

Supplementary Information

Vacancy formation, stability, and electronic properties of nickel on equimolar ceria-zirconia mixed oxide (111) catalyst

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DFT optimization

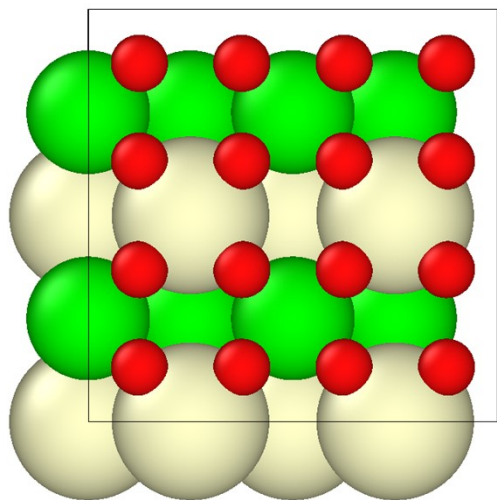
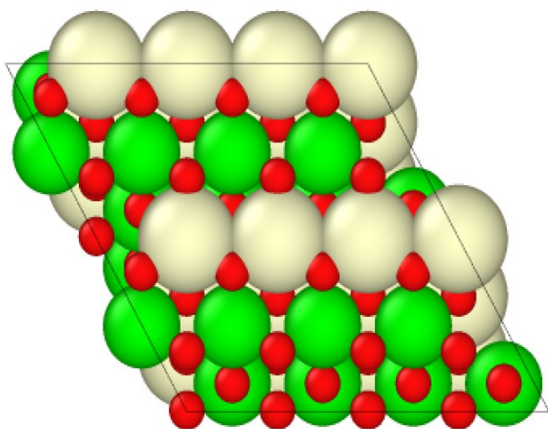


Figure S1. Bulk CZO structure in the cubic-fluorite unit cell with a Ce:Zr ratio of 1:1 (O, red; Ce, yellow; Zr, green).

a



b

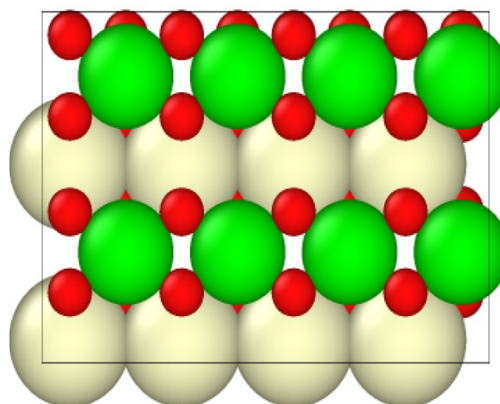
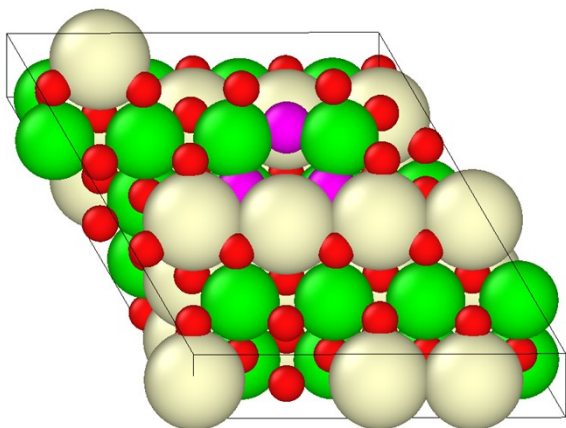


Figure S2. View along the surface normal of the carved out (a) (111) surface, (b) (110) surface. (O, red; Ce, yellow; Zr, green).

a



b

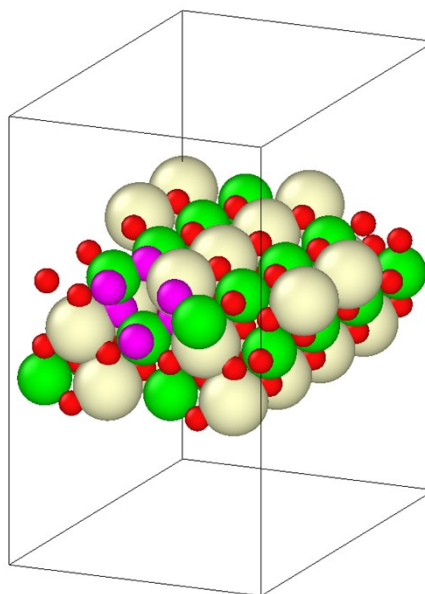


Figure S3. Oxygen atoms comprising the first coordination shell of a (a) surface vacancy and (b) subsurface vacancy highlighted in purple. (O, red and purple; Ce, yellow; Zr, green).

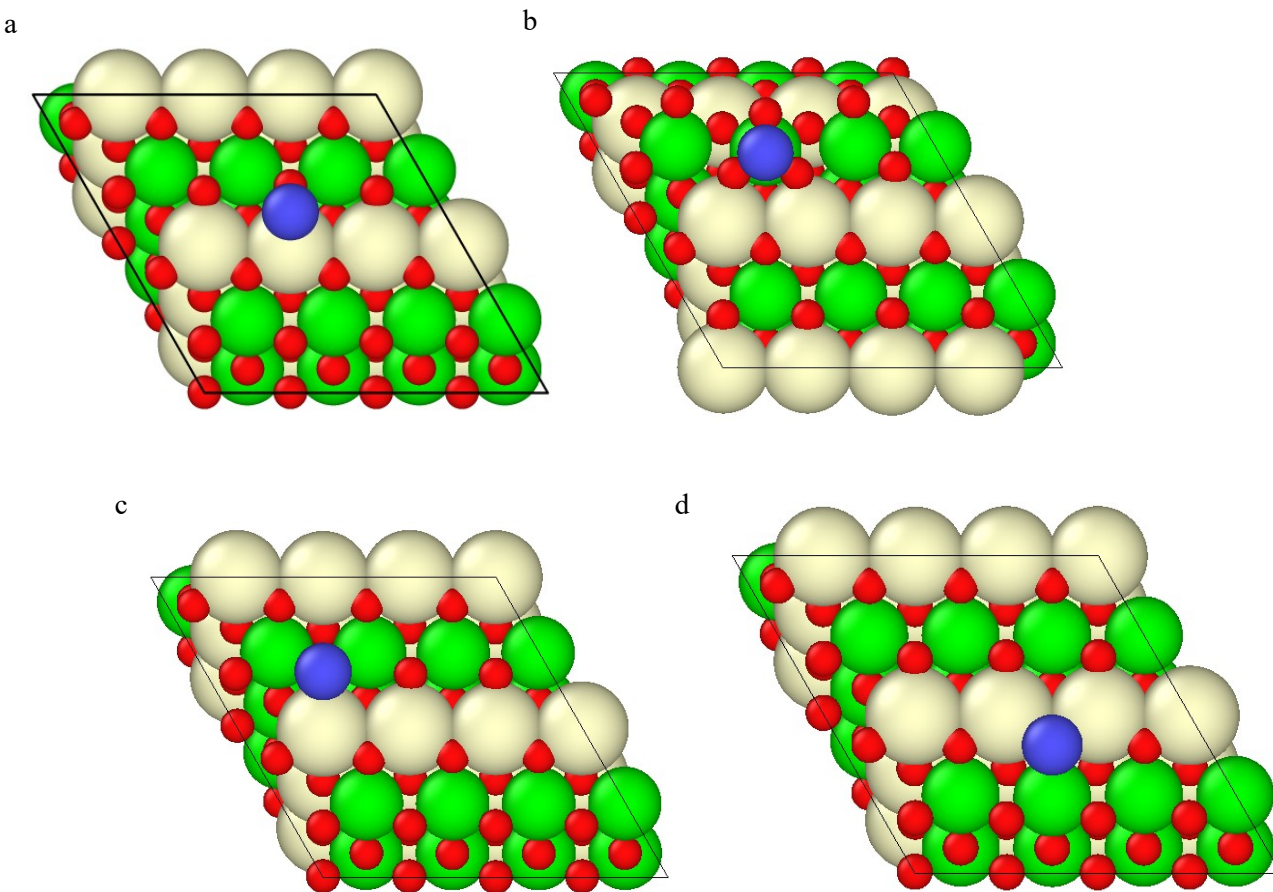
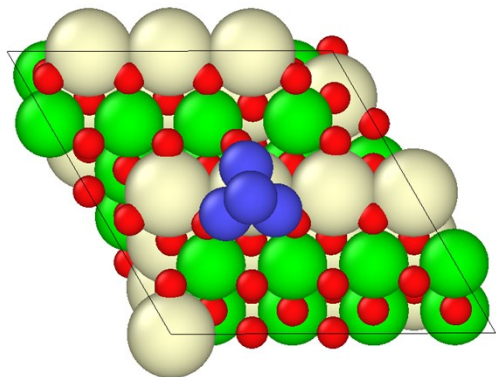
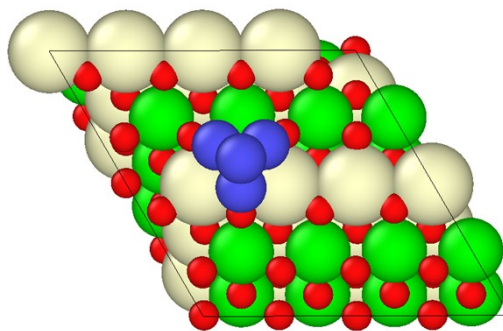


Figure S4. Nickel binding sites on the pristine CZO(111) surface. (a) Ni_{Ce} , (b) Ni_{Zr} , (c) $Ni_{O_{Zr}}$, and (d) $Ni_{O_{Ce}}$. (O, red; Ce, yellow; Zr, green; Ni, blue).

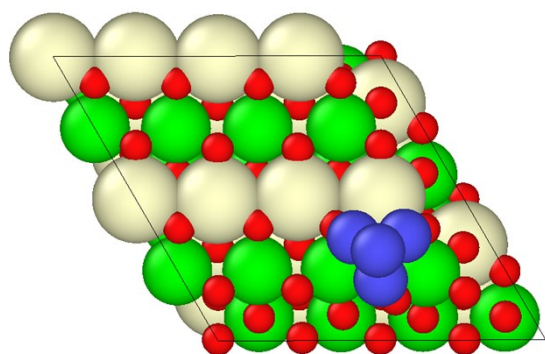
a



b



c



d

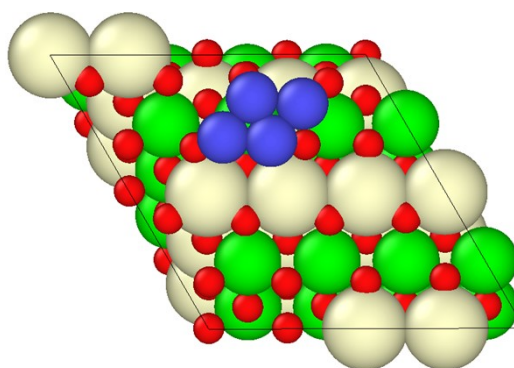


Figure S5. Nickel cluster binding sites on the pristine CZO(111) surface. (a) Ni_4Ce , (b) Ni_4Ce_2Zr , (c) Ni_4Zr_2Ce , and (d) planar Ni_4 . (O, red; Ce, yellow; Zr, green; Ni, blue).

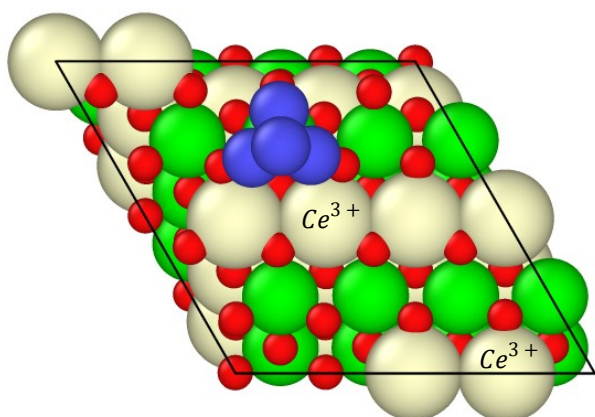


Figure S6. Ni_4 cluster binding on the pristine CZO(111) surface, with polarons indicated. (O, red; Ce, yellow; Zr, green; Ni, blue).

