342798756	0.031611921	0.324287280			
O	0.348800841	0.488689514	0.316460055			
O	0.843967440	-0.007034093	0.317642816			
O	0.849710565	0.501362656	0.319954033			
O	0.000000000	0.148190588	0.105812597	0	0	0
O	-0.000000000	0.648190856	0.105812597	0	0	0
O	0.500000119	0.148190632	0.105812597	0	0	0
O	0.500000238	0.648190796	0.105812610	0	0	0
O	0.011603029	0.357690422	0.316552976			
O	-0.001225343	0.849737943	0.318508144			
O	0.503274371	0.344542346	0.315477476			
O	0.480957497	0.827373846	0.324270629			
O	0.351809531	0.351809412	0.105812597	0	0	0
O	0.351809502	0.851809621	0.105812610	0	0	0
O	0.851809680	0.351809412	0.105812597	0	0	0
O	0.851809740	0.851809621	0.105812597	0	0	0
O	0.149924609	0.154532914	0.314263812			
O	0.149557484	0.657245987	0.317523242			
O	0.683254319	0.157142916	0.326809083			
O	0.651921609	0.647696914	0.319477669			
O	0.479264335	0.157915126	0.251891069			

O	0.481584707	0.665645966	0.246983696			
O	0.982509537	0.162899576	0.245604488			
O	0.983502122	0.668518739	0.246431883			
O	0.185142860	0.166666567	0.035270844	0	0	0
O	0.185142875	0.666666746	0.035270834	0	0	0
O	0.685143173	0.166666582	0.035270844	0	0	0
O	0.685143113	0.666666746	0.035270840	0	0	0
O	0.338595524	0.315624073	0.246511933			
O	0.340547280	0.822974265	0.250127043			
O	0.834669745	0.316831792	0.247299609			
O	0.835346775	0.814940291	0.245976529			
O	0.333333671	0.018475870	0.035270840	0	0	0
O	0.333333641	0.518476009	0.035270834	0	0	0
O	0.833333790	0.018475881	0.035270844	0	0	0
O	0.833333790	0.518476069	0.035270844	0	0	0
O	0.189475169	0.023054371	0.247254164			
O	0.182511641	0.521484052	0.245539516			
O	0.679280553	0.018371396	0.250786239			
O	0.686362935	0.518427922	0.246851356			
O	0.481524259	0.314857274	0.035270844	0	0	0
O	0.481524289	0.814857364	0.035270834	0	0	0
O	0.981524408	0.314857274	0.035270840	0	0	0
O	0.981524467	0.814857364	0.035270844	0	0	0
O	0.319086265	0.282648901	0.380705350			
O	0.315059058	0.880398934	0.390527137			
O	0.829923099	0.343209275	0.391472570			
O	0.828034512	0.841483690	0.390183572			
O	0.018497200	0.332345754	0.176819281			
O	0.024810846	0.834846301	0.174712966			
O	0.518304027	0.331999346	0.177533178			
O	0.518779968	0.835052273	0.176889403			
O	0.204024228	0.520375837	0.383102337			
O	0.148783303	0.984685956	0.390576650			
O	0.653445816	0.482395023	0.390263212			
O	0.649703137	0.955644366	0.395310182			
O	0.165316298	0.183681658	0.176563780			
O	0.169802103	0.690987504	0.174581196			
O	0.664691575	0.185736108	0.177752604			
O	0.667507331	0.686520763	0.176731065			
O	-0.023810892	0.182484505	0.381832096			
O	0.013307808	0.667809651	0.391430710			
O	0.548307521	0.190901289	0.394153812			
O	0.513389677	0.669291457	0.390195484			
O	0.315278593	0.481238554	0.177087074			
O	0.311994464	0.977721945	0.174651255			
O	0.815732931	0.480673158	0.176656402			
O	0.812369116	0.982352759	0.177394955			

Model ITO_{33v}

In	0.000000000	0.000000000	0.151330020	0	0	0
In	0.000000000	0.500000120	0.151330020	0	0	0
In	0.500000240	0.000000000	0.151330020	0	0	0
In	0.500000180	0.500000120	0.151330020	0	0	0
In	-0.003893372	-0.000342631	0.275083737			
In	-0.001054584	0.499137924	0.275278557			
In	0.500771039	-0.000699316	0.276029496			

In	0.503246987	0.504003898	0.276079525			
In	0.000000000	0.000000000	0.060295180	0	0	0
In	0.000000000	0.500000180	0.060295200	0	0	0
In	0.500000180	0.000000000	0.060295200	0	0	0
In	0.500000120	0.500000180	0.060295200	0	0	0
In	-0.005099334	-0.000563624	0.368574447			
In	-0.001575032	0.497466591	0.368884831			
In	0.500810196	0.000609850	0.370727104			
In	0.498800675	0.508387031	0.370941813			
Sn	0.333281103	0.169160188	0.292401882			
In	0.333562053	0.667041727	0.297928416			
In	0.829387372	0.166245137	0.296916043			
In	0.835155553	0.666674748	0.297475727			
Sn	0.327938268	0.167053820	0.424077771			
Sn	0.837397155	0.165628610	0.421203219			
In	0.839050902	0.662587911	0.420021071			
In	0.333584522	0.169055552	0.202372820			
In	0.335603601	0.666772025	0.205163477			
In	0.833260408	0.166779289	0.204460571			
In	0.830685364	0.664345712	0.204881738			
In	0.333333550	0.166666540	0.080788260	0	0	0
In	0.333333640	0.666666750	0.080788260	0	0	0
In	0.833333850	0.166666570	0.080788260	0	0	0
In	0.833333850	0.666666810	0.080788260	0	0	0
In	0.167483009	0.355571347	0.432100074			
In	0.175708381	0.832638411	0.432588887			
In	0.656524440	0.329497888	0.439651749			
In	0.661859545	0.830146931	0.437663833			
In	0.166666520	0.333333520	0.130836940	0	0	0
Sn	0.166666490	0.833333730	0.130836940	0	0	0
In	0.666666750	0.333333580	0.130836930	0	0	0
In	0.666666810	0.833333790	0.130836940	0	0	0
In	0.166508843	0.335469021	0.344039828			
In	0.168249582	0.836310393	0.344225284			
In	0.661465686	0.331888136	0.347251680			
In	0.666380227	0.832742544	0.347001054			
In	0.165378755	0.333774010	0.224145140			
In	0.167023819	0.833495737	0.226118908			
In	0.666251760	0.333156718	0.224264608			
In	0.667402845	0.834263490	0.224187730			
O	0.148190630	0.000000000	0.105812600	0	0	0
O	0.148190660	0.500000120	0.105812610	0	0	0
O	0.648190980	0.000000000	0.105812600	0	0	0
O	0.648190920	0.500000240	0.105812600	0	0	0
O	0.344809625	0.006275175	0.315272950			
O	0.356242663	0.500310209	0.319711437			
O	0.850025207	-0.002137218	0.318655661			
O	0.848299386	0.495421411	0.319487277			
O	0.000000000	0.148190590	0.105812600	0	0	0
O	0.000000000	0.648190860	0.105812600	0	0	0
O	0.500000120	0.148190630	0.105812600	0	0	0
O	0.500000240	0.648190800	0.105812610	0	0	0
O	0.000972742	0.351675698	0.316652304			
O	0.004379324	0.857434126	0.317940024			
O	0.493613180	0.342543975	0.316850096			
O	0.499994444	0.854937795	0.319958458			
O	0.351809530	0.351809410	0.105812600	0	0	0
O	0.351809500	0.851809620	0.105812610	0	0	0

O	0.851809680	0.351809410	0.105812600	0	0	0
O	0.851809740	0.851809620	0.105812600	0	0	0
O	0.157463089	0.155659457	0.316099060			
O	0.146723026	0.651536692	0.316660558			
O	0.642601884	0.148969881	0.319049927			
O	0.648620616	0.648504651	0.318811849			
O	0.476668125	0.164769440	0.247428063			
O	0.482481730	0.667438191	0.248355750			
O	0.981411720	0.164962396	0.247170684			
O	0.980594162	0.665684391	0.247513682			
O	0.176961141	0.185702447	0.458360130			
O	0.274774193	0.639402086	0.476489420			
O	0.681755017	0.160110726	0.456573791			
O	0.690598139	0.668797005	0.461043111			
O	0.335418849	0.315051285	0.247967744			
O	0.336491433	0.818189388	0.247304700			
O	0.832673984	0.315179927	0.247410618			
O	0.834727801	0.815345318	0.247267827			
O	0.329287189	0.014368162	0.456819767			
O	0.305319952	0.543997071	0.473706651			
O	0.858250447	0.011717331	0.447728436			
O	0.854785198	0.497209053	0.447351540			
O	0.186209044	0.023706968	0.247316812			
O	0.185556255	0.519228652	0.247528834			
O	0.684151240	0.019200042	0.247912863			
O	0.683626427	0.517317498	0.247944690			
O	0.475729047	0.317216155	0.458059872			
O	0.551626818	0.893330390	0.472537040			
O	0.982183298	0.320491621	0.455166378			
O	0.997061100	0.761938160	0.464070200			
O	0.314887791	0.330904128	0.392089415			
O	0.309125368	0.837684451	0.387246003			
O	0.811004139	0.316117041	0.388149841			
O	0.818643038	0.821343179	0.388450055			
O	0.018475950	0.333333700	0.176354340	0	0	0
O	0.018475850	0.833333790	0.176354340	0	0	0
O	0.518476130	0.333333700	0.176354340	0	0	0
O	0.518476130	0.833333850	0.176354330	0	0	0
O	0.171108038	0.483305583	0.385708358			
O	0.171029598	0.999152153	0.390585258			
O	0.666562053	0.483096370	0.388726644			
O	0.678285235	0.994898244	0.388801095			
O	0.166666490	0.185142860	0.176354340	0	0	0
O	0.166666430	0.685143110	0.176354330	0	0	0
O	0.666666690	0.185142910	0.176354340	0	0	0
O	0.666666690	0.685143110	0.176354340	0	0	0
O	0.009229151	0.187793600	0.385219884			
O	0.020086541	0.689518017	0.386308378			
O	0.504210504	0.184624824	0.389792703			
O	0.530436657	0.697172200	0.391555033			
O	0.314857240	0.481524230	0.176354330	0	0	0
O	0.314857300	0.981524470	0.176354340	0	0	0
O	0.814857420	0.481524230	0.176354340	0	0	0
O	0.814857480	0.981524470	0.176354340	0	0	0
H	0.080582948	0.107796576	0.460016933			
H	0.458446829	0.823160464	0.480534177			
H	0.610759329	0.063490927	0.465271572			
H	0.736804711	0.691204811	0.486097507			