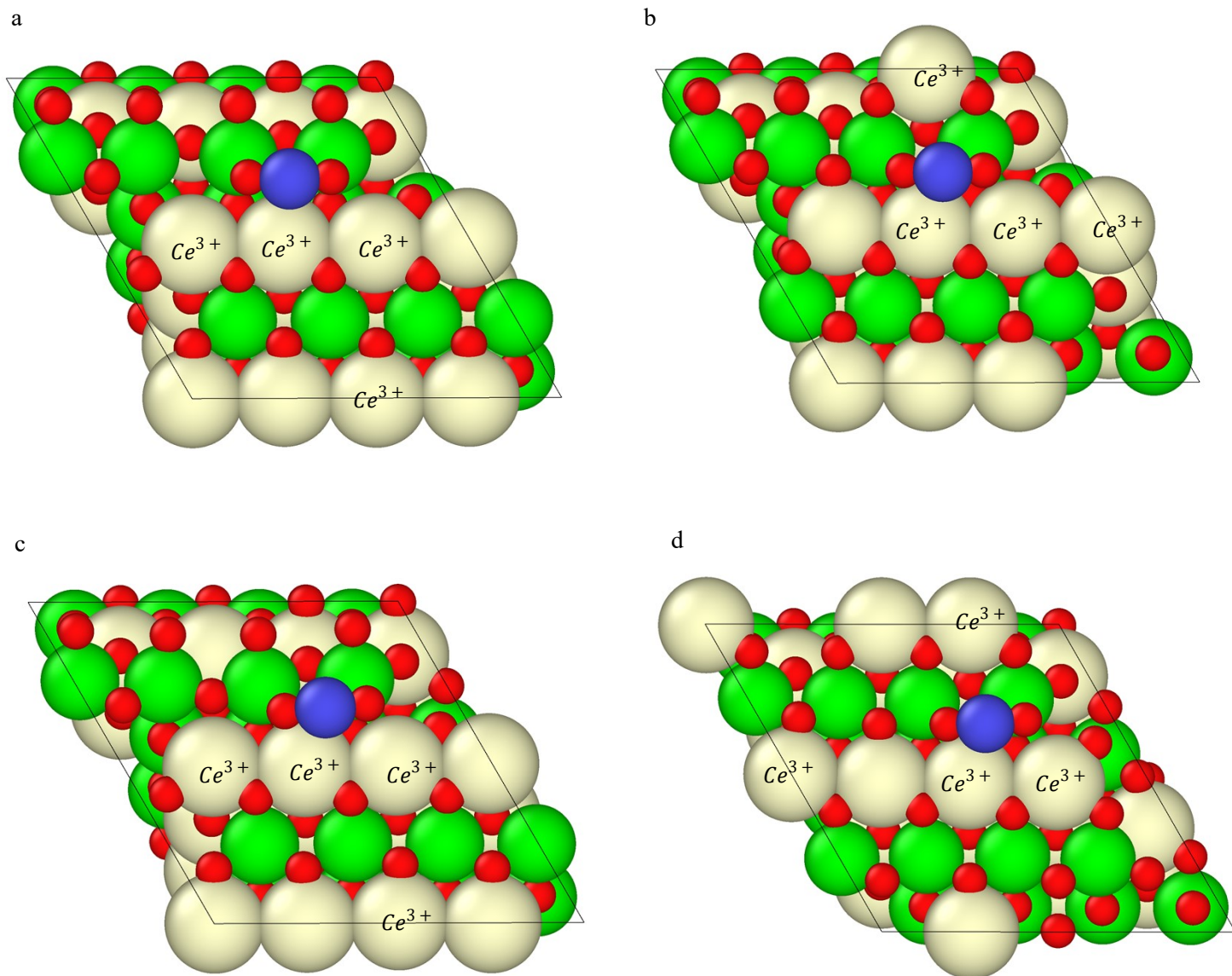


Figure S7. Ni/CZO(111) with an O_{Zr} vacancy at different distances from Ni, polarons indicated. (a) NN – surface, (b) NNN – surface, (c) NN – subsurface, and (d) NNN – subsurface. (O, red; Ce, yellow; Zr, green; Ni, blue)

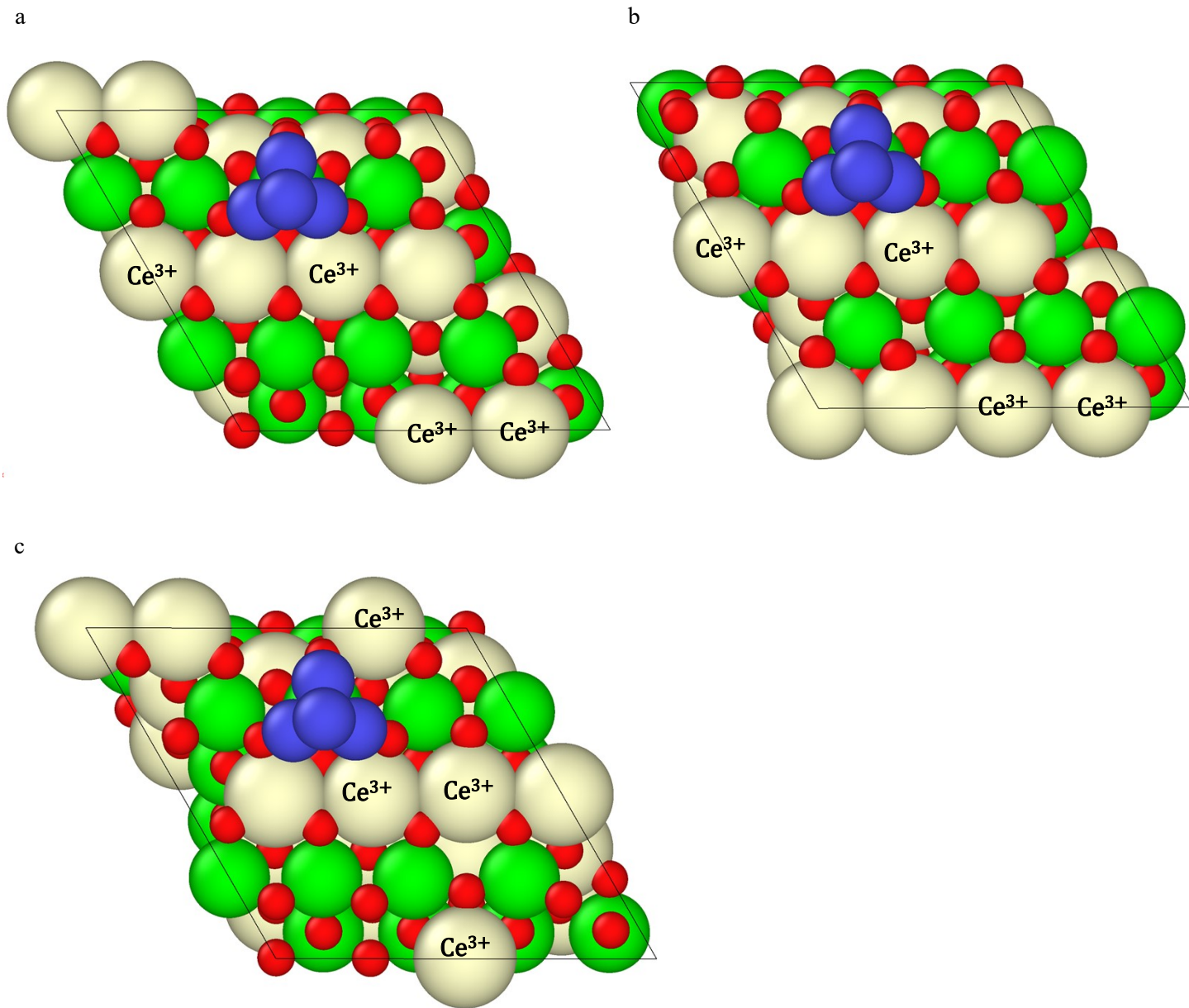


Figure S8. $\text{Ni}_4/\text{CZO}(111)$ with an O_{Zr} vacancy at different distances from Ni, polarons indicated. (a) NNN – surface, (b) NN – subsurface, and (c) NNN – subsurface. (O, red; Ce, yellow; Zr, green; Ni, blue)

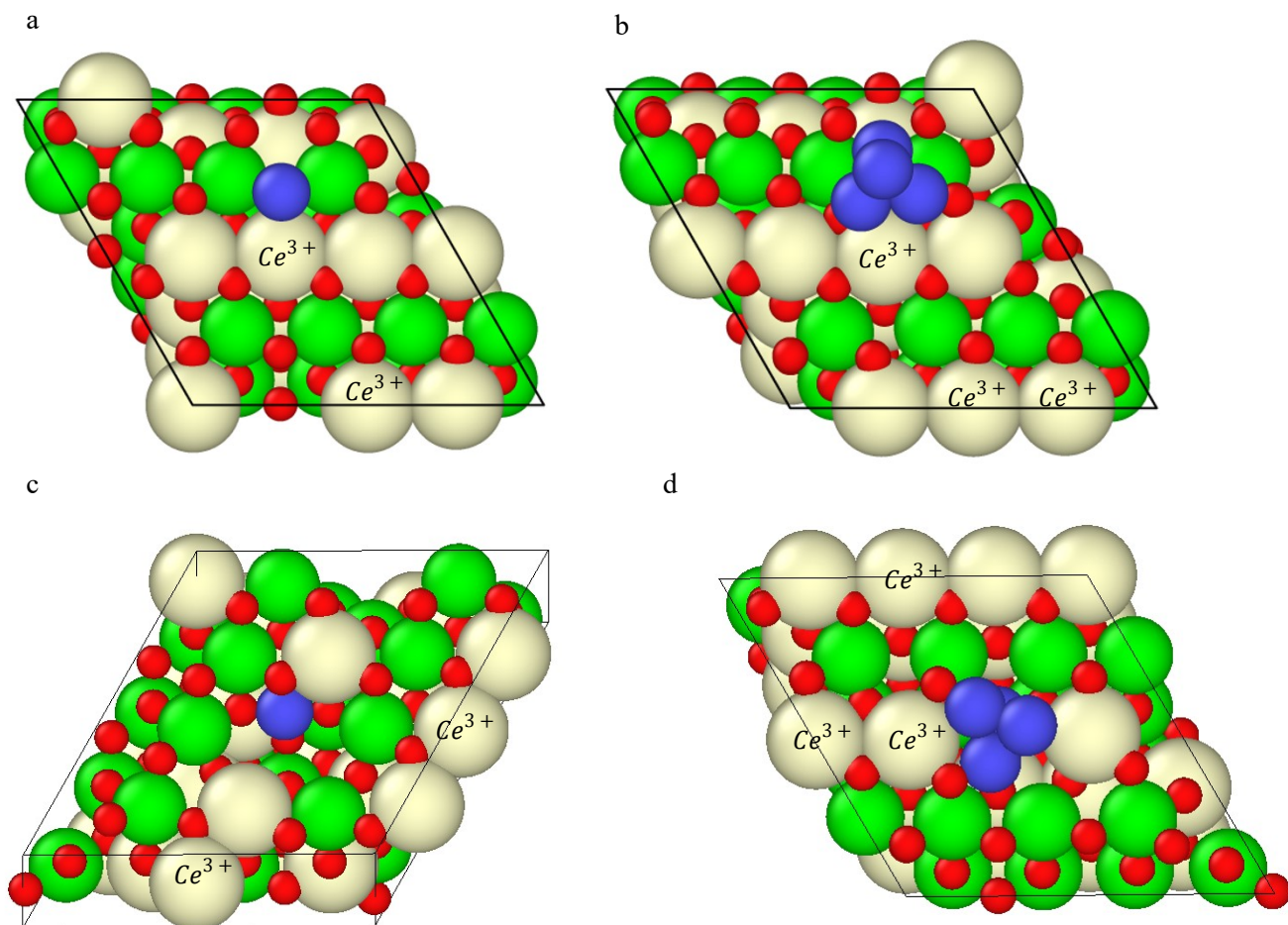


Figure S9. Top-view of (a) $Ni/O_v - CZO$, (b) $Ni_4/O_v - CZO$, (c) $Ni/Ce_v(O_v)_2 - CZO$ and (d) $Ni_4/Ce_v(O_v)_2 - CZO$. (O, red; Ce, yellow; Zr, green; Ni, blue). Polarons indicated.

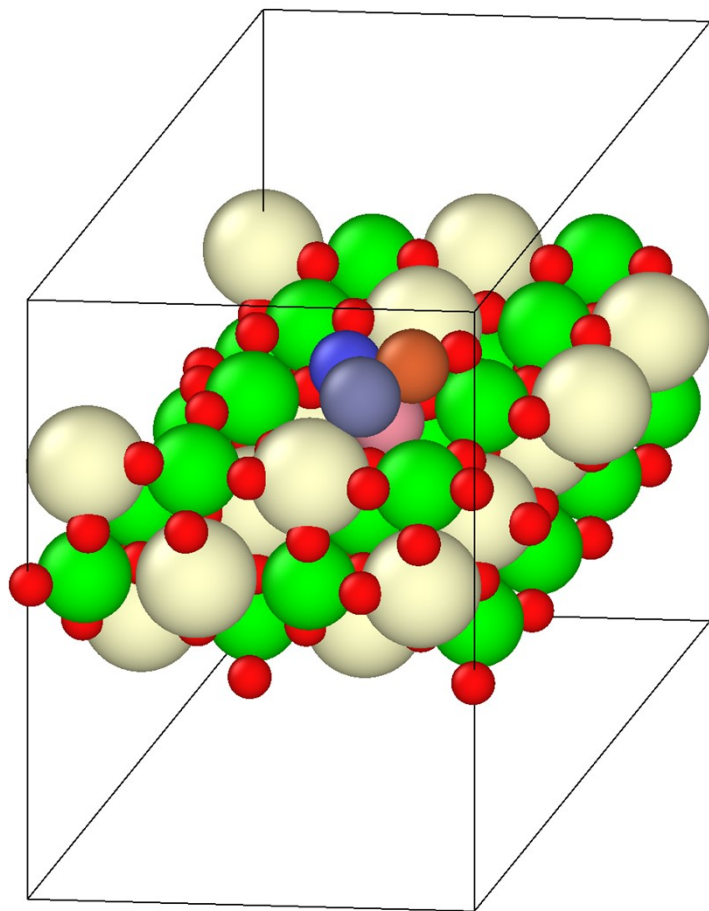


Figure S10. $Ni_4/Ce_v(O_v)_2 - CZO$ slab showing the asymm
(O, red; Ce, yellow; Zr, green; Ni: $q_{Ni} = 0.7$, pink; Ni: q_{Ni}

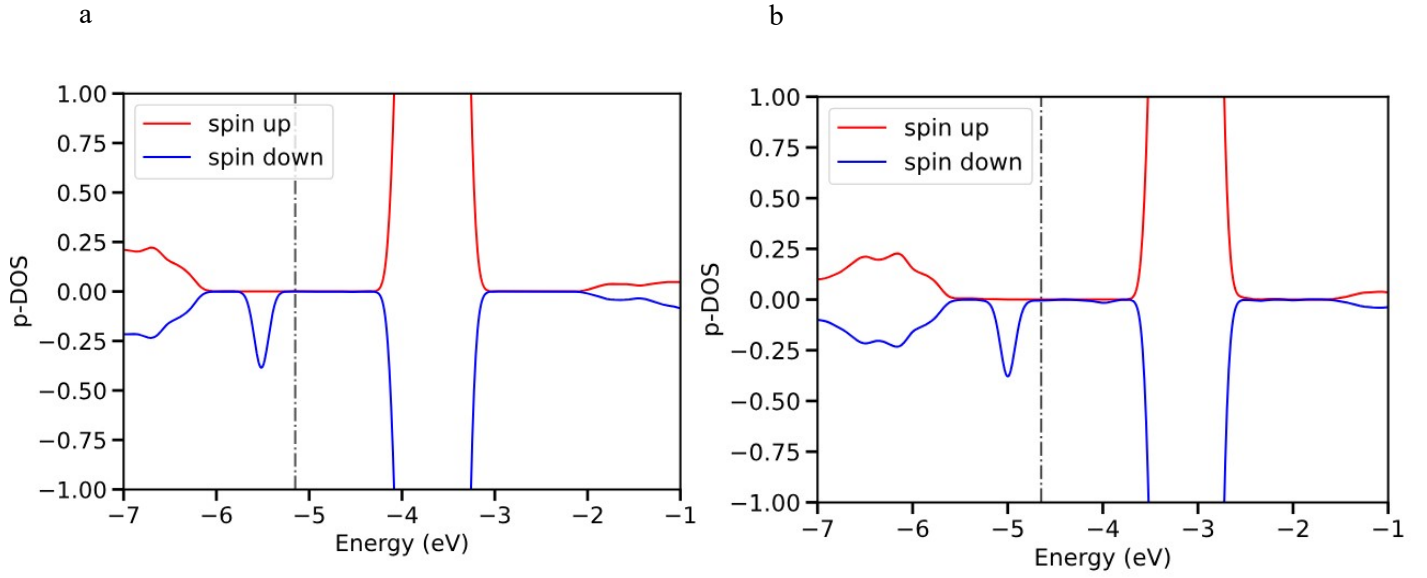


Figure S11. p-DOS on Ce f-states for (a) $Ni/s - CZO$ and (b) $Ni_4/s - CZO$.

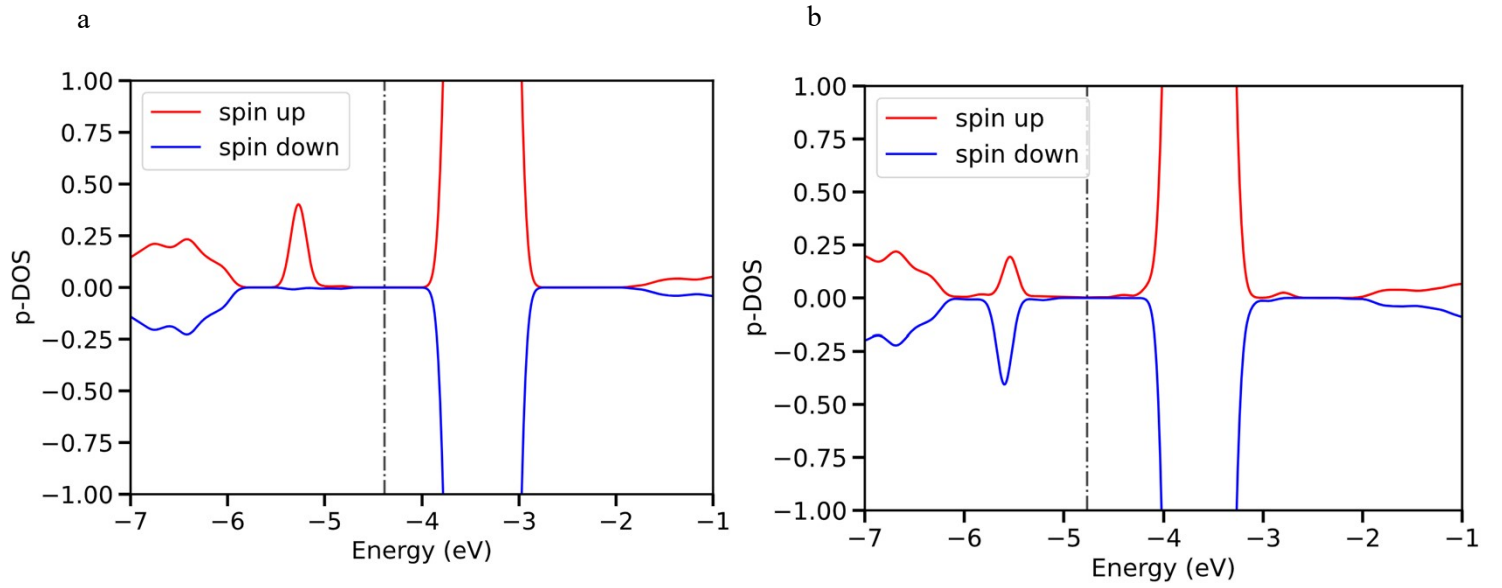


Figure S12. p-DOS on Ce f-states for (a) $Ni/Ce_v(O_v)_2 - CZO$ and (b) $Ni_4/Ce_v(O_v)_2 - CZO$.

Table S1. z-coordinate of the O_{Ce}^s , O_{Ce}^{sub} , O_{Zr}^s , and O_{Zr}^{sub} atoms.

Oxygen atom location	O_{Ce}	O_{Zr}
Surface	19.6 Å	19.5 Å
Subsurface	18.1 Å	18.0 Å

Table S2. Oxygen vacancy formation energy (in eV) dependence on choice of Ce f-orbital's U value.

Energies (in eV)	$U = 3 \text{ eV}$	$U = 6 \text{ eV}$
O_{Zr}^s	2.37	0.95
O_{Zr}^{sub}	2.18	0.74
O_{Ce}^s	2.97	1.6
O_{Ce}^{sub}	2.77	1.33

Table S3. ΔE^{strain} values for the single oxygen vacancies on Ni/CZO.

Oxygen atom removed	$\Delta E^{strain}(\text{eV})$
$Ni - O_{Zr}^{sub} - NN$	-2.7
$Ni - O_{Zr}^{surf} - NNN$	-3.66
$Ni - O_{Zr}^{sub} - NNN$	-2.84
$Ni_4 - O_{Zr}^{sub} - NN$	-3.1
$Ni_4 - O_{Zr}^{sub} - NNN$	-3
$Ni - O_{Zr}^{surf} - NN$	-3.3
$Ni_4 - O_{Zr}^{surf} - NNN$	-3.16

Table S4. Number of reduced cerium atoms and nickel oxidation states on the different CZO supports.

Surface	Number of Ce^{3+} species at the surface (with Ni)	Ni adatom oxidation state	Number of Ce^{3+} species at the surface (with Ni_4)	Ni_4 cluster oxidation state
$s - \text{CZO}$	2	+2	2	+2
$O_{Zr} - Ni - \text{CZO}$	2	0	3	+1

$O_{Zr-NN} - CZO$	4	+2	–	
$O_{Zr-NNN} - CZO$	4	+2	4	+2
$Ce_v(O_v)_2 - CZO$	2	+2	3	+3

Coordinates of all the stable geometries referenced in manuscript

CZO (111)

Ce O Zr

1.0000000000000000

15.0049857511559779 0.0000000000000000 0.0000000000000000

-7.5024928755779881 13.0447800098917028 0.0000000000000000

0.0000000000000000 0.0000000000000000 31.5474089986390567

Ce O Zr

24 96 24

Selective dynamics

Direct

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0.6655744207272837	0.5811488414545680	0.4995533650727875	T	T	T
0.9155744207272837	0.5811488414545680	0.4995533650727875	T	T	T
-0.0015927411716732	0.7468145176566463	0.5939913329828640	T	T	T
0.7484072588283268	0.7468145176566463	0.5939913329828640	T	T	T

CZO(110)

Ce O Zr

1.0000000000000000

15.0049857511559779 0.0000000000000000 0.0000000000000000

0.0000000000000000 10.6714050695478573 0.0000000000000000

0.0000000000000000 0.0000000000000000 33.1293625322614815

Ce O Zr

24 96 24

Selective dynamics

Direct

0.3125000000000000	0.0657280964396918	0.3575778659265509	F	F	F
0.5625000000000000	0.0657280964396918	0.3575778659265509	F	F	F
0.0625000000000000	0.0657280964396918	0.4720447732694801	T	T	T
0.3125000000000000	0.0657280964396918	0.4720447732694801	T	T	T
0.3125000000000000	0.0657280964396918	0.5890294241903098	T	T	T
0.5625000000000000	0.0657280964396918	0.5890294241903098	T	T	T
0.3125000000000000	0.5657280964396918	0.3575778659265509	F	F	F
0.5625000000000000	0.5657280964396918	0.3575778659265509	F	F	F
0.0625000000000000	0.5657280964396918	0.4720447732694801	T	T	T
0.3125000000000000	0.5657280964396918	0.4720447732694801	T	T	T
0.3125000000000000	0.5657280964396918	0.5890294241903098	T	T	T
0.5625000000000000	0.5657280964396918	0.5890294241903098	T	T	T
0.8125000000000000	0.0657280964396918	0.3575778659265509	F	F	F
0.0625000000000000	0.0657280964396918	0.3575778659265509	F	F	F
0.5625000000000000	0.0657280964396918	0.4720447732694801	T	T	T
0.8125000000000000	0.0657280964396918	0.4720447732694801	T	T	T
0.8125000000000000	0.0657280964396918	0.5890294241903098	T	T	T
0.0625000000000000	0.0657280964396918	0.5890294241903098	T	T	T
0.8125000000000000	0.5657280964396918	0.3575778659265509	F	F	F
0.0625000000000000	0.5657280964396918	0.3575778659265509	F	F	F
0.5625000000000000	0.5657280964396918	0.4720447732694801	T	T	T
0.8125000000000000	0.5657280964396918	0.4720447732694801	T	T	T
0.8125000000000000	0.5657280964396918	0.5890294241903098	T	T	T
0.0625000000000000	0.5657280964396918	0.5890294241903098	T	T	T
0.3125000000000000	0.4342719035603082	0.4141929975056158	F	F	F
0.4375000000000000	0.1971842893190683	0.3575778659265509	F	F	F
0.1875000000000000	0.1971842893190683	0.3575778659265509	F	F	F
0.5625000000000000	0.4342719035603082	0.4141929975056158	F	F	F

0.5625000000000000	0.1971842893190683	0.4141929975056158	F	F	F
0.1875000000000000	0.4342719035603082	0.3575778659265509	F	F	F
0.4375000000000000	0.4342719035603082	0.3575778659265509	F	F	F
0.3125000000000000	0.1971842893190683	0.4141929975056158	F	F	F
0.0625000000000000	0.4346466230298395	0.5281609597633423	T	T	T
0.1875000000000000	0.1972423251017672	0.4710993121075280	T	T	T
0.4375000000000000	0.1972423251017672	0.4710993121075280	T	T	T
0.3125000000000000	0.4346466230298395	0.5281609597633423	T	T	T
0.3125000000000000	0.1968095698495372	0.5281609597633423	T	T	T
0.4375000000000000	0.4342138677776093	0.4710993121075280	T	T	T
0.1875000000000000	0.4342138677776093	0.4710993121075280	T	T	T
0.0625000000000000	0.1968095698495372	0.5281609597633423	T	T	T
0.3125000000000000	0.4305988001731906	0.6422116618432201	T	T	T
0.4375000000000000	0.1967938161118522	0.5836482043156883	T	T	T
0.1875000000000000	0.1967938161118522	0.5836482043156883	T	T	T
0.0625000000000000	0.4305988001731906	0.6422116618432201	T	T	T
0.0625000000000000	0.2008573927061858	0.6422116618432201	T	T	T
0.1875000000000000	0.4346623767675243	0.5836482043156883	T	T	T
0.4375000000000000	0.4346623767675243	0.5836482043156883	T	T	T
0.3125000000000000	0.2008573927061858	0.6422116618432201	T	T	T
0.3125000000000000	0.9342719035603082	0.4141929975056158	F	F	F
0.4375000000000000	0.6971842893190683	0.3575778659265509	F	F	F
0.1875000000000000	0.6971842893190683	0.3575778659265509	F	F	F
0.5625000000000000	0.9342719035603082	0.4141929975056158	F	F	F
0.5625000000000000	0.6971842893190683	0.4141929975056158	F	F	F
0.1875000000000000	0.9342719035603082	0.3575778659265509	F	F	F
0.4375000000000000	0.9342719035603082	0.3575778659265509	F	F	F
0.3125000000000000	0.6971842893190683	0.4141929975056158	F	F	F

0.0625000000000000	0.9346466230298393	0.5281609597633423	T	T	T
0.1875000000000000	0.6972423251017672	0.4710993121075280	T	T	T
0.4375000000000000	0.6972423251017672	0.4710993121075280	T	T	T
0.3125000000000000	0.9346466230298393	0.5281609597633423	T	T	T
0.3125000000000000	0.6968095698495372	0.5281609597633423	T	T	T
0.4375000000000000	0.9342138677776093	0.4710993121075280	T	T	T
0.1875000000000000	0.9342138677776093	0.4710993121075280	T	T	T
0.0625000000000000	0.6968095698495372	0.5281609597633423	T	T	T
0.3125000000000000	0.9305988001731907	0.6422116618432201	T	T	T
0.4375000000000000	0.6967938161118523	0.5836482043156883	T	T	T
0.1875000000000000	0.6967938161118523	0.5836482043156883	T	T	T
0.0625000000000000	0.9305988001731907	0.6422116618432201	T	T	T
0.0625000000000000	0.7008573927061857	0.6422116618432201	T	T	T
0.1875000000000000	0.9346623767675242	0.5836482043156883	T	T	T
0.4375000000000000	0.9346623767675242	0.5836482043156883	T	T	T
0.3125000000000000	0.7008573927061857	0.6422116618432201	T	T	T
0.8125000000000000	0.4342719035603082	0.4141929975056158	F	F	F
0.9375000000000000	0.1971842893190683	0.3575778659265509	F	F	F
0.6875000000000000	0.1971842893190683	0.3575778659265509	F	F	F
0.0625000000000000	0.4342719035603082	0.4141929975056158	F	F	F
0.0625000000000000	0.1971842893190683	0.4141929975056158	F	F	F
0.6875000000000000	0.4342719035603082	0.3575778659265509	F	F	F
0.9375000000000000	0.4342719035603082	0.3575778659265509	F	F	F
0.8125000000000000	0.1971842893190683	0.4141929975056158	F	F	F
0.5625000000000000	0.4346466230298395	0.5281609597633423	T	T	T
0.6875000000000000	0.1972423251017672	0.4710993121075280	T	T	T
0.9375000000000000	0.1972423251017672	0.4710993121075280	T	T	T
0.8125000000000000	0.4346466230298395	0.5281609597633423	T	T	T