I	0.185142860	0.166666567	0.035270844	0	0	0
I	0.185142875	0.666666746	0.035270834	0	0	0
I	0.685143173	0.166666582	0.035270844	0	0	0
I	0.685143113	0.666666746	0.035270840	0	0	0

Model ITO_{66v}

In	0.000000000	0.000000000	0.151330020	0	0	0
In	0.000000000	0.500000120	0.151330020	0	0	0
In	0.500000240	0.000000000	0.151330020	0	0	0
In	0.500000180	0.500000120	0.151330020	0	0	0
In	-0.003298283	0.000367150	0.275987713			
In	-0.000248974	0.497798174	0.274179411			
In	0.502736804	0.000418651	0.274789761			
In	0.504868557	0.505957052	0.278938493			
In	0.000000000	0.000000000	0.060295180	0	0	0
In	0.000000000	0.500000180	0.060295200	0	0	0
In	0.500000180	0.000000000	0.060295200	0	0	0
In	0.500000120	0.500000180	0.060295200	0	0	0
In	-0.009592890	0.000197535	0.368121150			
In	-0.002819539	0.492593159	0.364384318			
In	0.505905957	0.005032357	0.365203318			
In	0.513873301	0.503724369	0.407079797			
Sn	0.331522364	0.165062716	0.292232232			
In	0.332076579	0.673461115	0.296070185			
In	0.830898626	0.165004450	0.296138302			
In	0.842305749	0.669655613	0.295752865			
Sn	0.324863631	0.167147433	0.419335014			
Sn	0.819332724	0.159954252	0.422007217			
In	0.867619497	0.680192171	0.421589526			
In	0.333385309	0.169693772	0.202218271			
In	0.337390674	0.666650223	0.204400843			
In	0.833984471	0.167170542	0.203916447			
In	0.829656051	0.663668701	0.204311624			
In	0.333333550	0.166666540	0.080788260	0	0	0
In	0.333333640	0.666666750	0.080788260	0	0	0
In	0.833333850	0.166666570	0.080788260	0	0	0
In	0.833333850	0.666666810	0.080788260	0	0	0
In	0.157991770	0.347751747	0.432996451			
In	0.263988338	0.814962948	0.444901626			
In	0.658573467	0.324267671	0.436445666			
In	0.622502429	0.825492588	0.437234632			
In	0.166666520	0.333333520	0.130836940	0	0	0
Sn	0.166666490	0.833333730	0.130836940	0	0	0
In	0.666666750	0.333333580	0.130836930	0	0	0
In	0.666666810	0.833333790	0.130836940	0	0	0
In	0.182824551	0.347497474	0.343204248			
In	0.165546858	0.836631226	0.349980889			
In	0.659757915	0.339819887	0.345975947			
In	0.662053688	0.816051437	0.347676399			
In	0.167734164	0.334870269	0.224555096			
In	0.167037694	0.833510522	0.225693894			
In	0.665270502	0.333539687	0.224162820			
In	0.668852322	0.833187766	0.224183011			
O	0.148190630	0.000000000	0.105812600	0	0	0
O	0.148190660	0.500000120	0.105812610	0	0	0
O	0.648190980	0.000000000	0.105812600	0	0	0
O	0.648190920	0.500000240	0.105812600	0	0	0

O	0.344774932	0.002254766	0.315906593			
O	0.346554411	0.503872515	0.313300954			
O	0.849402130	-0.003185846	0.320946846			
O	0.847353548	0.492637256	0.318096279			
O	0.000000000	0.148190590	0.105812600	0	0	0
O	0.000000000	0.648190860	0.105812600	0	0	0
O	0.500000120	0.148190630	0.105812600	0	0	0
O	0.500000240	0.648190800	0.105812610	0	0	0
O	0.002634520	0.349103942	0.317026106			
O	0.005473039	0.858424849	0.320091434			
O	0.493342621	0.336792349	0.315061090			
O	0.505984343	0.856514328	0.319449135			
O	0.351809530	0.351809410	0.105812600	0	0	0
O	0.351809500	0.851809620	0.105812610	0	0	0
O	0.851809680	0.351809410	0.105812600	0	0	0
O	0.851809740	0.851809620	0.105812600	0	0	0
O	0.157377670	0.157934114	0.317478373			
O	0.144683647	0.653917430	0.317288289			
O	0.645717023	0.152577616	0.319489251			
O	0.661707885	0.656237949	0.316399972			
O	0.476065892	0.161269575	0.246784328			
O	0.484248144	0.668621498	0.247468273			
O	0.981852541	0.165463612	0.247845954			
O	0.981026616	0.665668349	0.247396806			
O	0.183073368	0.184074623	0.460274123			
O	0.193941577	0.601010440	0.466665380			
O	0.669940493	0.156117672	0.456777989			
O	0.654314746	0.656602810	0.457267291			
O	0.335111139	0.312083811	0.248140772			
O	0.337011910	0.818646707	0.247115843			
O	0.831643526	0.313674922	0.247432816			
O	0.840956551	0.819919395	0.246322946			
O	0.329500608	0.029529218	0.461453574			
O	0.285102600	0.554052337	0.463695717			
O	0.806149211	-0.001265221	0.462264178			
O	0.823859393	0.510718835	0.465282685			
O	0.185615941	0.022391665	0.248201121			
O	0.181437932	0.520706063	0.245367991			
O	0.686715992	0.019506296	0.248260901			
O	0.683322991	0.517763935	0.247668468			
O	0.478949453	0.340329960	0.449104643			
O	0.476276480	0.870617854	0.464823674			
O	0.972288996	0.301842241	0.462983656			
O	1.060199964	0.776762275	0.464818681			
O	0.309704060	0.332241131	0.392029857			
O	0.321635494	0.847539669	0.387751023			
O	0.811088756	0.320496050	0.390592603			
O	0.822068857	0.827481413	0.395867419			
O	0.018475950	0.333333700	0.176354340	0	0	0
O	0.018475850	0.833333790	0.176354340	0	0	0
O	0.518476130	0.333333700	0.176354340	0	0	0
O	0.518476130	0.833333850	0.176354330	0	0	0
O	0.158457167	0.469320233	0.386357950			
O	0.170637240	1.006088017	0.389136776			
O	0.691021438	0.491104562	0.392218456			
O	0.672166367	0.984096078	0.390099973			
O	0.166666490	0.185142860	0.176354340	0	0	0
O	0.166666430	0.685143110	0.176354330	0	0	0

O	0.666666690	0.185142910	0.176354340	0	0	0
O	0.666666690	0.685143110	0.176354340	0	0	0
O	-0.007028252	0.173423630	0.395532409			
O	0.019981233	0.675631075	0.388021585			
O	0.500126280	0.182775347	0.388829172			
O	0.517472059	0.684729369	0.391860921			
O	0.314857240	0.481524230	0.176354330	0	0	0
O	0.314857300	0.981524470	0.176354340	0	0	0
O	0.814857420	0.481524230	0.176354340	0	0	0
O	0.814857480	0.981524470	0.176354340	0	0	0
H	0.089489461	0.102871854	0.460718930			
H	0.530035143	-0.025307353	0.465385124			
H	0.619465357	0.612688508	0.482261677			
H	0.265692864	0.026460011	0.481332789			
H	0.783429525	0.030182486	0.486110128			
H	0.787090972	0.525416874	0.489221407			
H	0.964043049	0.383896416	0.468150706			
H	1.021267972	0.690542926	0.479740343			
I	0.481524259	0.314857274	0.035270844	0	0	0
I	0.481524289	0.814857364	0.035270834	0	0	0
I	0.981524408	0.314857274	0.035270840	0	0	0
I	0.981524467	0.814857364	0.035270844	0	0	0
I	0.333333671	0.018475870	0.035270840	0	0	0
I	0.333333641	0.518476009	0.035270834	0	0	0
I	0.833333790	0.018475881	0.035270844	0	0	0
I	0.833333790	0.518476069	0.035270844	0	0	0

Model ITO_{100v}

In	0.000000000	0.000000000	0.151330020	0	0	0
In	0.000000000	0.500000120	0.151330020	0	0	0
In	0.500000240	0.000000000	0.151330020	0	0	0
In	0.500000180	0.500000120	0.151330020	0	0	0
In	-0.003347999	-0.001602002	0.273827576			
In	0.000315649	0.498327952	0.274022117			
In	0.500267275	-0.001034779	0.274797198			
In	0.500911602	0.503488296	0.274821117			
In	0.000000000	0.000000000	0.060295180	0	0	0
In	0.000000000	0.500000180	0.060295200	0	0	0
In	0.500000180	0.000000000	0.060295200	0	0	0
In	0.500000120	0.500000180	0.060295200	0	0	0
In	-0.009965950	-0.005908658	0.365143527			
In	0.001406514	0.497065704	0.364600229			
In	0.502622504	0.001714277	0.367206915			
In	0.503246103	0.505653798	0.367637302			
Sn	0.332016440	0.168000106	0.292392626			
In	0.331635865	0.666035288	0.297400795			
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Model ITO_{0v}-bcc