0.8125000000000000	0.1968095698495372	0.5281609597633423	T	T	T
0.9375000000000000	0.4342138677776093	0.4710993121075280	T	T	T
0.6875000000000000	0.4342138677776093	0.4710993121075280	T	T	T
0.5625000000000000	0.1968095698495372	0.5281609597633423	T	T	T
0.8125000000000000	0.4305988001731906	0.6422116618432201	T	T	T
0.9375000000000000	0.1967938161118522	0.5836482043156883	T	T	T
0.6875000000000000	0.1967938161118522	0.5836482043156883	T	T	T
0.5625000000000000	0.4305988001731906	0.6422116618432201	T	T	T
0.5625000000000000	0.2008573927061858	0.6422116618432201	T	T	T
0.6875000000000000	0.4346623767675243	0.5836482043156883	T	T	T
0.9375000000000000	0.4346623767675243	0.5836482043156883	T	T	T
0.8125000000000000	0.2008573927061858	0.6422116618432201	T	T	T
0.8125000000000000	0.9342719035603082	0.4141929975056158	F	F	F
0.9375000000000000	0.6971842893190683	0.3575778659265509	F	F	F
0.6875000000000000	0.6971842893190683	0.3575778659265509	F	F	F
0.0625000000000000	0.9342719035603082	0.4141929975056158	F	F	F
0.0625000000000000	0.6971842893190683	0.4141929975056158	F	F	F
0.6875000000000000	0.9342719035603082	0.3575778659265509	F	F	F
0.9375000000000000	0.9342719035603082	0.3575778659265509	F	F	F
0.8125000000000000	0.6971842893190683	0.4141929975056158	F	F	F
0.5625000000000000	0.9346466230298393	0.5281609597633423	T	T	T
0.6875000000000000	0.6972423251017672	0.4710993121075280	T	T	T
0.9375000000000000	0.6972423251017672	0.4710993121075280	T	T	T
0.8125000000000000	0.9346466230298393	0.5281609597633423	T	T	T
0.8125000000000000	0.6968095698495372	0.5281609597633423	T	T	T
0.9375000000000000	0.9342138677776093	0.4710993121075280	T	T	T
0.6875000000000000	0.9342138677776093	0.4710993121075280	T	T	T
0.5625000000000000	0.6968095698495372	0.5281609597633423	T	T	T

0.8125000000000000	0.9305988001731907	0.6422116618432201	T	T	T
0.9375000000000000	0.6967938161118523	0.5836482043156883	T	T	T
0.6875000000000000	0.6967938161118523	0.5836482043156883	T	T	T
0.5625000000000000	0.9305988001731907	0.6422116618432201	T	T	T
0.5625000000000000	0.7008573927061857	0.6422116618432201	T	T	T
0.6875000000000000	0.9346623767675242	0.5836482043156883	T	T	T
0.9375000000000000	0.9346623767675242	0.5836482043156883	T	T	T
0.8125000000000000	0.7008573927061857	0.6422116618432201	T	T	T
0.1875000000000000	0.3157280964396918	0.4141929975056158	F	F	F
0.4375000000000000	0.3157280964396918	0.4141929975056158	F	F	F
0.4375000000000000	0.3157280964396918	0.5257350761765036	T	T	T
0.1875000000000000	0.3157280964396918	0.5257350761765036	T	T	T
0.1875000000000000	0.3157280964396918	0.6332143038312309	T	T	T
0.4375000000000000	0.3157280964396918	0.6332143038312309	T	T	T
0.1875000000000000	0.8157280964396918	0.4141929975056158	F	F	F
0.4375000000000000	0.8157280964396918	0.4141929975056158	F	F	F
0.4375000000000000	0.8157280964396918	0.5257350761765036	T	T	T
0.1875000000000000	0.8157280964396918	0.5257350761765036	T	T	T
0.1875000000000000	0.8157280964396918	0.6332143038312309	T	T	T
0.4375000000000000	0.8157280964396918	0.6332143038312309	T	T	T
0.6875000000000000	0.3157280964396918	0.4141929975056158	F	F	F
0.9375000000000000	0.3157280964396918	0.4141929975056158	F	F	F
0.9375000000000000	0.3157280964396918	0.5257350761765036	T	T	T
0.6875000000000000	0.3157280964396918	0.5257350761765036	T	T	T
0.6875000000000000	0.3157280964396918	0.6332143038312309	T	T	T
0.9375000000000000	0.3157280964396918	0.6332143038312309	T	T	T
0.6875000000000000	0.8157280964396918	0.4141929975056158	F	F	F
0.9375000000000000	0.8157280964396918	0.4141929975056158	F	F	F

0.9375000000000000	0.8157280964396918	0.5257350761765036	T	T	T
0.6875000000000000	0.8157280964396918	0.5257350761765036	T	T	T
0.6875000000000000	0.8157280964396918	0.6332143038312309	T	T	T
0.9375000000000000	0.8157280964396918	0.6332143038312309	T	T	T

O_{Zr}^s vacancy

Ce O Zr

1.0000000000000000

15.0049857511559779 0.0000000000000000 0.0000000000000000

-7.5024928755779881 13.0447800098917028 0.0000000000000000

0.0000000000000000 0.0000000000000000 31.5474089986390567

Ce O Zr

24 95 24

Selective dynamics

Direct

0.3332909580984804	0.1665819161969608	0.4027260065404690	F	F	F
0.0832909580984804	0.1665819161969608	0.4027260065404690	F	F	F
0.1664505698948478	0.3329051133419106	0.4992119179534675	T	T	T
0.4163869965590659	0.3328290776490623	0.4991275855445174	T	T	T
0.4920422882982226	0.4842159292599417	0.6006988086248557	T	T	T
0.2477484637521423	0.4963895975731880	0.5993375845751794	T	T	T
0.3332909580984804	0.6665819161969608	0.4027260065404690	F	F	F
0.0832909580984804	0.6665819161969608	0.4027260065404690	F	F	F
0.1663334568309521	0.8330529232354472	0.4987925887114461	T	T	T
0.4156770345233992	0.8352635632461506	0.4980687092384304	T	T	T
0.4991597816122619	0.0012045025912472	0.6019737482348699	T	T	T
0.2491225214904307	0.9976579318772332	0.5991668778848995	T	T	T
0.8332909580984804	0.1665819161969608	0.4027260065404690	F	F	F

0.5832909580984804	0.1665819161969608	0.4027260065404690	F	F	F
0.6669736503129310	0.3339763936786586	0.4986844111631350	T	T	T
0.9160633496370938	0.3321156889564247	0.4991521801208680	T	T	T
0.9980108554445781	0.4961048440326141	0.5981899923620285	T	T	T
0.7486802755173492	0.4968506514332761	0.5991250287484919	T	T	T
0.8332909580984804	0.6665819161969608	0.4027260065404690	F	F	F
0.5832909580984804	0.6665819161969608	0.4027260065404690	F	F	F
0.6647620675920808	0.8293088618339920	0.5003161773803571	T	T	T
0.9191089644412676	0.8344774419288861	0.4973599232906354	T	T	T
0.0026377819278644	0.0015289298404651	0.5981645241764063	T	T	T
0.7493739168304073	-0.0011207491396739	0.5998115245649839	T	T	T
0.4979569726550324	0.4959139453100718	0.3796635475034336	F	F	F
0.0022775938153288	0.2545551876306504	0.3771514688477424	F	F	F
0.2522775938153288	0.2545551876306504	0.3771514688477424	F	F	F
0.2479569726550324	0.4959139453100718	0.3796635475034336	F	F	F
0.3314714849772605	0.1630728911569217	0.4757353152394632	T	T	T
0.3351843450046547	0.4202761145257516	0.4730660597960934	T	T	T
0.0863312587214443	0.4205807385131357	0.4738590526127571	T	T	T
0.0803830258497740	0.1624286133342701	0.4755061666096146	T	T	T
0.1686249435419285	0.3372498870838498	0.4257884655775115	F	F	F
0.1643043223816321	0.0786086447632712	0.4283005442331955	F	F	F
0.4143043223816321	0.0786086447632712	0.4283005442331955	F	F	F
0.4186249435419285	0.3372498870838498	0.4257884655775115	F	F	F
0.1614790897303971	0.3301022709136096	0.5704813677608631	T	T	T
0.1664493037775457	0.0826297082117035	0.5716497584085175	T	T	T
0.4142670979769575	0.0848081730902150	0.5713009398859591	T	T	T
0.4119810914263429	0.3242018587586116	0.5712018070712875	T	T	T
0.0032766327270622	0.0053427795913960	0.5227531145901996	T	T	T

0.4981661055070569	0.2436337195575479	0.5246405016639152	T	T	T
0.2447568763079092	0.2417489294818622	0.5249992480188875	T	T	T
0.2511888747847943	0.0042434042186704	0.5227526840929243	T	T	T
0.3342828619414371	0.1722547966787407	0.6220502023229250	T	T	T
0.3137833627764735	0.3950112663380906	0.6235759528362120	T	T	T
0.0766384351609496	0.4040247706057410	0.6223955007839144	T	T	T
0.0860230173996303	0.1732148317254563	0.6205490272414935	T	T	T
0.4979569726550324	0.9959139453100718	0.3796635475034336	F	F	F
0.0022775938153288	0.7545551876306504	0.3771514688477424	F	F	F
0.2522775938153288	0.7545551876306504	0.3771514688477424	F	F	F
0.2479569726550324	0.9959139453100718	0.3796635475034336	F	F	F
0.3301319892100633	0.6616558228457290	0.4754392305827613	T	T	T
0.3339608411256276	0.9200932971522235	0.4728420713015974	T	T	T
0.0853866738302451	0.9201683627416677	0.4725974904656182	T	T	T
0.0800318037049591	0.6608403735197356	0.4756922633852432	T	T	T
0.1686249435419285	0.8372498870838498	0.4257884655775115	F	F	F
0.1643043223816321	0.5786086447632712	0.4283005442331955	F	F	F
0.4143043223816321	0.5786086447632712	0.4283005442331955	F	F	F
0.4186249435419285	0.8372498870838498	0.4257884655775115	F	F	F
0.1635723516309228	0.8308062823187503	0.5702841504363800	T	T	T
0.1645642018178194	0.5801386200320282	0.5712774724238947	T	T	T
0.4253205707228251	0.5927280934272364	0.5792795264066838	T	T	T
0.4096993437605555	0.8302630259062234	0.5702585004655605	T	T	T
0.0012724142920158	0.5030482371047418	0.5230648628432751	T	T	T
0.4936108598384567	0.7436819289741786	0.5238744019084584	T	T	T
0.2437274750064373	0.7410110788660615	0.5247269663637296	T	T	T
0.2597196223534754	0.5073467972568363	0.5249197815119336	T	T	T
0.3310493875902539	0.6773021470561100	0.6219587479163879	T	T	T

0.3158663976205251	0.8981278249287558	0.6238499353139697	T	T	T
0.0776909624529574	0.9050478849381929	0.6222076413068671	T	T	T
0.0859011021295639	0.6738321401110533	0.6203992773535517	T	T	T
0.9979569726550324	0.4959139453100718	0.3796635475034336	F	F	F
0.5022775938153288	0.2545551876306504	0.3771514688477424	F	F	F
0.7522775938153288	0.2545551876306504	0.3771514688477424	F	F	F
0.7479569726550324	0.4959139453100718	0.3796635475034336	F	F	F
0.8283058006804875	0.1563168958200300	0.4770802099674833	T	T	T
0.8349709990352697	0.4212471172535606	0.4735931408833086	T	T	T
0.5850153095655266	0.4208888956349456	0.4728896702125170	T	T	T
0.5822551337780799	0.1632339882089933	0.4755424071815595	T	T	T
0.6686249435419285	0.3372498870838498	0.4257884655775115	F	F	F
0.6643043223816321	0.0786086447632712	0.4283005442331955	F	F	F
0.9143043223816321	0.0786086447632712	0.4283005442331955	F	F	F
0.9186249435419285	0.3372498870838498	0.4257884655775115	F	F	F
0.6700806339628784	0.3330823920411436	0.5696726619398532	T	T	T
0.6714594889703516	0.0858385187455077	0.5709797433796112	T	T	T
0.9165989344566615	0.0838807180639826	0.5713044949234047	T	T	T
0.9145956469418756	0.3285151467608494	0.5714350429985492	T	T	T
0.5021412314855729	0.0053266838653060	0.5219395610882408	T	T	T
0.9949387523345572	0.2414282695775999	0.5245647164314798	T	T	T
0.7468459201199191	0.2428554877281101	0.5240985678559852	T	T	T
0.7472113031197960	-0.0080119702287145	0.5265778451401716	T	T	T
0.8367400783344592	0.1705794013392002	0.6213678223235752	T	T	T
0.8283714155985371	0.4051889909901721	0.6221291155176462	T	T	T
0.5818838194387592	0.3964313486336948	0.6231898386906047	T	T	T
0.5923926234146764	0.1830608339914829	0.6209819993071076	T	T	T
0.9979569726550324	0.9959139453100718	0.3796635475034336	F	F	F

0.5022775938153288	0.7545551876306504	0.3771514688477424	F	F	F
0.7522775938153288	0.7545551876306504	0.3771514688477424	F	F	F
0.7479569726550324	0.9959139453100718	0.3796635475034336	F	F	F
0.8316835852840666	0.6617836243725007	0.4750099122421619	T	T	T
0.8340743771076241	0.9197534934478107	0.4731454746464823	T	T	T
0.5863557165551989	0.9196033294650778	0.4733852276447762	T	T	T
0.5814713495152231	0.6626359620198945	0.4760549335437921	T	T	T
0.6686249435419285	0.8372498870838498	0.4257884655775115	F	F	F
0.6643043223816321	0.5786086447632712	0.4283005442331955	F	F	F
0.9143043223816321	0.5786086447632712	0.4283005442331955	F	F	F
0.9186249435419285	0.8372498870838498	0.4257884655775115	F	F	F
0.6461886505707397	0.7881666613099224	0.5803174124164902	T	T	T
0.6677154668629796	0.5933631822084311	0.5795932025085048	T	T	T
0.9157961345725765	0.5810318379740127	0.5712263828500429	T	T	T
0.9222399742702332	0.8340478773739270	0.5695663570386760	T	T	T
0.5026794085766660	0.5048251259262437	0.5233638666517222	T	T	T
0.9955168705547585	0.7409078371113998	0.5245575271191613	T	T	T
0.7512873248503593	0.7433594694983194	0.5235700283648861	T	T	T
0.7482338326425346	0.5085266836796926	0.5246543718204059	T	T	T
0.8476326058120219	0.6795475309666084	0.6211449587388267	T	T	T
0.8314998736299570	0.9063793334954250	0.6201589894156740	T	T	T
0.5811365890545407	0.9007500230506343	0.6211007104627549	T	T	T
0.3332909580984804	0.4165819161969608	0.4027260065404690	F	F	F
0.0832909580984804	0.4165819161969608	0.4027260065404690	F	F	F
0.1671401051106298	0.0823716325065733	0.4993845176263975	T	T	T
0.4162716060626286	0.0821851192354657	0.5001644457007723	T	T	T
0.5004187664107906	0.2459691252472956	0.5942341034181573	T	T	T
0.2472718205222714	0.2451144672642699	0.5947006772480899	T	T	T

0.3332909580984804	0.9165819161969608	0.4027260065404690	F	F	F
0.0832909580984804	0.9165819161969608	0.4027260065404690	F	F	F
0.1658571780399813	0.5823881150927519	0.4997552197043559	T	T	T
0.4159341267377418	0.5808899427006551	0.4991648005014896	T	T	T
0.4841494654937462	0.7532364478900194	0.5915173617978580	T	T	T
0.2448522730376972	0.7483973964267568	0.5946971701718904	T	T	T
0.8332909580984804	0.4165819161969608	0.4027260065404690	F	F	F
0.5832909580984804	0.4165819161969608	0.4027260065404690	F	F	F
0.6631328267144052	0.0807805875702161	0.5000517720478543	T	T	T
0.9160547408502996	0.0807303047117162	0.4994724339325096	T	T	T
0.9977786960835997	0.2468088741286366	0.5936607072192864	T	T	T
0.7475233161390773	0.2472100919518100	0.5934041624152050	T	T	T
0.8332909580984804	0.9165819161969608	0.4027260065404690	F	F	F
0.5832909580984804	0.9165819161969608	0.4027260065404690	F	F	F
0.6646301915126059	0.5807495365643613	0.4989151431360894	T	T	T
0.9163795096718287	0.5822123851237684	0.4995141200376406	T	T	T
0.0026957350917960	0.7475528623096692	0.5939896764247358	T	T	T
0.7696580190289692	0.7537219965318548	0.5909448876043426	T	T	T

O_{Zr}^{sub} vacancy

Ce O Zr

1.0000000000000000

15.0049857511559779 0.0000000000000000 0.0000000000000000

-7.5024928755779881 13.0447800098917028 0.0000000000000000

0.0000000000000000 0.0000000000000000 31.5474089986390567

Ce O Zr

24 95 24

Selective dynamics

Direct

0.3332909580984804	0.1665819161969608	0.4027260065404690	F	F	F
0.0832909580984804	0.1665819161969608	0.4027260065404690	F	F	F
0.1667801733925808	0.3335575098381127	0.4989851681904607	T	T	T
0.4162642812074068	0.3327125449613922	0.4990782852744647	T	T	T
0.4998155033118722	0.4970434602459367	0.5978560936782603	T	T	T
0.2543507657430682	0.5086855735830856	0.6031770181942480	T	T	T
0.3332909580984804	0.6665819161969608	0.4027260065404690	F	F	F
0.0832909580984804	0.6665819161969608	0.4027260065404690	F	F	F
0.1664742315687646	0.8325279409237322	0.4989287577173457	T	T	T
0.4165447783444360	0.8331070284575959	0.4986545226462086	T	T	T
0.4987513586438150	0.9975076593180729	0.5981423184843333	T	T	T
0.2481185388032362	0.9932667150527091	0.5988734202516051	T	T	T
0.8332909580984804	0.1665819161969608	0.4027260065404690	F	F	F
0.5832909580984804	0.1665819161969608	0.4027260065404690	F	F	F
0.6663465225162968	0.3326959038163984	0.4985285590469075	T	T	T
0.9164306326584030	0.3327108660165956	0.4990788118207783	T	T	T
-0.0027861863208412	0.4970330583793130	0.5978486168881287	T	T	T
0.7486642907090670	0.4973421263491775	0.5989371779520850	T	T	T
0.8332909580984804	0.6665819161969608	0.4027260065404690	F	F	F
0.5832909580984804	0.6665819161969608	0.4027260065404690	F	F	F
0.6660520133662683	0.8325179704609527	0.4989293345550509	T	T	T
0.9159590383425484	0.8318902294828261	0.4990434473345345	T	T	T
0.9955678378040043	0.9911272206474059	0.5976297690912342	T	T	T
0.7451526103053843	0.9932523867854290	0.5988828619005706	T	T	T
0.4979569726550324	0.4959139453100718	0.3796635475034336	F	F	F
0.0022775938153288	0.2545551876306504	0.3771514688477424	F	F	F
0.2522775938153288	0.2545551876306504	0.3771514688477424	F	F	F

0.2479569726550324	0.4959139453100718	0.3796635475034336	F	F	F
0.3294195931582843	0.1626193427500028	0.4761265207314713	T	T	T
0.3398190102151974	0.4224870387187109	0.4730739374273943	T	T	T
0.0826575201594811	0.4224801646735892	0.4730748201426008	T	T	T
0.0781113588865950	0.1562243238215891	0.4760190370453165	T	T	T
0.1686249435419285	0.3372498870838498	0.4257884655775115	F	F	F
0.1643043223816321	0.0786086447632712	0.4283005442331955	F	F	F
0.4143043223816321	0.0786086447632712	0.4283005442331955	F	F	F
0.4186249435419285	0.3372498870838498	0.4257884655775115	F	F	F
0.1649490080384414	0.0760477702562754	0.5741628142433962	T	T	T
0.4163776613443754	0.0819695797903877	0.5720474524563495	T	T	T
0.4218236417603222	0.3270935662786967	0.5714547137779293	T	T	T
0.0016043551521540	0.0032398286584555	0.5247708464113005	T	T	T
0.4970024400065328	0.2397982041108534	0.5244882976624945	T	T	T
0.2455010005128643	0.2413950631679275	0.5290017494095377	T	T	T
0.2526994450837804	0.0037965834259073	0.5233815313535443	T	T	T
0.3397963448918671	0.1708633742899310	0.6228532918346912	T	T	T
0.3206581520352170	0.3940847813745694	0.6158378308318426	T	T	T
0.0733875107076120	0.3940370276284915	0.6158313772461015	T	T	T
0.1025077069412509	0.2050413382632611	0.6095465909164480	T	T	T
0.4979569726550324	0.9959139453100718	0.3796635475034336	F	F	F
0.0022775938153288	0.7545551876306504	0.3771514688477424	F	F	F
0.2522775938153288	0.7545551876306504	0.3771514688477424	F	F	F
0.2479569726550324	0.9959139453100718	0.3796635475034336	F	F	F
0.3298968127666846	0.6598389346251329	0.4762453463017180	T	T	T
0.3346759332642623	0.9199654282634293	0.4729138726195510	T	T	T
0.0847992500525927	0.9204549371545112	0.4736608534938648	T	T	T
0.0803425704619017	0.6607881914064677	0.4762359030149276	T	T	T

0.1686249435419285	0.8372498870838498	0.4257884655775115	F	F	F
0.1643043223816321	0.5786086447632712	0.4283005442331955	F	F	F
0.4143043223816321	0.5786086447632712	0.4283005442331955	F	F	F
0.4186249435419285	0.8372498870838498	0.4257884655775115	F	F	F
0.1652128810570801	0.8296185420571915	0.5712555492425946	T	T	T
0.1634354271332582	0.5881873778981362	0.5726194441194472	T	T	T
0.4247864055935023	0.5882299045510962	0.5726411094354550	T	T	T
0.4167112471193493	0.8333863770385674	0.5704727360311582	T	T	T
0.0006522773770708	0.5025471174466484	0.5241687378591451	T	T	T
0.4962640103749483	0.7439703514071928	0.5247584976227302	T	T	T
0.2476945368332560	0.7439806328784689	0.5247568693292173	T	T	T
0.2522927184490067	0.5045262721771593	0.5263415171325792	T	T	T
0.3424125892251685	0.6848295981587389	0.6217507790217820	T	T	T
0.3268941261140178	0.9042127807326545	0.6224285663549147	T	T	T
0.0746250955348746	0.9006502610206647	0.6229010136872133	T	T	T
0.0832801370673064	0.6744625791149019	0.6217376109540242	T	T	T
0.9979569726550324	0.4959139453100718	0.3796635475034336	F	F	F
0.5022775938153288	0.2545551876306504	0.3771514688477424	F	F	F
0.7522775938153288	0.2545551876306504	0.3771514688477424	F	F	F
0.7479569726550324	0.4959139453100718	0.3796635475034336	F	F	F
0.8331973407618066	0.1626104913664461	0.4761334981743243	T	T	T
0.8353768046404664	0.4197705256822426	0.4733002120517568	T	T	T
0.5843437671752396	0.4197531244009952	0.4732914843718803	T	T	T
0.5810818236818008	0.1621332662800701	0.4749884827680247	T	T	T
0.6686249435419285	0.3372498870838498	0.4257884655775115	F	F	F
0.6643043223816321	0.0786086447632712	0.4283005442331955	F	F	F
0.9143043223816321	0.0786086447632712	0.4283005442331955	F	F	F
0.9186249435419285	0.3372498870838498	0.4257884655775115	F	F	F

0.6647272227242017	0.3294596806714569	0.5712904065327328	T	T	T
0.6655931571157113	0.0819267525527588	0.5720449248150367	T	T	T
0.9110890583948636	0.0760376991570739	0.5741478347336820	T	T	T
0.9053097012588888	0.3271023187107519	0.5714582484843270	T	T	T
0.5028788204646719	0.0058208071815370	0.5227298946115019	T	T	T
0.9958967573342868	0.2414231460289188	0.5290327812725285	T	T	T
0.7427806660235754	0.2398020594995260	0.5244971423172674	T	T	T
0.7511431569591350	0.0038415706403012	0.5233721464792026	T	T	T
0.8310399690710003	0.1707684540653798	0.6228388690481116	T	T	T
0.8253334559048501	0.4045760914639704	0.6227994391574946	T	T	T
0.5792498845127642	0.4045848794335167	0.6228056169244877	T	T	T
0.5867453418992639	0.1734965338168226	0.6211162420650675	T	T	T
0.9979569726550324	0.9959139453100718	0.3796635475034336	F	F	F
0.5022775938153288	0.7545551876306504	0.3771514688477424	F	F	F
0.7522775938153288	0.7545551876306504	0.3771514688477424	F	F	F
0.7479569726550324	0.9959139453100718	0.3796635475034336	F	F	F
0.8310001369491780	0.6619379083557686	0.4757853298484616	T	T	T
0.8356764203437013	0.9204558518610216	0.4736672285553025	T	T	T
0.5853040877399590	0.9199396519165829	0.4729360220638998	T	T	T
0.5804302267051868	0.6607803565187964	0.4762286490290166	T	T	T
0.6686249435419285	0.8372498870838498	0.4257884655775115	F	F	F
0.6643043223816321	0.5786086447632712	0.4283005442331955	F	F	F
0.9143043223816321	0.5786086447632712	0.4283005442331955	F	F	F
0.9186249435419285	0.8372498870838498	0.4257884655775115	F	F	F
0.6644071718693904	0.8296326325377689	0.5712467612664718	T	T	T
0.6659635496814317	0.5814629263827881	0.5719100339983840	T	T	T
0.9154997082554940	0.5814278734626869	0.5718850082221405	T	T	T
0.9152974431109462	0.8305867462364409	0.5710192619449670	T	T	T

0.5018967034302777	0.5025970597592777	0.5241595410373319	T	T	T
0.9955970181116258	0.7411346000510295	0.5253497226612572	T	T	T
0.7455123693685578	0.7411157007441115	0.5253335579347818	T	T	T
0.7518808189897050	0.5038330358371128	0.5231824461738381	T	T	T
0.8370726828454633	0.6740830087368714	0.6203554132514185	T	T	T
0.8260285829927334	0.9006045565735865	0.6229260179905352	T	T	T
0.5773179117681607	0.9042033730357590	0.6224427490841855	T	T	T
0.5912149871668881	0.6744955400753899	0.6217384031442236	T	T	T
0.3332909580984804	0.4165819161969608	0.4027260065404690	F	F	F
0.0832909580984804	0.4165819161969608	0.4027260065404690	F	F	F
0.1648871444562168	0.0811718565079115	0.4995970649848289	T	T	T
0.4157537311307964	0.0811476348543154	0.4993141778315967	T	T	T
0.5019985118832537	0.2465981466917412	0.5937316206645502	T	T	T
0.2595541877248249	0.2405132718264676	0.5957552725594153	T	T	T
0.3332909580984804	0.9165819161969608	0.4027260065404690	F	F	F
0.0832909580984804	0.9165819161969608	0.4027260065404690	F	F	F
0.1661551767542749	0.5802330079653099	0.5002487571130690	T	T	T
0.4140719173575010	0.5802330104317485	0.5002481545913322	T	T	T
0.4995278625109936	0.7482998032737738	0.5936964168692609	T	T	T
0.2487964920464472	0.7483087733133093	0.5936965249272325	T	T	T
0.8332909580984804	0.4165819161969608	0.4027260065404690	F	F	F
0.5832909580984804	0.4165819161969608	0.4027260065404690	F	F	F
0.6653861079927541	0.0811372245740234	0.4993171021140053	T	T	T
0.9162817025979477	0.0811703832532171	0.4995855392664696	T	T	T
0.9809379109236065	0.2405227302057028	0.5957449694368768	T	T	T
0.7445976470409787	0.2465886708256208	0.5937374698280086	T	T	T
0.8332909580984804	0.9165819161969608	0.4027260065404690	F	F	F
0.5832909580984804	0.9165819161969608	0.4027260065404690	F	F	F