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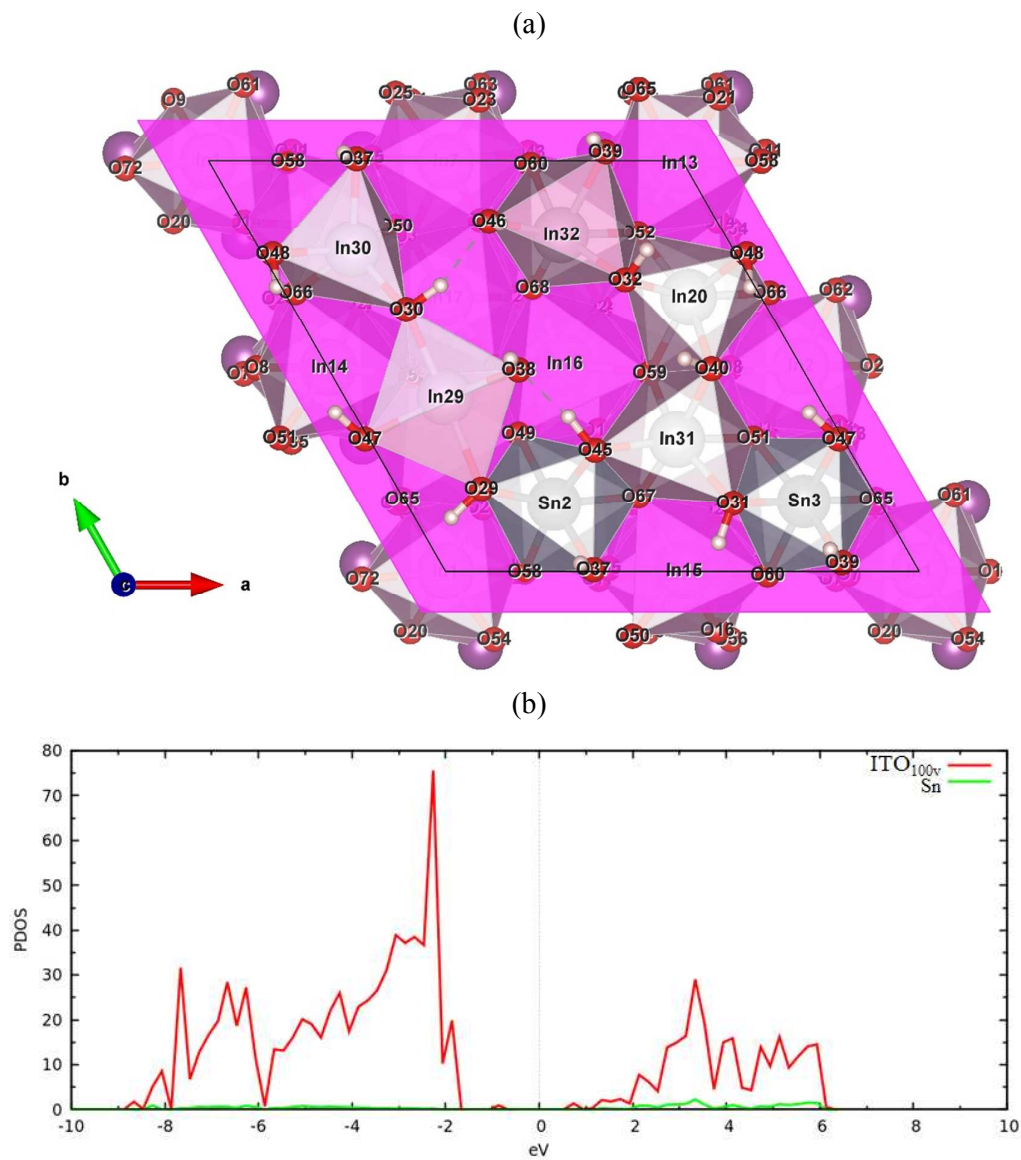


Figure S1: Surface structure (a) and PDOS (b) of ITO_{100v} . The Fermi energy is set to zero.

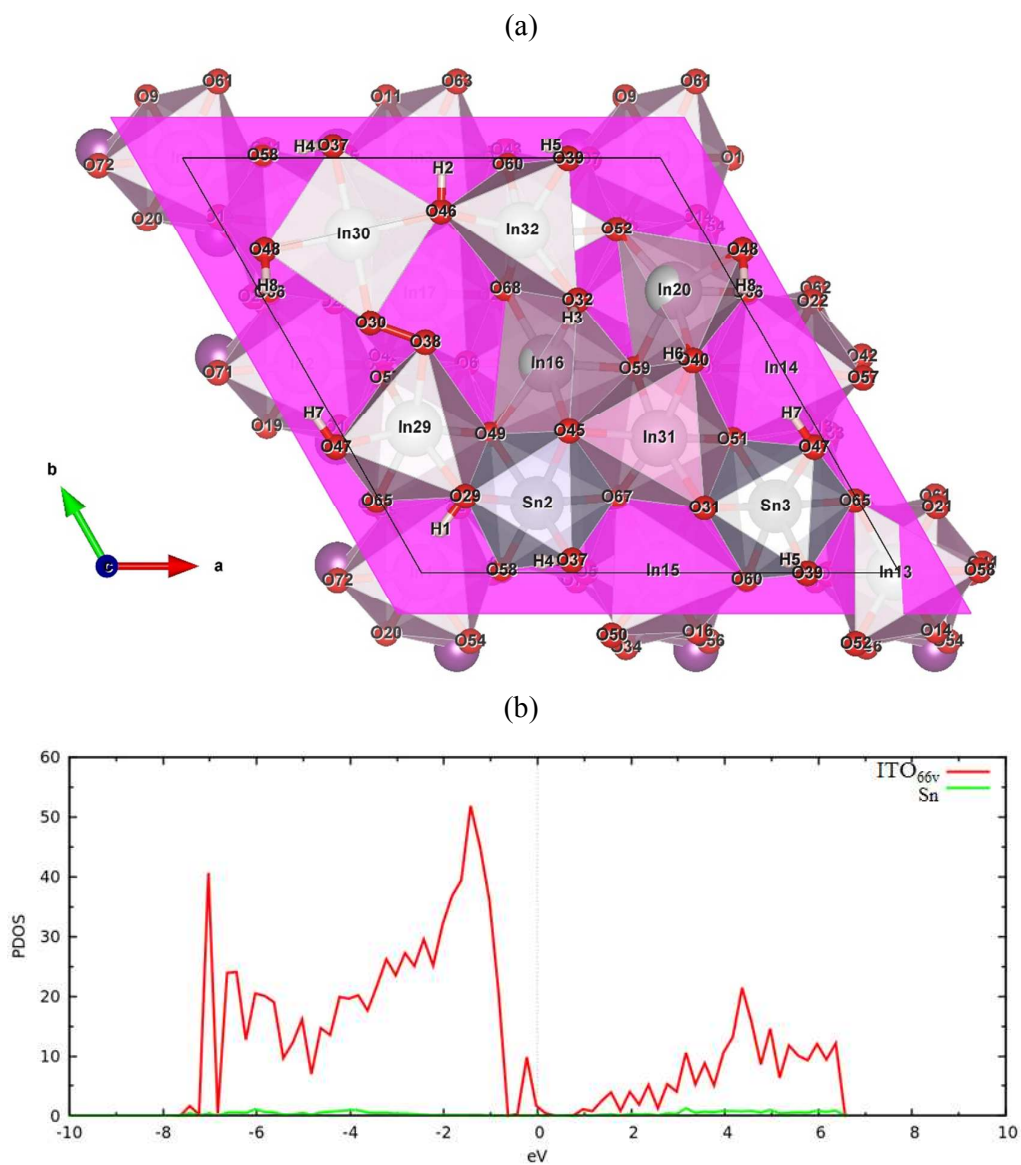


Figure S2: Surface structure (a) and PDOS (b) of ITO_{66v}. The Fermi energy is set to zero.

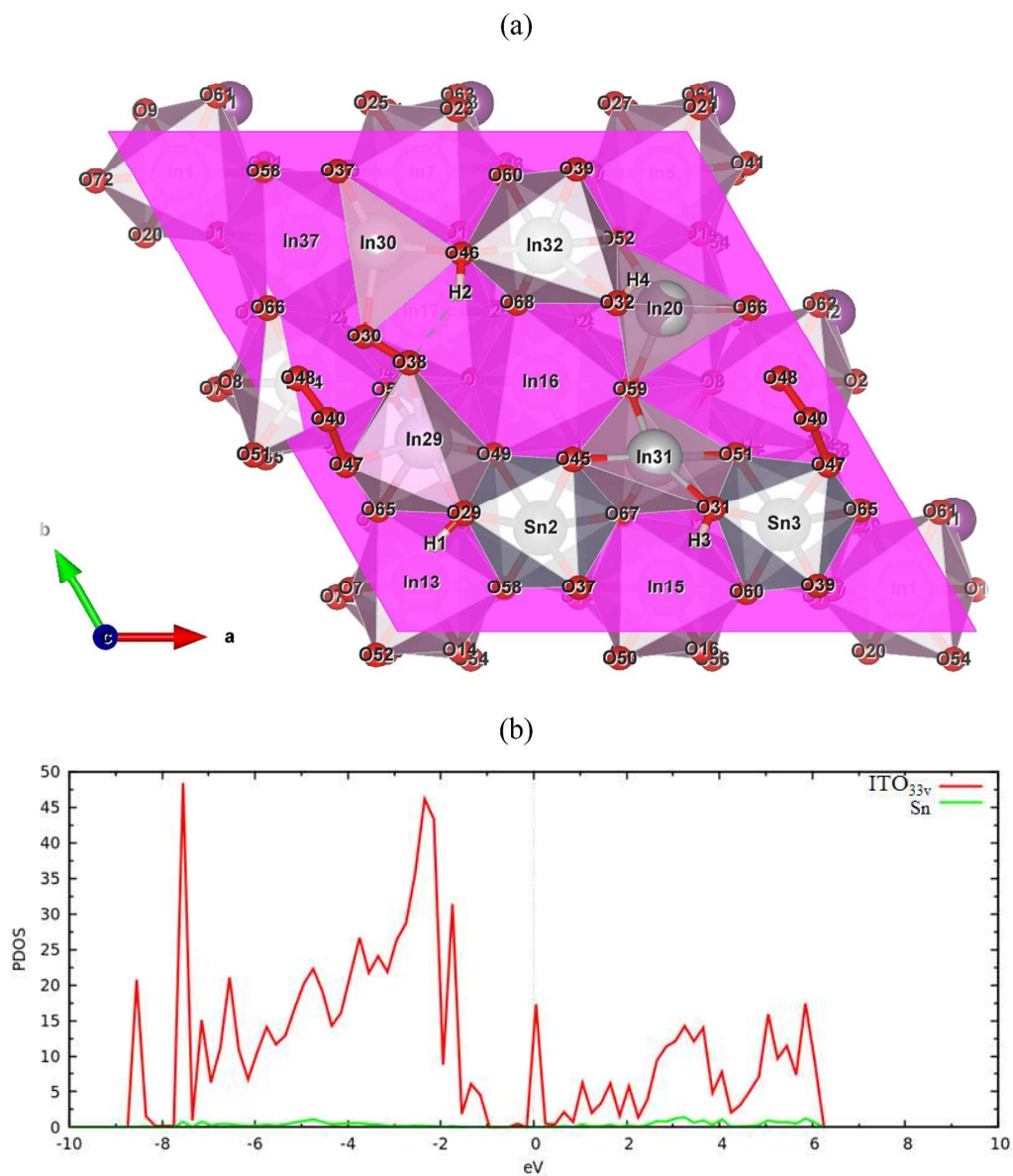


Figure S3: Surface structure (a) and PDOS (b) of ITO_{33v} . The Fermi energy is set to zero.

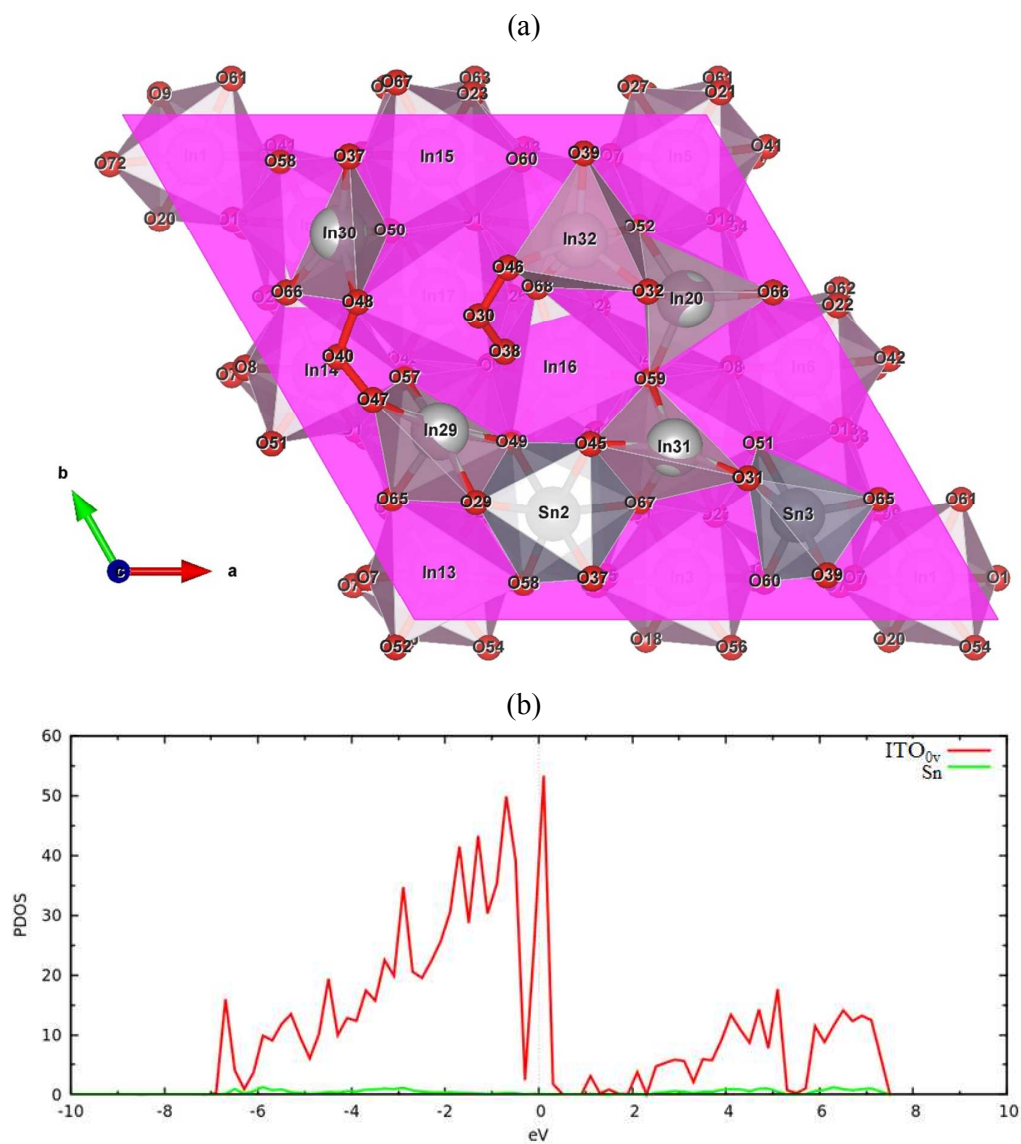


Figure S4: Surface structure (a) and PDOS (b) of ITO_{0v} . The Fermi energy is set to zero.

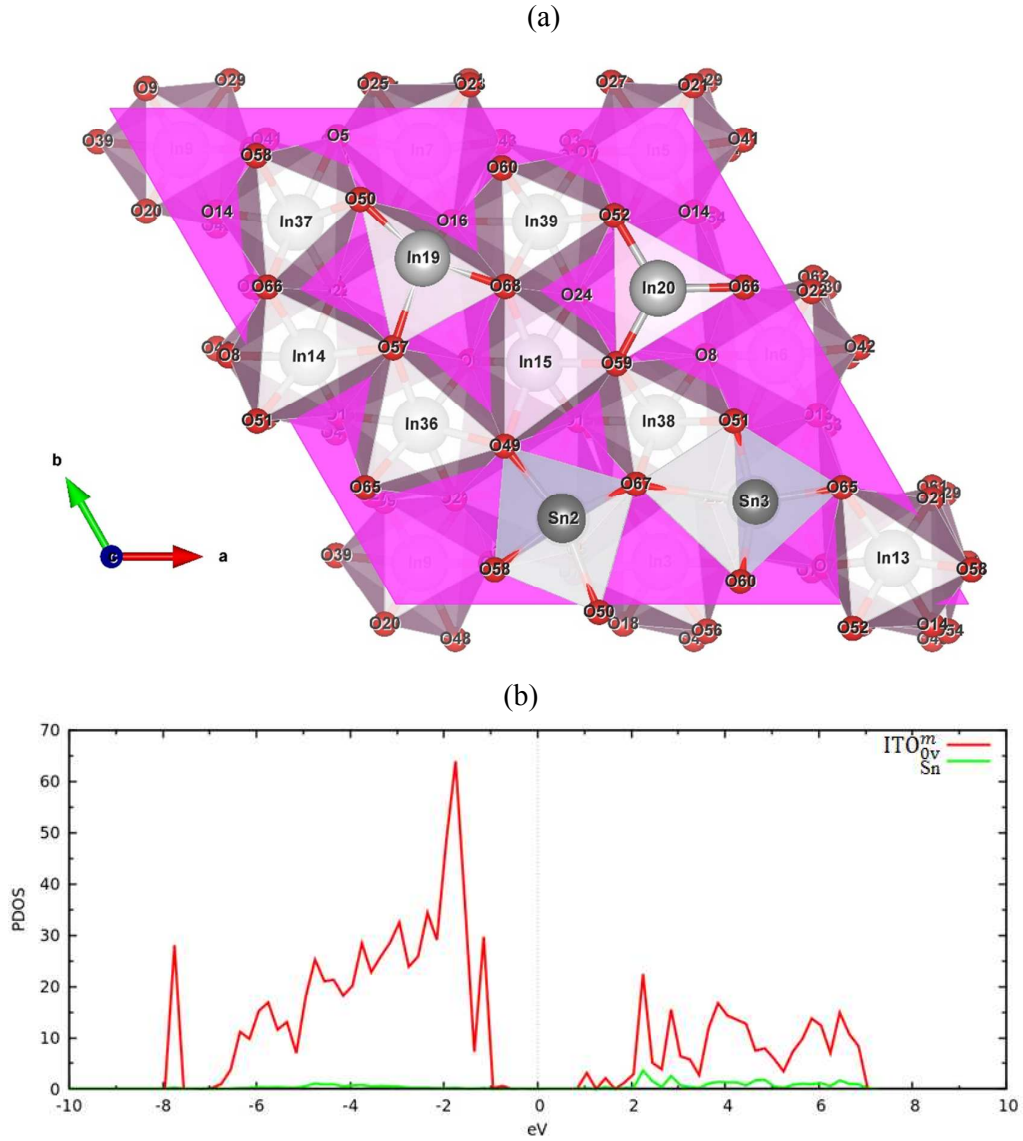


Figure S5: Surface structure (a) and PDOS (b) of ITO_{0v}^m . The Fermi energy is set to zero.