0.6653846486918933	0.5811010627928532	0.4994754284478171	T	T	T
0.9157129519013861	0.5811065871395124	0.4994724438882333	T	T	T
0.9981567933698426	0.7448790120195188	0.5947189325368901	T	T	T
0.7467298277419931	0.7449008084181542	0.5947195154611716	T	T	T

O_{Ce}^s vacancy

Ce O Zr

1.0000000000000000

15.0049857511559779 0.0000000000000000 0.0000000000000000

-7.5024928755779881 13.0447800098917028 0.0000000000000000

0.0000000000000000 0.0000000000000000 31.5474089986390567

Ce O Zr

24 95 24

Selective dynamics

Direct

0.3332909580984804	0.1665819161969608	0.4027260065404690	F	F	F
0.0832909580984804	0.1665819161969608	0.4027260065404690	F	F	F
0.1672206995420746	0.3332186124999708	0.4988512614326505	T	T	T
0.4184674265539231	0.3344951198870761	0.5006665246769961	T	T	T
0.4961241089403269	0.5070762665934206	0.5991366474763461	T	T	T
0.2461067379392316	0.4962062998371498	0.5984461773668472	T	T	T
0.3332909580984804	0.6665819161969608	0.4027260065404690	F	F	F
0.0832909580984804	0.6665819161969608	0.4027260065404690	F	F	F
0.1654776980842839	0.8317301649688893	0.4989551332659602	T	T	T
0.4162524668845984	0.8317301649688893	0.4989551332659602	T	T	T
0.4981316969224507	0.9923935918386879	0.5984438848418868	T	T	T
0.2442618949162370	0.9923935918386879	0.5984438848418868	T	T	T
0.8332909580984804	0.1665819161969608	0.4027260065404690	F	F	F

0.5832909580984804	0.1665819161969608	0.4027260065404690	F	F	F
0.6660276933331458	0.3344951198870761	0.5006665246769961	T	T	T
0.9159979129578893	0.3332186124999708	0.4988512614326505	T	T	T
0.0000995618979181	0.4962062998371498	0.5984461773668472	T	T	T
0.7609521576530937	0.5070762665934206	0.5991366474763461	T	T	T
0.8332909580984804	0.6665819161969608	0.4027260065404690	F	F	F
0.5832909580984804	0.6665819161969608	0.4027260065404690	F	F	F
0.6670923887551418	0.8336173373926185	0.4986274922944730	T	T	T
0.9165249486374698	0.8336173373926185	0.4986274922944730	T	T	T
0.9980944010361751	0.9970427205215645	0.5980107680484856	T	T	T
0.7489483194853891	0.9970427205215645	0.5980107680484856	T	T	T
0.4979569726550324	0.4959139453100718	0.3796635475034336	F	F	F
0.0022775938153288	0.2545551876306504	0.3771514688477424	F	F	F
0.2522775938153288	0.2545551876306504	0.3771514688477424	F	F	F
0.2479569726550324	0.4959139453100718	0.3796635475034336	F	F	F
0.3286649873053467	0.1625353629851356	0.4754938346320442	T	T	T
0.3350753616526814	0.4189662597945833	0.4732902200668889	T	T	T
0.0849117675062888	0.4198235350125846	0.4731769487320500	T	T	T
0.0858148802933968	0.1642386872580773	0.4758847716572777	T	T	T
0.1686249435419285	0.3372498870838498	0.4257884655775115	F	F	F
0.1643043223816321	0.0786086447632712	0.4283005442331955	F	F	F
0.4143043223816321	0.0786086447632712	0.4283005442331955	F	F	F
0.4186249435419285	0.3372498870838498	0.4257884655775115	F	F	F
0.1588545099301299	0.3280930499163296	0.5706152925415060	T	T	T
0.1629875741347301	0.0787720690317016	0.5709688221756116	T	T	T
0.4114306273629476	0.0728612547259022	0.5703135513408074	T	T	T
0.4418754773828101	0.3362710076349671	0.5757408383284350	T	T	T
0.0002448090269345	0.0060916546089921	0.5224338451110603	T	T	T

0.4911751440182426	0.2323502880364850	0.5221565791393130	T	T	T
0.2529839237345228	0.2463423238039477	0.5285310197906355	T	T	T
0.2513448528670706	0.0028943575618759	0.5223859313093461	T	T	T
0.3326088574211297	0.1671640169709840	0.6192810851992169	T	T	T
0.3166030480885603	0.3959740612847416	0.6213167474466567	T	T	T
0.0771622992403402	0.4043245984806731	0.6229778807965930	T	T	T
0.0893674587702136	0.1736057215374208	0.6212423990936299	T	T	T
0.4979569726550324	0.9959139453100718	0.3796635475034336	F	F	F
0.0022775938153288	0.7545551876306504	0.3771514688477424	F	F	F
0.2522775938153288	0.7545551876306504	0.3771514688477424	F	F	F
0.2479569726550324	0.9959139453100718	0.3796635475034336	F	F	F
0.3306016146629805	0.6619478193566150	0.4756205158952982	T	T	T
0.3339064696082188	0.9178129392164447	0.4724951182131951	T	T	T
0.0851122712405457	0.9205230224566477	0.4732951335471899	T	T	T
0.0813462046936200	0.6619478193566150	0.4756205158952982	T	T	T
0.1686249435419285	0.8372498870838498	0.4257884655775115	F	F	F
0.1643043223816321	0.5786086447632712	0.4283005442331955	F	F	F
0.4143043223816321	0.5786086447632712	0.4283005442331955	F	F	F
0.4186249435419285	0.8372498870838498	0.4257884655775115	F	F	F
0.1639608615327184	0.8299568509672651	0.5710802529802432	T	T	T
0.1650565097513985	0.5801130195028043	0.5715124164658719	T	T	T
0.4131610089358871	0.5862467291319351	0.5719524321457503	T	T	T
0.4159959894345470	0.8299568509672651	0.5710802529802432	T	T	T
0.0016252350141672	0.5034551377626884	0.5229921603743753	T	T	T
0.4966242439686777	0.7422199556013341	0.5246619794632023	T	T	T
0.2454926534479485	0.7409853068958974	0.5256353357101256	T	T	T
0.2518299027485207	0.5034551377626884	0.5229921603743753	T	T	T
0.3343566990441278	0.6743179055946046	0.6212350768850093	T	T	T

0.3253743938404826	0.9007487876809580	0.6225462662861195	T	T	T
0.0769899900420619	0.9039321670386651	0.6227273462218160	T	T	T
0.0899612065504769	0.6743179055946046	0.6212350768850093	T	T	T
0.9979569726550324	0.4959139453100718	0.3796635475034336	F	F	F
0.5022775938153288	0.2545551876306504	0.3771514688477424	F	F	F
0.7522775938153288	0.2545551876306504	0.3771514688477424	F	F	F
0.7479569726550324	0.4959139453100718	0.3796635475034336	F	F	F
0.8284238069646663	0.1642386872580773	0.4758847716572777	T	T	T
0.8338908981418948	0.4189662597945833	0.4732902200668889	T	T	T
0.5849837554257752	0.4199675108515571	0.4744069649924442	T	T	T
0.5838703756797746	0.1625353629851356	0.4754938346320442	T	T	T
0.6686249435419285	0.3372498870838498	0.4257884655775115	F	F	F
0.6643043223816321	0.0786086447632712	0.4283005442331955	F	F	F
0.9143043223816321	0.0786086447632712	0.4283005442331955	F	F	F
0.9186249435419285	0.3372498870838498	0.4257884655775115	F	F	F
0.6443955302521571	0.3362710076349671	0.5757408383284350	T	T	T
0.6657844948969645	0.0787720690317016	0.5709688221756116	T	T	T
0.9175576097105315	0.0851152194210706	0.5725576052878916	T	T	T
0.9192385399861995	0.3280930499163296	0.5706152925415060	T	T	T
0.5015495046948052	0.0028943575618759	0.5223859313093461	T	T	T
0.9949336799046249	0.2398673598092498	0.5235543816918060	T	T	T
0.7433584000694250	0.2463423238039477	0.5285310197906355	T	T	T
0.7558468455820578	0.0060916546089921	0.5224338451110603	T	T	T
0.8342382627672070	0.1736057215374208	0.6212423990936299	T	T	T
0.8293710131961887	0.3959740612847416	0.6213167474466567	T	T	T
0.5845551595498546	0.1671640169709840	0.6192810851992169	T	T	T
0.9979569726550324	0.9959139453100718	0.3796635475034336	F	F	F
0.5022775938153288	0.7545551876306504	0.3771514688477424	F	F	F

0.7522775938153288	0.7545551876306504	0.3771514688477424	F	F	F
0.7479569726550324	0.9959139453100718	0.3796635475034336	F	F	F
0.8310429444590978	0.6630213805044050	0.4755351285393654	T	T	T
0.8346315271045504	0.9192630542091083	0.4725198762202681	T	T	T
0.5854107512160949	0.9205230224566477	0.4732951335471899	T	T	T
0.5819784360452923	0.6630213805044050	0.4755351285393654	T	T	T
0.6686249435419285	0.8372498870838498	0.4257884655775115	F	F	F
0.6643043223816321	0.5786086447632712	0.4283005442331955	F	F	F
0.9143043223816321	0.5786086447632712	0.4283005442331955	F	F	F
0.9186249435419285	0.8372498870838498	0.4257884655775115	F	F	F
0.6666532041685573	0.8344402144097618	0.5700755670451809	T	T	T
0.6673314871673790	0.5846629743347654	0.5734613079205313	T	T	T
0.9230857201960407	0.5862467291319351	0.5719524321457503	T	T	T
0.9177870102412041	0.8344402144097618	0.5700755670451809	T	T	T
0.5004639037141223	0.5060491693662198	0.5225168368764097	T	T	T
0.9955957116326565	0.7422199556013341	0.5246619794632023	T	T	T
0.7461025890571081	0.7422051781142163	0.5255086723985726	T	T	T
0.7555852656520976	0.5060491693662198	0.5225168368764097	T	T	T
0.8454768530230978	0.6867808503669496	0.6216428600260179	T	T	T
0.8279013339752869	0.9058026679505671	0.6218934684319410	T	T	T
0.5769421769966104	0.9039321670386651	0.6227273462218160	T	T	T
0.5913039973438519	0.6867808503669496	0.6216428600260179	T	T	T
0.3332909580984804	0.4165819161969608	0.4027260065404690	F	F	F
0.0832909580984804	0.4165819161969608	0.4027260065404690	F	F	F
0.1665270198814739	0.0813497108549185	0.4992558653980504	T	T	T
0.4132695128824975	0.0765390257650020	0.4974359083443953	T	T	T
0.4881592636635961	0.2263185273271778	0.5891137300639732	T	T	T
0.2430190260414381	0.2440122676610476	0.5960813122901359	T	T	T

0.3332909580984804	0.9165819161969608	0.4027260065404690	F	F	F
0.0832909580984804	0.9165819161969608	0.4027260065404690	F	F	F
0.1654697449924278	0.5809394899848629	0.4993391265436131	T	T	T
0.4159969949523790	0.5818080135869481	0.4991201307988782	T	T	T
0.4997035500508519	0.7490740316029079	0.5941728225578855	T	T	T
0.2476024293969939	0.7452048587939732	0.5950821067808172	T	T	T
0.8332909580984804	0.4165819161969608	0.4027260065404690	F	F	F
0.5832909580984804	0.4165819161969608	0.4027260065404690	F	F	F
0.6648226909734373	0.0813497108549185	0.4992558653980504	T	T	T
0.9156340996807126	0.0812681993614324	0.4993008275647910	T	T	T
0.9989158366829540	0.2478316733658939	0.5928041330700332	T	T	T
0.7509932416196238	0.2440122676610476	0.5960813122901359	T	T	T
0.8332909580984804	0.9165819161969608	0.4027260065404690	F	F	F
0.5832909580984804	0.9165819161969608	0.4027260065404690	F	F	F
0.6663081686669502	0.5826163373339075	0.5007035364566087	T	T	T
0.9158110186345617	0.5818080135869481	0.4991201307988782	T	T	T
-0.0006295184479299	0.7490740316029079	0.5941728225578855	T	T	T
0.7493847892310197	0.7487695784620255	0.5942562298001837	T	T	T