Table S1. The calculated work functions ϕ (in eV) for all IO and ITO models considered in this paper.

IO	IO_0	IO_0^m	IO_{100}	IO_{66}	IO_{33}	$\text{IO}_0\text{-bcc}$
	8.4135	6.3152	4.6669	5.8506	6.4757	5.7197
ITO	ITO_0	ITO_0^m	ITO_{100}	ITO_{66}	ITO_{33}	$\text{ITO}_0\text{-bcc}$
	7.4297	5.1195	2.9238	5.4523	7.3948	4.8264
ITO	ITO_{0v}	ITO_{0v}^m	ITO_{100v}	ITO_{66v}	ITO_{33v}	$\text{ITO}_{0v}\text{-bcc}$
	7.4307	5.7028	4.1385	5.5073	5.3730	5.5762

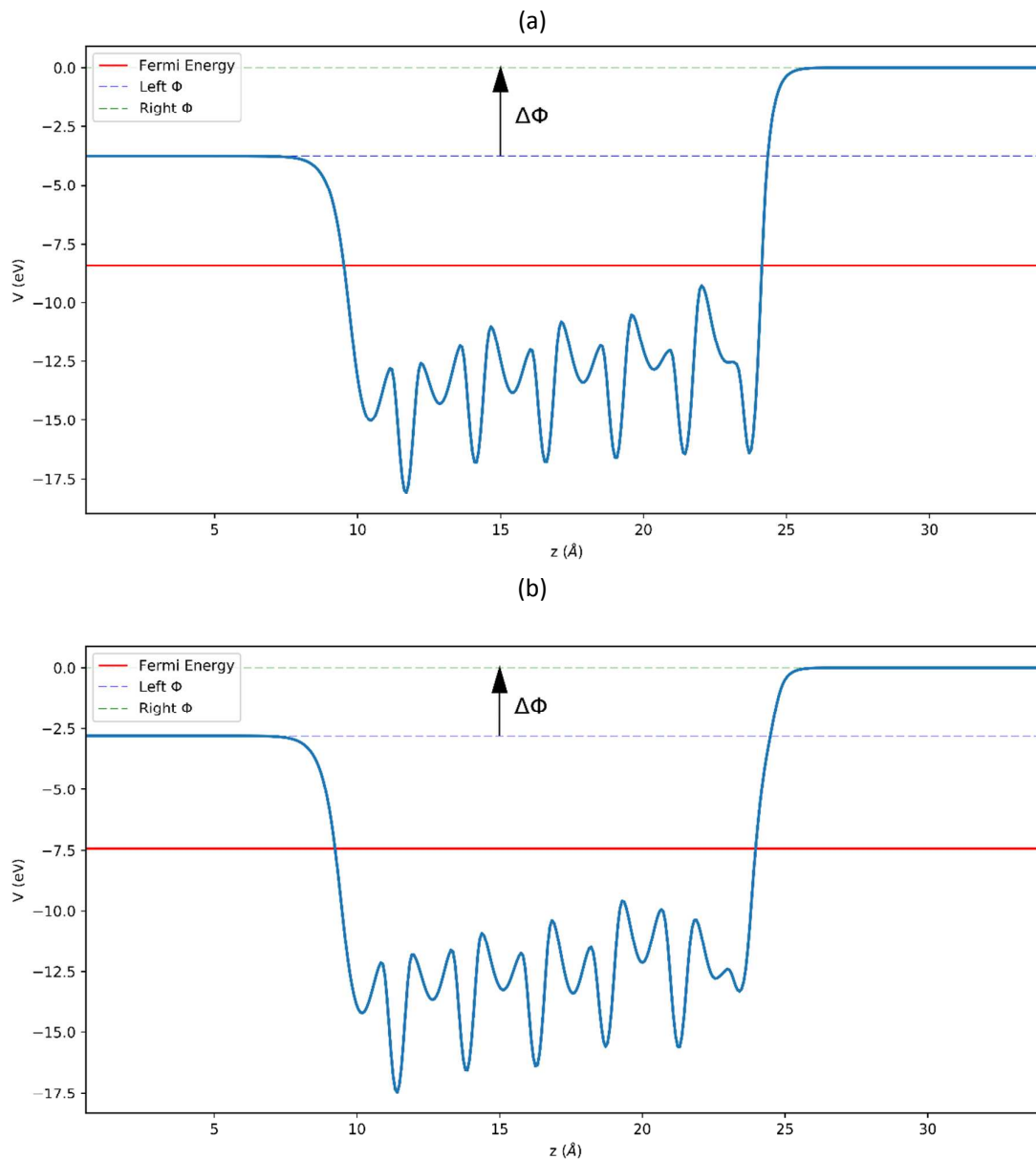


Figure S6: Surface-averaged electrostatic potential computed by DFT as a function of distance from the surface. The surface atoms are located at z values around 15 Angstroms. (a) IO_0 -dipole and (b) ITO_0 -dipole, where the vertical arrow shows the amplitude of the work-function change due to dipole correction.

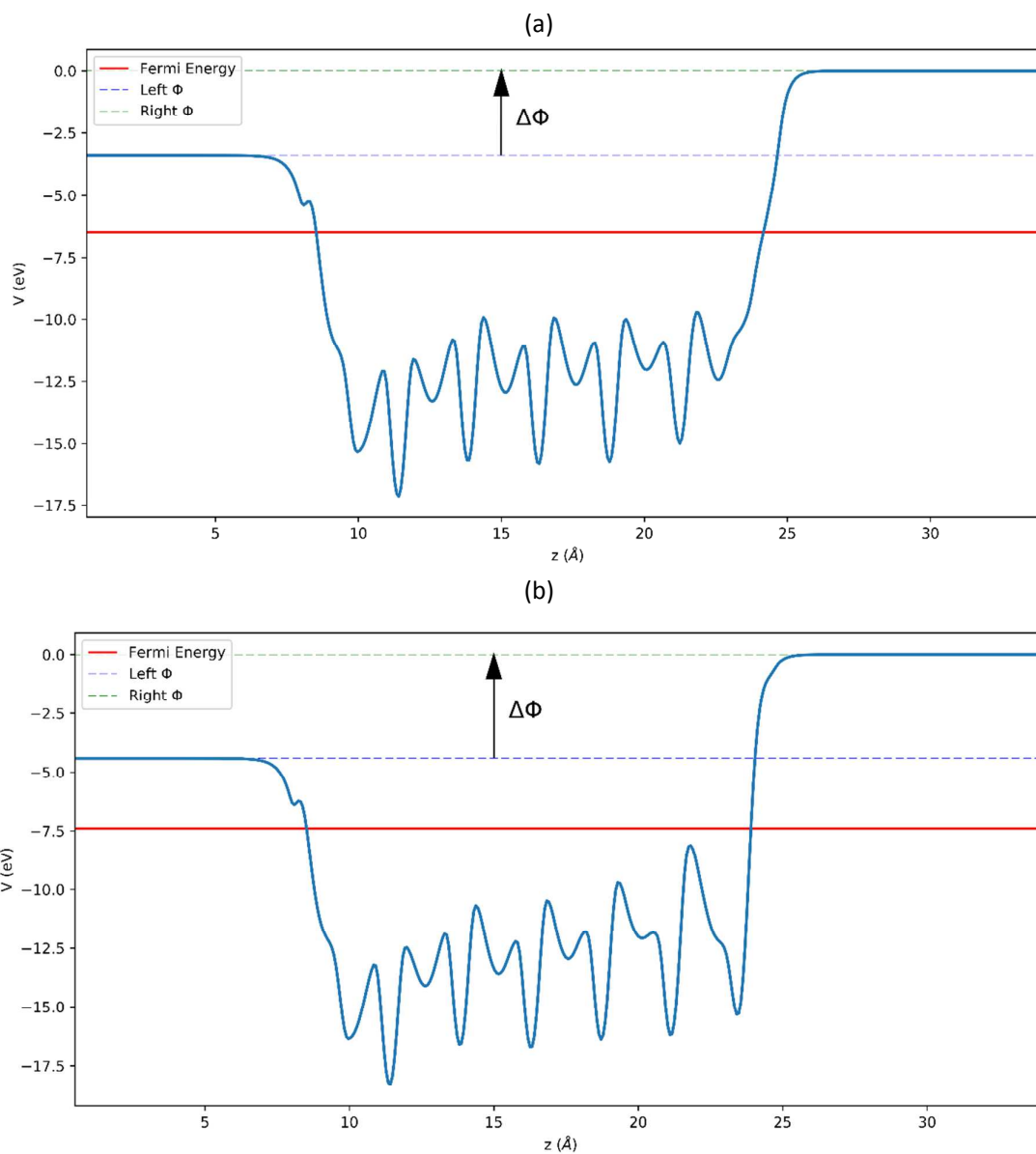


Figure S7: Surface-averaged electrostatic potential computed by DFT as a function of distance from the surface. The surface atoms are located at z values around 15 Angstroms. (a) IO_{33} -dipole and (b) ITO_{33} -dipole, where the vertical arrow shows the amplitude of the work-function change due to dipole correction.

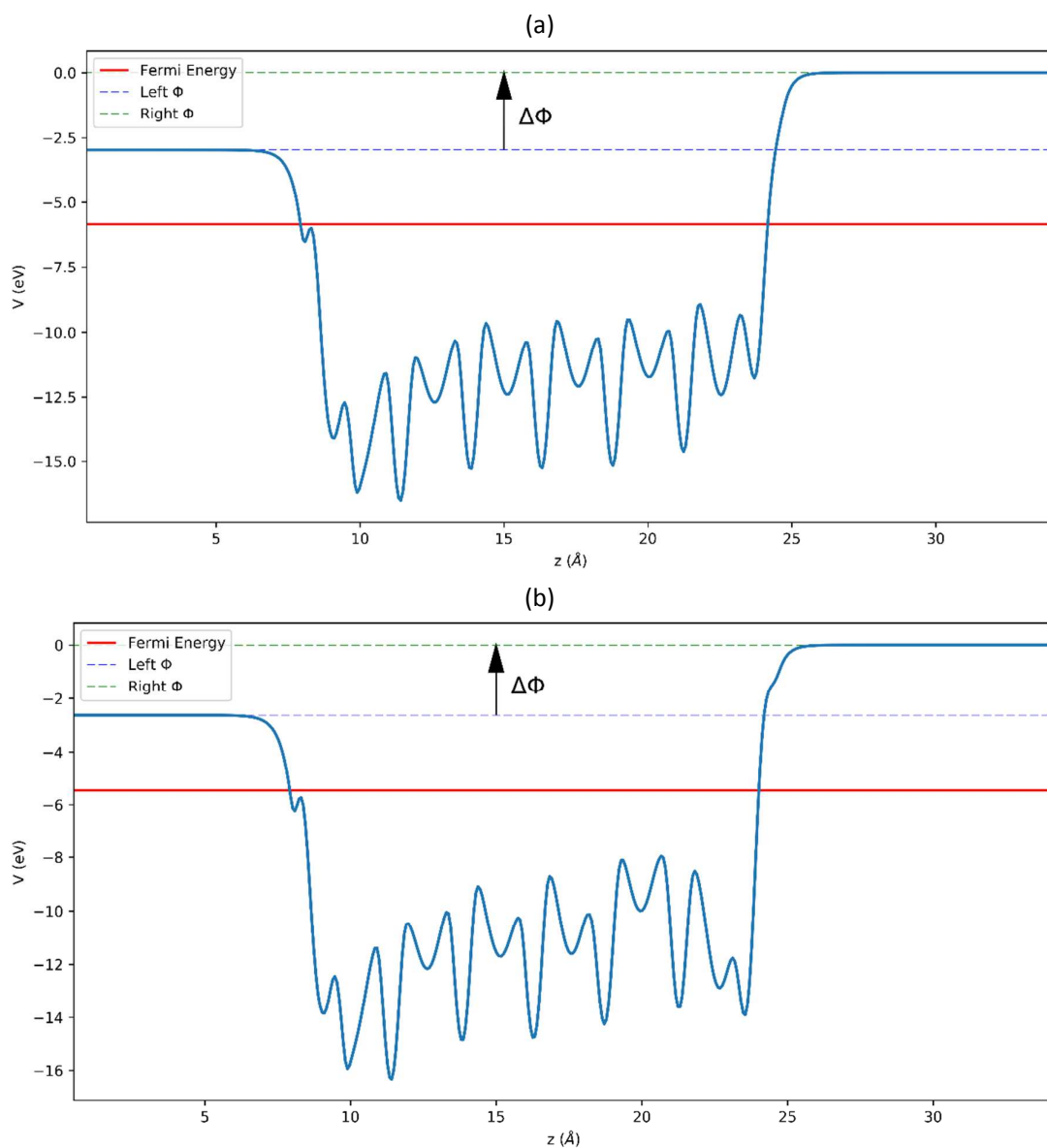


Figure S8: Surface-averaged electrostatic potential computed by DFT as a function of distance from the surface. The surface atoms are located at z values around 15 Angstroms. (a) IO₆₆-dipole and (b) ITO₆₆-dipole, where the vertical arrow shows the amplitude of the work-function change due to dipole correction.

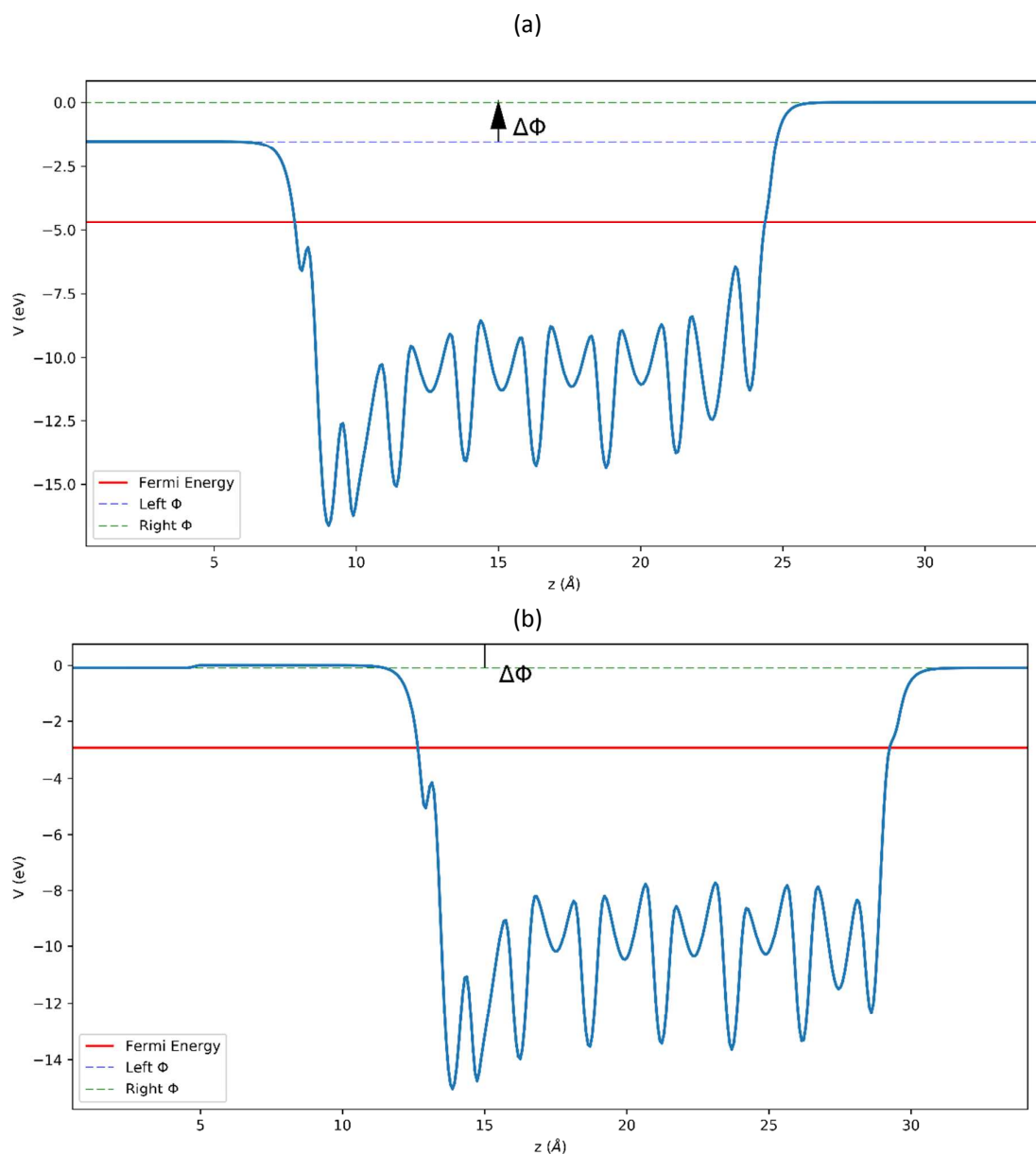


Figure S9: Surface-averaged electrostatic potential computed by DFT as a function of distance from the surface. The surface atoms are located at z values around 15 Å. (a) IO₁₀₀-dipole and (b) ITO₁₀₀-dipole, where the vertical arrow shows the amplitude of the work-function change due to dipole correction.