O_{Ce}^{sub} vacancy

Ce O Zr

1.0000000000000000

15.0049857511559779 0.0000000000000000 0.0000000000000000

-7.5024928755779881 13.0447800098917028 0.0000000000000000

0.0000000000000000 0.0000000000000000 31.5474089986390567

Ce O Zr

24 95 24

Selective dynamics

Direct

0.3332909580984804	0.1665819161969608	0.4027260065404690	F	F	F
0.0832909580984804	0.1665819161969608	0.4027260065404690	F	F	F
0.1661761174151379	0.3336471547206548	0.5001893430136013	T	T	T
0.4165332318527384	0.3333713823939047	0.4987611552249914	T	T	T
0.4990945046041724	0.4964719113623845	0.5983832594281885	T	T	T
0.2496641041638082	0.4893541478994128	0.6046063040184511	T	T	T
0.3332909580984804	0.6665819161969608	0.4027260065404690	F	F	F
0.0832909580984804	0.6665819161969608	0.4027260065404690	F	F	F
0.1666718178866395	0.8325833711266175	0.4995493063060137	T	T	T
0.4159115532399711	0.8325833711266175	0.4995493063060137	T	T	T
0.5018004893500749	0.0015517820499885	0.5983396386991262	T	T	T
0.2497512926999137	0.0015517820499885	0.5983396386991262	T	T	T
0.8332909580984804	0.1665819161969608	0.4027260065404690	F	F	F
0.5832909580984804	0.1665819161969608	0.4027260065404690	F	F	F
0.6668381505411592	0.3333713823939047	0.4987611552249914	T	T	T
0.9174710373055099	0.3336471547206548	0.5001893430136013	T	T	T
0.9896900437356049	0.4893541478994128	0.6046063040184511	T	T	T
0.7473774067582123	0.4964719113623845	0.5983832594281885	T	T	T
0.8332909580984804	0.6665819161969608	0.4027260065404690	F	F	F
0.5832909580984804	0.6665819161969608	0.4027260065404690	F	F	F
0.6669074138956053	0.8338406639421660	0.4988327818390740	T	T	T
0.9169332500465539	0.8338406639421660	0.4988327818390740	T	T	T
0.9985566702223514	0.9974282663121702	0.5986763071385413	T	T	T
0.7488715960898185	0.9974282663121702	0.5986763071385413	T	T	T
0.4979569726550324	0.4959139453100718	0.3796635475034336	F	F	F
0.0022775938153288	0.2545551876306504	0.3771514688477424	F	F	F
0.2522775938153288	0.2545551876306504	0.3771514688477424	F	F	F

0.2479569726550324	0.4959139453100718	0.3796635475034336	F	F	F
0.3317260918827340	0.1631299059608796	0.4748799308503603	T	T	T
0.3338914869815618	0.4235075207486275	0.4750153609194786	T	T	T
0.0840071037741155	0.4180142075482380	0.4718066596172545	T	T	T
0.0813920043198145	0.1633211986688417	0.4758631561621818	T	T	T
0.1686249435419285	0.3372498870838498	0.4257884655775115	F	F	F
0.1643043223816321	0.0786086447632712	0.4283005442331955	F	F	F
0.4143043223816321	0.0786086447632712	0.4283005442331955	F	F	F
0.4186249435419285	0.3372498870838498	0.4257884655775115	F	F	F
0.1658482905137768	0.3225399872844649	0.5711035949737397	T	T	T
0.1661426637177543	0.0822988522236828	0.5716379514510512	T	T	T
0.4164987085402394	0.0829974170804856	0.5710583952470218	T	T	T
0.4163124321338684	0.3295326684114132	0.5703053383508268	T	T	T
0.0026507339198612	0.0042500512742088	0.5228377460511863	T	T	T
0.4957037288166838	0.2414074576333677	0.5242355845113428	T	T	T
0.2474572549707279	0.2405900493294825	0.5242874142411921	T	T	T
0.2534075280861899	0.0066916481081306	0.5223483298368141	T	T	T
0.3380146254407858	0.1734200543114487	0.6202895303128462	T	T	T
0.3316382740100199	0.3972861102620406	0.6240473660584845	T	T	T
0.0711998500222349	0.3923997000444627	0.6224632779075352	T	T	T
0.0844644162114187	0.1687997918316495	0.6212554126347718	T	T	T
0.4979569726550324	0.9959139453100718	0.3796635475034336	F	F	F
0.0022775938153288	0.7545551876306504	0.3771514688477424	F	F	F
0.2522775938153288	0.7545551876306504	0.3771514688477424	F	F	F
0.2479569726550324	0.9959139453100718	0.3796635475034336	F	F	F
0.3322427980696642	0.6625684967009031	0.4753154614828826	T	T	T
0.3333743515115753	0.9167487030231577	0.4740045596787508	T	T	T
0.0854670766260434	0.9188698174326609	0.4732635808582750	T	T	T

0.0803256986312249	0.6625684967009031	0.4753154614828826	T	T	T
0.1686249435419285	0.8372498870838498	0.4257884655775115	F	F	F
0.1643043223816321	0.5786086447632712	0.4283005442331955	F	F	F
0.4143043223816321	0.5786086447632712	0.4283005442331955	F	F	F
0.4186249435419285	0.8372498870838498	0.4257884655775115	F	F	F
0.1688616807087818	0.8378149379238721	0.5709708249335431	T	T	T
0.4197508692591101	0.5836315229326303	0.5716496093901441	T	T	T
0.4189532572150901	0.8378149379238721	0.5709708249335431	T	T	T
0.0181648239504269	0.5089010757727341	0.5276132720590884	T	T	T
0.4952762704930772	0.7434221522959277	0.5253549511240624	T	T	T
0.2371349692738649	0.7242699385477298	0.5310607729635948	T	T	T
0.2407362518223072	0.5089010757727341	0.5276132720590884	T	T	T
0.3249331981763007	0.6749226709796589	0.6173616375918271	T	T	T
0.3304711745404687	0.9109423490809303	0.6246112587763508	T	T	T
0.0759902195966940	0.9034179602336790	0.6223006479736268	T	T	T
0.0999894728033584	0.6749226709796589	0.6173616375918271	T	T	T
0.9979569726550324	0.4959139453100718	0.3796635475034336	F	F	F
0.5022775938153288	0.2545551876306504	0.3771514688477424	F	F	F
0.7522775938153288	0.2545551876306504	0.3771514688477424	F	F	F
0.7479569726550324	0.4959139453100718	0.3796635475034336	F	F	F
0.8319291943490131	0.1633211986688417	0.4758631561621818	T	T	T
0.8396160337670583	0.4235075207486275	0.4750153609194786	T	T	T
0.5849945041370160	0.4199890082740388	0.4728749369181042	T	T	T
0.5814038140781316	0.1631299059608796	0.4748799308503603	T	T	T
0.6686249435419285	0.3372498870838498	0.4257884655775115	F	F	F
0.6643043223816321	0.0786086447632712	0.4283005442331955	F	F	F
0.9143043223816321	0.0786086447632712	0.4283005442331955	F	F	F
0.9186249435419285	0.3372498870838498	0.4257884655775115	F	F	F

0.6632202362775449	0.3295326684114132	0.5703053383508268	T	T	T
0.6661561885059216	0.0822988522236828	0.5716379514510512	T	T	T
0.9151274350146152	0.0802548700292376	0.5712129759922812	T	T	T
0.9066916967706878	0.3225399872844649	0.5711035949737397	T	T	T
0.5032841200219406	0.0066916481081306	0.5223483298368141	T	T	T
0.9961610254642395	0.2423220509284791	0.5255006689557639	T	T	T
0.7431327943587543	0.2405900493294825	0.5242874142411921	T	T	T
0.7515993173543475	0.0042500512742088	0.5228377460511863	T	T	T
0.8343353756202309	0.1687997918316495	0.6212554126347718	T	T	T
0.8156478362520277	0.3972861102620406	0.6240473660584845	T	T	T
0.5767746038023922	0.4035492076047765	0.6218937410949980	T	T	T
0.5854054288706626	0.1734200543114487	0.6202895303128462	T	T	T
0.9979569726550324	0.9959139453100718	0.3796635475034336	F	F	F
0.5022775938153288	0.7545551876306504	0.3771514688477424	F	F	F
0.7522775938153288	0.7545551876306504	0.3771514688477424	F	F	F
0.7479569726550324	0.9959139453100718	0.3796635475034336	F	F	F
0.8326755290561196	0.6624199428587207	0.4761960525185894	T	T	T
0.8349465692717154	0.9198931385434383	0.4730945591514267	T	T	T
0.5834027408066103	0.9188698174326609	0.4732635808582750	T	T	T
0.5797444138025870	0.6624199428587207	0.4761960525185894	T	T	T
0.6686249435419285	0.8372498870838498	0.4257884655775115	F	F	F
0.6643043223816321	0.5786086447632712	0.4283005442331955	F	F	F
0.9143043223816321	0.5786086447632712	0.4283005442331955	F	F	F
0.9186249435419285	0.8372498870838498	0.4257884655775115	F	F	F
0.6636916472260997	0.8300206471707272	0.5708552201888629	T	T	T
0.6662444999018232	0.5824889998036539	0.5721689826861172	T	T	T
0.9138806536735131	0.5836315229326303	0.5716496093901441	T	T	T
0.9163289999446278	0.8300206471707272	0.5708552201888629	T	T	T

0.5034187302998486	0.5043679712698321	0.5230407342913055	T	T	T
0.9981458818028506	0.7434221522959277	0.5253549511240624	T	T	T
0.7458952017847940	0.7417904035695883	0.5252327453801358	T	T	T
0.7509492409699836	0.5043679712698321	0.5230407342913055	T	T	T
0.8378541183535255	0.6756294239100957	0.6207856167727662	T	T	T
0.8259302961864894	0.9018605923729718	0.6215039970557844	T	T	T
0.5774277406369920	0.9034179602336790	0.6223006479736268	T	T	T
0.5877753055565701	0.6756294239100957	0.6207856167727662	T	T	T
0.3332909580984804	0.4165819161969608	0.4027260065404690	F	F	F
0.0832909580984804	0.4165819161969608	0.4027260065404690	F	F	F
0.1661020576800587	0.0819590097732201	0.4991175847010998	T	T	T
0.4162125312213066	0.0824250624426202	0.4992205366338950	T	T	T
0.4987104440383472	0.2474208880766804	0.5931492179244237	T	T	T
0.2487427941642548	0.2457449217229133	0.5936751571752427	T	T	T
0.3332909580984804	0.9165819161969608	0.4027260065404690	F	F	F
0.0832909580984804	0.9165819161969608	0.4027260065404690	F	F	F
0.1646952491480559	0.5793904982961190	0.4956500739556448	T	T	T
0.4162638166329180	0.5827969495628068	0.5008543982432206	T	T	T
0.5011329486986198	0.7484828565486253	0.5934188164479424	T	T	T
0.2558562526957561	0.7617125053914980	0.5977722229938061	T	T	T
0.8332909580984804	0.4165819161969608	0.4027260065404690	F	F	F
0.5832909580984804	0.4165819161969608	0.4027260065404690	F	F	F
0.6658569520931543	0.0819590097732201	0.4991175847010998	T	T	T
0.9160411665447196	0.0820823330894461	0.4995302887155666	T	T	T
-0.0026403902973397	0.2447192194053062	0.5947128055440075	T	T	T
0.7470021275586728	0.2457449217229133	0.5936751571752427	T	T	T
0.8332909580984804	0.9165819161969608	0.4027260065404690	F	F	F
0.5832909580984804	0.9165819161969608	0.4027260065404690	F	F	F

0.6656592714654879	0.5813185429309826	0.4997140935382020	T	T	T
0.9165331329298818	0.5827969495628068	0.5008543982432206	T	T	T
0.9973499078500195	0.7484828565486253	0.5934188164479424	T	T	T
0.7483768588148356	0.7467537176296569	0.5942696417902922	T	T	T

CeO_2 vacancy

Ce O Zr

1.0000000000000000

15.0049857511559779 0.0000000000000000 0.0000000000000000

-7.5024928755779881 13.0447800098917028 0.0000000000000000

0.0000000000000000 0.0000000000000000 31.5474089986390567

Ce O Zr

23 94 24

Selective dynamics

Direct

0.3332909580984804	0.1665819161969608	0.4027260065404690	F	F	F
0.0832909580984804	0.1665819161969608	0.4027260065404690	F	F	F
0.1664951013467828	0.3326966667405742	0.4981253117426334	T	T	T
0.4176828679361293	0.3368069846771959	0.5013800401628572	T	T	T
0.2553236250983844	0.4931586096349392	0.5996551873622380	T	T	T
0.3332909580984804	0.6665819161969608	0.4027260065404690	F	F	F
0.0832909580984804	0.6665819161969608	0.4027260065404690	F	F	F
0.1659979737315425	0.8316165616959168	0.4988654110970003	T	T	T
0.4150277583566719	0.8325335616194920	0.4975425019172519	T	T	T
0.4993328895569462	0.9982794893494784	0.5969993841379093	T	T	T
0.2463750214631233	0.9940225150170008	0.5996757264259429	T	T	T
0.8332909580984804	0.1665819161969608	0.4027260065404690	F	F	F
0.5832909580984804	0.1665819161969608	0.4027260065404690	F	F	F

0.6650217994304413	0.3356083541451724	0.5001097933993890	T	T	T
0.9148678901004033	0.3320020994433506	0.4995457364995062	T	T	T
0.0014350314677642	0.4943348580949163	0.5978560442923637	T	T	T
0.7579714764476435	0.5107554811325912	0.5959131205638712	T	T	T
0.8332909580984804	0.6665819161969608	0.4027260065404690	F	F	F
0.5832909580984804	0.6665819161969608	0.4027260065404690	F	F	F
0.6665716087064766	0.8315996373089405	0.4986988805909505	T	T	T
0.9195061395492701	0.8346551401188407	0.4975174190501903	T	T	T
0.0034713645507765	0.0025924150746022	0.5979218386938783	T	T	T
0.7482461925655528	0.9950126941873236	0.5999107625369007	T	T	T
0.4979569726550324	0.4959139453100718	0.3796635475034336	F	F	F
0.0022775938153288	0.2545551876306504	0.3771514688477424	F	F	F
0.2522775938153288	0.2545551876306504	0.3771514688477424	F	F	F
0.2479569726550324	0.4959139453100718	0.3796635475034336	F	F	F
0.3299443046387793	0.1616592735894358	0.4757937709607276	T	T	T
0.3340946579724928	0.4192822420111568	0.4730996176913251	T	T	T
0.0837018066702555	0.4198611796606144	0.4732913429892349	T	T	T
0.0806600423438653	0.1607125545322177	0.4753381564391361	T	T	T
0.1686249435419285	0.3372498870838498	0.4257884655775115	F	F	F
0.1643043223816321	0.0786086447632712	0.4283005442331955	F	F	F
0.4143043223816321	0.0786086447632712	0.4283005442331955	F	F	F
0.4186249435419285	0.3372498870838498	0.4257884655775115	F	F	F
0.1594997914022898	0.3256105145944233	0.5694786298477581	T	T	T
0.1674428629526545	0.0812746107832041	0.5710612449025163	T	T	T
0.4116575927737358	0.0774301433610631	0.5703492195283459	T	T	T
0.4098296925195442	0.3168972523601568	0.5729509735688509	T	T	T
0.0015337662746120	0.0057970639593847	0.5234502992188936	T	T	T
0.4948191452584041	0.2352964709954293	0.5225612638903101	T	T	T