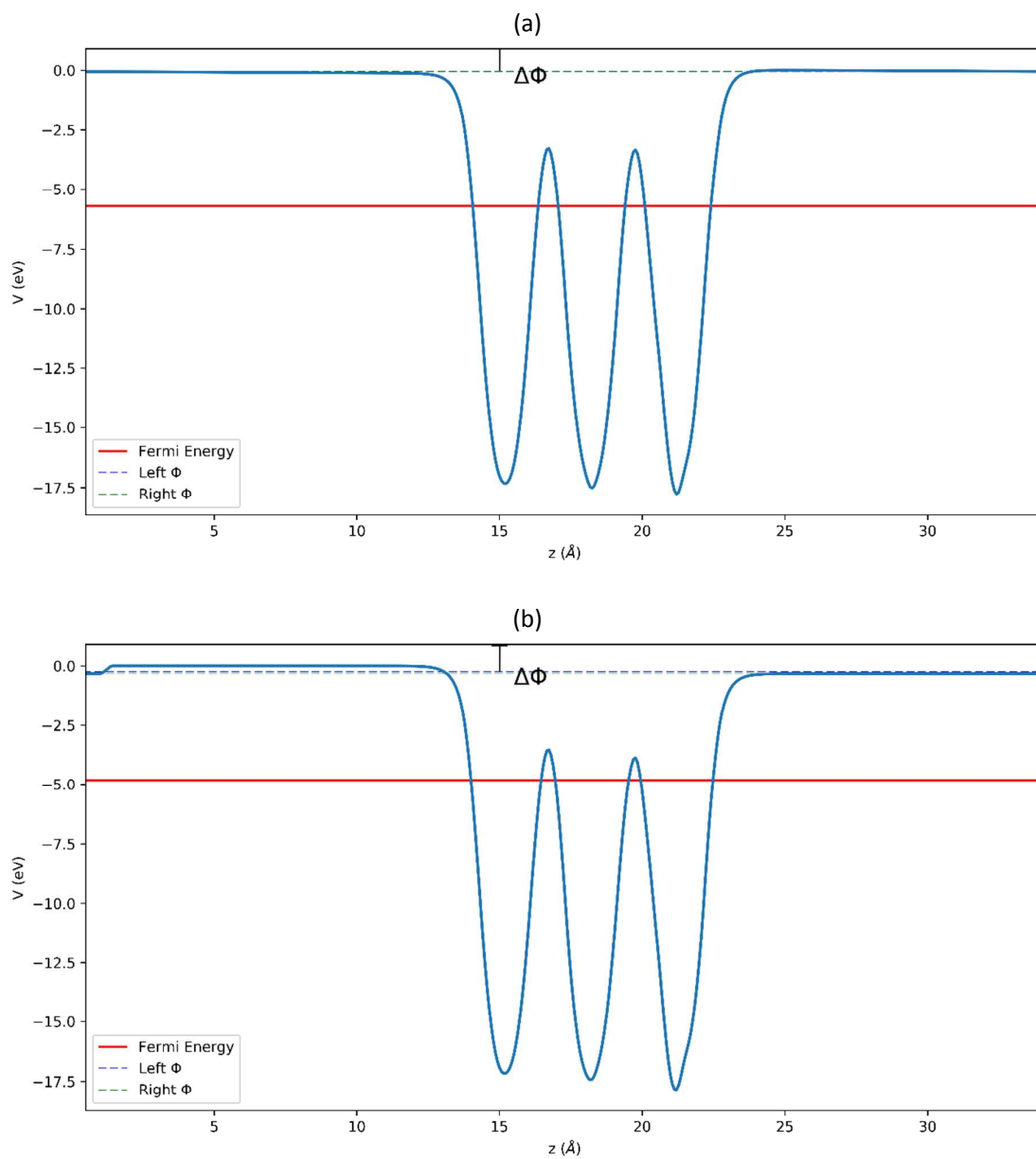


Figure S10: Surface-averaged electrostatic potential computed by DFT as a function of distance from the surface. The surface atoms are located at z values around 15 Angstroms. (a) $\text{IO}_0\text{-bcc}$ -dipole and (b) $\text{ITO}_0\text{-bcc}$ -dipole, where the vertical arrow shows the amplitude of the work-function change due to dipole correction.

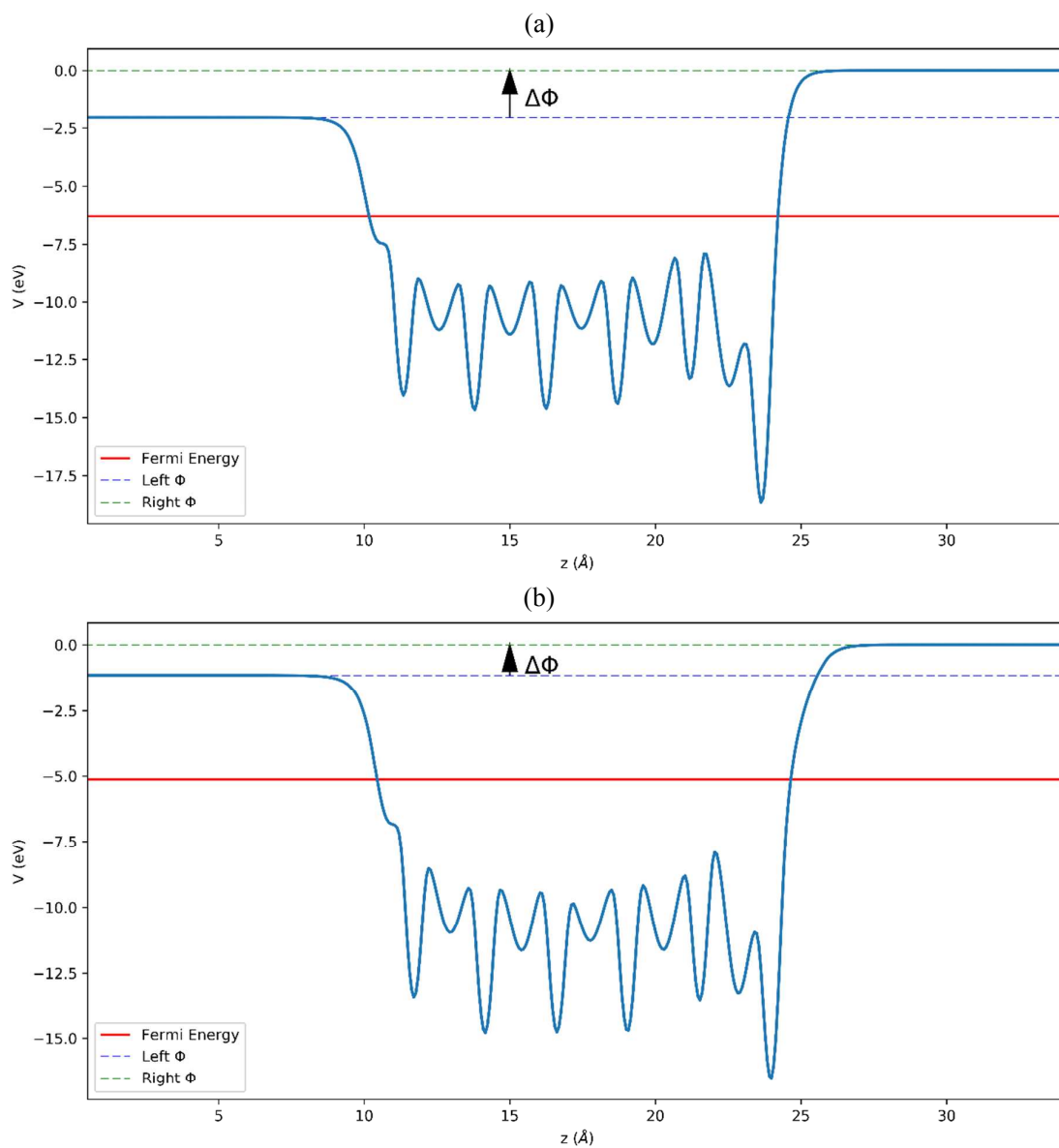


Figure S11: Surface-averaged electrostatic potential computed by DFT as a function of distance from the surface. The surface atoms are located at z values around 15 Å. (a) IO_0^m - dipole and (b) ITO_0^m - dipole, where the vertical arrow shows the amplitude of the work-function change due to dipole correction.

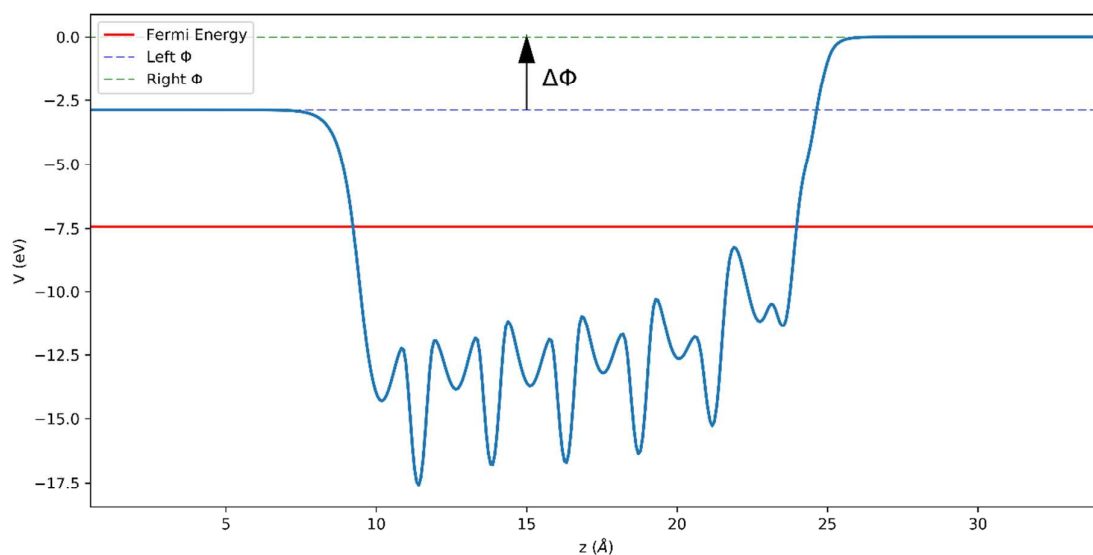


Figure S12: Surface-averaged electrostatic potential computed by DFT as a function of distance from the surface for ITO_{0v} - dipole. The surface atoms are located at z values around 15 Angstroms. The vertical arrow shows the amplitude of the work-function change due to dipole correction.

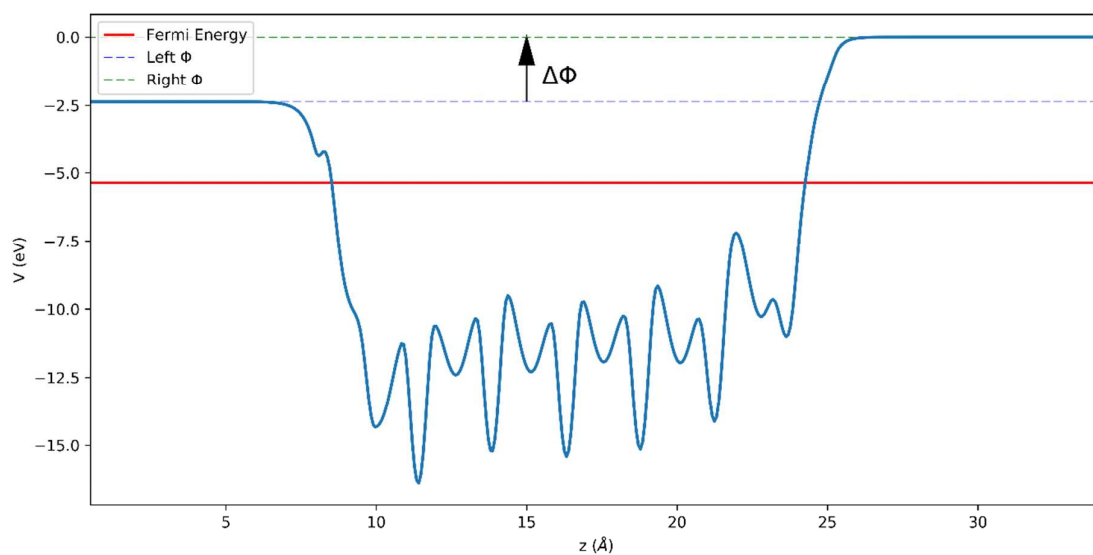


Figure S13: Surface-averaged electrostatic potential computed by DFT as a function of distance from the surface for ITO_{33v} - dipole. The surface atoms are located at z values around 15 Angstroms. The vertical arrow shows the amplitude of the work-function change due to dipole correction.

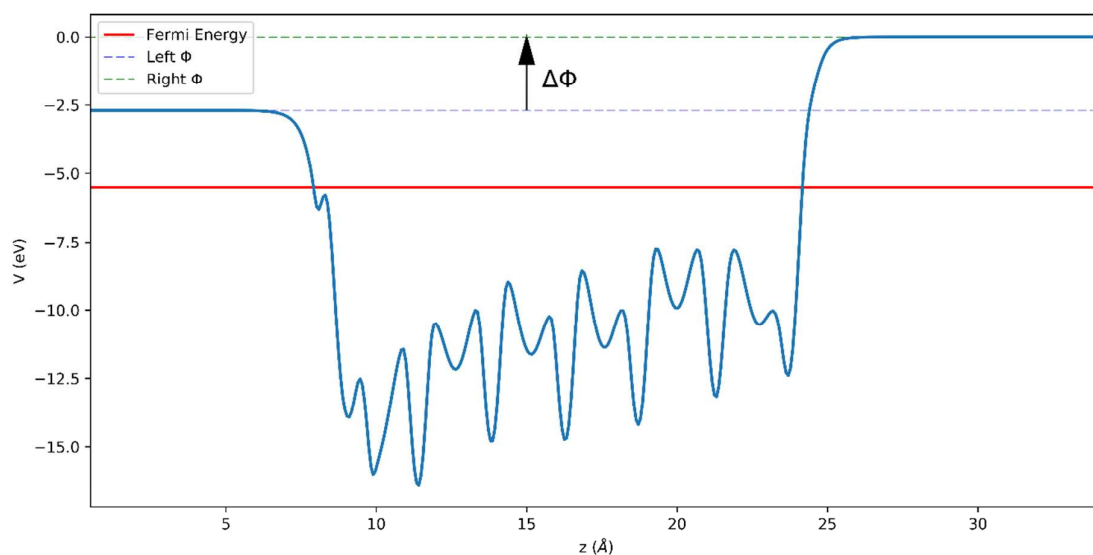


Figure S14: Surface-averaged electrostatic potential computed by DFT as a function of distance from the surface for ITO_{66v} - dipole. The surface atoms are located at z values around 15 Angstroms. The vertical arrow shows the amplitude of the work-function change due to dipole correction.

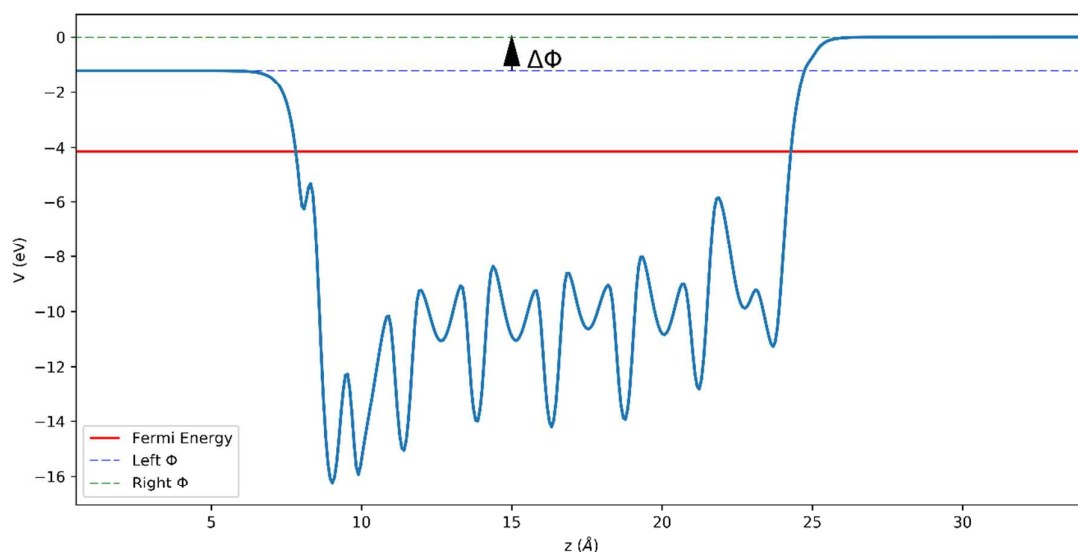


Figure S15: Surface-averaged electrostatic potential computed by DFT as a function of distance from the surface for ITO_{100v} - dipole. The surface atoms are located at z values around 15 Angstroms. The vertical arrow shows the amplitude of the work-function change due to dipole correction.

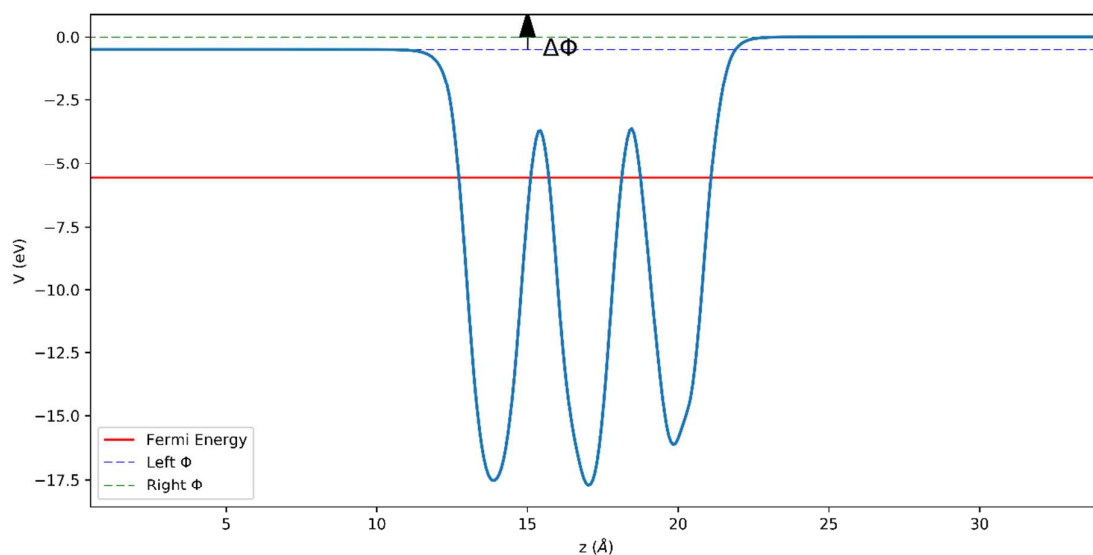


Figure S16: Surface-averaged electrostatic potential computed by DFT as a function of distance from the surface for $\text{ITO}_{0V}\text{-bcc}$ - dipole. The surface atoms are located at z values around 15 Angstroms. The vertical arrow shows the amplitude of the work-function change due to dipole correction.

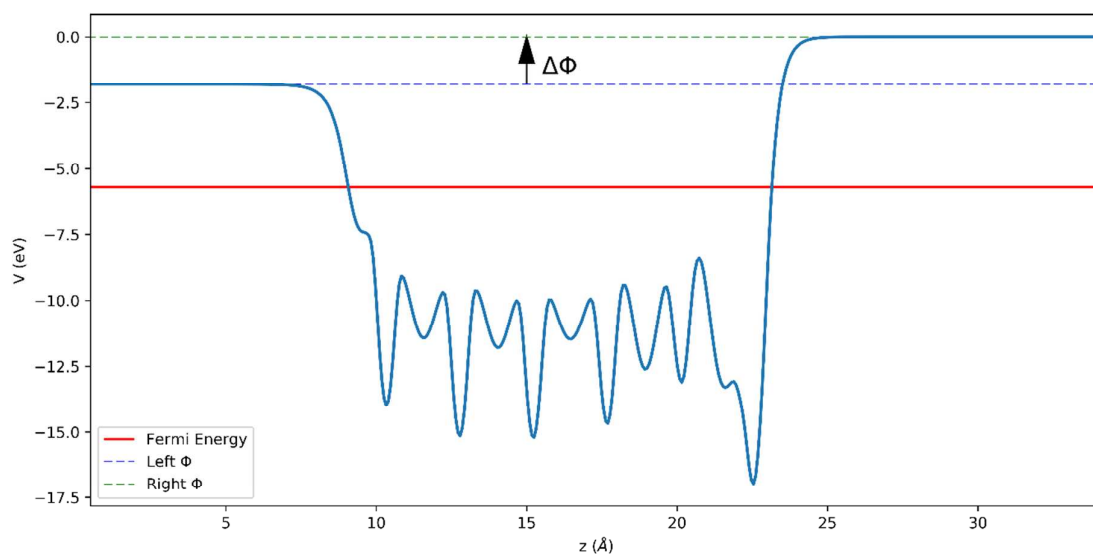


Figure S17: Surface-averaged electrostatic potential computed by DFT as a function of distance from the surface for ITO_{0V}^m - dipole. The surface atoms are located at z values around 15 Angstroms. The vertical arrow shows the amplitude of the work-function change due to dipole correction.