0.2455955575433038	0.2426905271728259	0.5247622706997959	T	T	T
0.2512549775512269	0.0019623564642046	0.5224987057977231	T	T	T
0.3332394771125564	0.1632763882481640	0.6237088386451575	T	T	T
0.2966477866267070	0.3856331077899071	0.6263564224710052	T	T	T
0.0766834387203019	0.4025749247067267	0.6222201153073499	T	T	T
0.0844258432557226	0.1695177196481197	0.6207633966239783	T	T	T
0.4979569726550324	0.9959139453100718	0.3796635475034336	F	F	F
0.0022775938153288	0.7545551876306504	0.3771514688477424	F	F	F
0.2522775938153288	0.7545551876306504	0.3771514688477424	F	F	F
0.2479569726550324	0.9959139453100718	0.3796635475034336	F	F	F
0.3302983614241768	0.6623488931298809	0.4759178352374036	T	T	T
0.3338526120143541	0.9184451285267414	0.4722791994339062	T	T	T
0.0857785463252867	0.9204152317570475	0.4728674494506038	T	T	T
0.0805661123049077	0.6595644128222773	0.4758440843290828	T	T	T
0.1686249435419285	0.8372498870838498	0.4257884655775115	F	F	F
0.1643043223816321	0.5786086447632712	0.4283005442331955	F	F	F
0.4143043223816321	0.5786086447632712	0.4283005442331955	F	F	F
0.4186249435419285	0.8372498870838498	0.4257884655775115	F	F	F
0.1659262341065499	0.8295227282576434	0.5715216073444154	T	T	T
0.1668282907883736	0.5802320961343526	0.5719257805304494	T	T	T
0.4171234807720623	0.5931344066809459	0.5717505886042673	T	T	T
0.4119238229759361	0.8305848982298514	0.5697805640090010	T	T	T
0.0005350762316141	0.5007631529581076	0.5242767937746180	T	T	T
0.4995872924424276	0.7498653976391125	0.5233340705642107	T	T	T
0.2442136112972690	0.7401554249010900	0.5251250100904414	T	T	T
0.2532722542303105	0.5023792897200394	0.5233376633691691	T	T	T
0.3347629342510956	0.6789514534437728	0.6224716948071602	T	T	T
0.3293082577257209	0.9046722951509878	0.6220086513448138	T	T	T

0.0791272381241086	0.9039662540204532	0.6229862607988750	T	T	T
0.0886971528173319	0.6730487006512860	0.6209885114546552	T	T	T
0.9979569726550324	0.4959139453100718	0.3796635475034336	F	F	F
0.5022775938153288	0.2545551876306504	0.3771514688477424	F	F	F
0.7522775938153288	0.2545551876306504	0.3771514688477424	F	F	F
0.7479569726550324	0.4959139453100718	0.3796635475034336	F	F	F
0.8237114542030142	0.1576723147884209	0.4786460389827951	T	T	T
0.8342937585878261	0.4189777338038851	0.4731043830716573	T	T	T
0.5870101113882669	0.4199628806613021	0.4740143233574443	T	T	T
0.5849438471230641	0.1624797017037380	0.4755702104177928	T	T	T
0.6686249435419285	0.3372498870838498	0.4257884655775115	F	F	F
0.6643043223816321	0.0786086447632712	0.4283005442331955	F	F	F
0.9143043223816321	0.0786086447632712	0.4283005442331955	F	F	F
0.9186249435419285	0.3372498870838498	0.4257884655775115	F	F	F
0.6283436912296878	0.3600430692672631	0.5795791455237236	T	T	T
0.6693692288595017	0.0802644016407896	0.5692926672560077	T	T	T
0.9163508176636839	0.0867704429552205	0.5719711659734728	T	T	T
0.9165510982269964	0.3217178238575542	0.5722447828952468	T	T	T
0.5000345238682655	0.0038737129622533	0.5227328080713463	T	T	T
0.9954726208846978	0.2409976937046920	0.5228619314051741	T	T	T
0.7418899410622615	0.2518681460252665	0.5297294065223070	T	T	T
0.7504725990830252	0.9903953300996520	0.5269721538503163	T	T	T
0.8256282292515067	0.1635459905608627	0.6242428485690894	T	T	T
0.8210079173807188	0.3988242839279295	0.6166148357830252	T	T	T
0.5911365267313968	0.1766083904442795	0.6149416577039730	T	T	T
0.9979569726550324	0.9959139453100718	0.3796635475034336	F	F	F
0.5022775938153288	0.7545551876306504	0.3771514688477424	F	F	F
0.7522775938153288	0.7545551876306504	0.3771514688477424	F	F	F

0.7479569726550324	0.9959139453100718	0.3796635475034336	F	F	F
0.8334482952048603	0.6637191584545619	0.4757383516601692	T	T	T
0.8359219699349865	0.9208859674749448	0.4721074519249910	T	T	T
0.5869273494226235	0.9230828654165251	0.4733329671687585	T	T	T
0.5847958006745344	0.6664737676461669	0.4759189192686293	T	T	T
0.6686249435419285	0.8372498870838498	0.4257884655775115	F	F	F
0.6643043223816321	0.5786086447632712	0.4283005442331955	F	F	F
0.9143043223816321	0.5786086447632712	0.4283005442331955	F	F	F
0.9186249435419285	0.8372498870838498	0.4257884655775115	F	F	F
0.6436429714023646	0.7859122984411542	0.5857509260604203	T	T	T
0.6799137697883495	0.5952513368516179	0.5723281974247385	T	T	T
0.9205725952522599	0.5852208287126359	0.5717687583547999	T	T	T
0.9227501308325046	0.8324273408265341	0.5701499104754078	T	T	T
0.5038068180210473	0.5062218554669755	0.5184971968089442	T	T	T
0.9982616836989848	0.7421823674519388	0.5247868653997045	T	T	T
0.7524726419158227	0.7511107506766024	0.5238242068695200	T	T	T
0.7568875986594676	0.5058221584921228	0.5228578905199228	T	T	T
0.8480406495314270	0.6806487516172339	0.6227982959949188	T	T	T
0.8327917170042483	0.9083655174192771	0.6195924722704689	T	T	T
0.5760544907428482	0.9075515223680668	0.6195473689311868	T	T	T
0.3332909580984804	0.4165819161969608	0.4027260065404690	F	F	F
0.0832909580984804	0.4165819161969608	0.4027260065404690	F	F	F
0.1682291379410330	0.0838610893599139	0.4993943917631825	T	T	T
0.4116662103121911	0.0788173892335138	0.4978481273588500	T	T	T
0.4818990184973373	0.2320076125453809	0.5900834945276614	T	T	T
0.2520470590465393	0.2494516133060642	0.5951207847958671	T	T	T
0.3332909580984804	0.9165819161969608	0.4027260065404690	F	F	F
0.0832909580984804	0.9165819161969608	0.4027260065404690	F	F	F

0.1678058070880084	0.5802687457438367	0.4998357332530929	T	T	T
0.4174377130170512	0.5791336251253867	0.5018340289134784	T	T	T
0.4837007342058826	0.7477636726269239	0.5907736840146001	T	T	T
0.2463181999472468	0.7441413477369920	0.5945445240232488	T	T	T
0.8332909580984804	0.4165819161969608	0.4027260065404690	F	F	F
0.5832909580984804	0.4165819161969608	0.4027260065404690	F	F	F
0.6615428868965409	0.0808156532661997	0.4989170436532930	T	T	T
0.9161355045360295	0.0803752618260489	0.4998986082038215	T	T	T
0.0057953514089064	0.2483489998199744	0.5926792522590461	T	T	T
0.7540041032280485	0.2398153238858498	0.5967024011454782	T	T	T
0.8332909580984804	0.9165819161969608	0.4027260065404690	F	F	F
0.5832909580984804	0.9165819161969608	0.4027260065404690	F	F	F
0.6614062789949458	0.5811290772334132	0.5012974278184146	T	T	T
0.9174205216525522	0.5826087253927525	0.4985367957306792	T	T	T
0.0055290660500305	0.7487806640436574	0.5943267903657627	T	T	T
0.7680705483395087	0.7527997295118851	0.5908566810574811	T	T	T

Ni/pristine-CZO

Ce Ni O Zr

1.0000000000000000

15.0049857511559779 0.0000000000000000 0.0000000000000000

-7.5024928755779881 13.0447800098917028 0.0000000000000000

0.0000000000000000 0.0000000000000000 31.5474089986390567

Ce Ni O Zr

24 1 96 24

Selective dynamics

Direct

0.3332909580984804	0.1665819161969608	0.4027260065404690	F	F	F
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0.0832909580984804	0.1665819161969608	0.4027260065404690	F	F	F
0.1653274669327781	0.3324804504212799	0.4988930946651463	T	T	T
0.4163291273201106	0.3335966065505528	0.4992721099823466	T	T	T
0.4900221369258325	0.4870058022419393	0.6018376375024598	T	T	T
0.2446674390657206	0.4950236329893973	0.5984310944071599	T	T	T
0.3332909580984804	0.6665819161969608	0.4027260065404690	F	F	F
0.0832909580984804	0.6665819161969608	0.4027260065404690	F	F	F
0.1687800618272050	0.8328712139774910	0.4978376952180498	T	T	T
0.4173464293246287	0.8334887772087967	0.4986661350976962	T	T	T
0.5002750664684592	0.0002332451562379	0.5985887492956565	T	T	T
0.2536894053743296	0.0022877608236951	0.5988615700567022	T	T	T
0.8332909580984804	0.1665819161969608	0.4027260065404690	F	F	F
0.5832909580984804	0.1665819161969608	0.4027260065404690	F	F	F
0.6669251191097874	0.3343123194549767	0.4997444178853517	T	T	T
0.9153884178089567	0.3335583279392807	0.4994463726354699	T	T	T
0.9952244656257682	0.4970151314468634	0.6006550650818958	T	T	T
0.7391149196683895	0.4871060496854798	0.6040885004275034	T	T	T
0.8332909580984804	0.6665819161969608	0.4027260065404690	F	F	F
0.5832909580984804	0.6665819161969608	0.4027260065404690	F	F	F
0.6649052529807199	0.8307396455148690	0.4994492651816128	T	T	T
0.9180965612342697	0.8311192957175946	0.4991537653055518	T	T	T
0.0025862204473011	0.0008996815790791	0.5988248838984414	T	T	T
0.7485384443578418	0.9993981962698173	0.5983886024162852	T	T	T
0.6304947159974511	0.6756082458180404	0.6625486106409569	T	T	T
0.4979569726550324	0.4959139453100718	0.3796635475034336	F	F	F
0.0022775938153288	0.2545551876306504	0.3771514688477424	F	F	F
0.2522775938153288	0.2545551876306504	0.3771514688477424	F	F	F
0.2479569726550324	0.4959139453100718	0.3796635475034336	F	F	F

0.3302847137797034	0.1623832700564587	0.4755541994044629	T	T	T
0.3344783085160846	0.4200155690686635	0.4731073311422566	T	T	T
0.0836709258987216	0.4235753235446177	0.4747211975875179	T	T	T
0.0782917753222741	0.1573298208381183	0.4764264161682127	T	T	T
0.1686249435419285	0.3372498870838498	0.4257884655775115	F	F	F
0.1643043223816321	0.0786086447632712	0.4283005442331955	F	F	F
0.4143043223816321	0.0786086447632712	0.4283005442331955	F	F	F
0.4186249435419285	0.3372498870838498	0.4257884655775115	F	F	F
0.1577523296546647	0.3258177424302229	0.5705838171238883	T	T	T
0.1663262114534168	0.0824010193921109	0.5704454325028814	T	T	T
0.4168550613369716	0.0830262217739098	0.5708156486377702	T	T	T
0.4077481144358569	0.3218278193684630	0.5709554159225332	T	T	T
0.9983727647973203	0.9965293080629570	0.5251702971565877	T	T	T
0.4958778671522440	0.2423283897409703	0.5242056387567464	T	T	T
0.2433033457330670	0.2417867756000668	0.5243459889420885	T	T	T
0.2531114609758046	0.0047576197999646	0.5222713819420608	T	T	T
0.3328084614790283	0.1687222077798194	0.6215948364674380	T	T	T
0.3118966275826470	0.3950085670673479	0.6222906348282184	T	T	T
0.0757742917980793	0.4048994331345240	0.6224832923582553	T	T	T
0.0849493739507912	0.1685606059597332	0.6205237483857023	T	T	T
0.4979569726550324	0.9959139453100718	0.3796635475034336	F	F	F
0.0022775938153288	0.7545551876306504	0.3771514688477424	F	F	F
0.2522775938153288	0.7545551876306504	0.3771514688477424	F	F	F
0.2479569726550324	0.9959139453100718	0.3796635475034336	F	F	F
0.3287913355643178	0.6600663665164342	0.4761189919780526	T	T	T
0.3352398600646709	0.9195867615881290	0.4726338822971531	T	T	T
0.0848832781636750	0.9189950303848963	0.4731829517629862	T	T	T
0.0823111032718553	0.6593343515373452	0.4751850167308795	T	T	T

0.1686249435419285	0.8372498870838498	0.4257884655775115	F	F	F
0.1643043223816321	0.5786086447632712	0.4283005442331955	F	F	F
0.4143043223816321	0.5786086447632712	0.4283005442331955	F	F	F
0.4186249435419285	0.8372498870838498	0.4257884655775115	F	F	F
0.1730788706137035	0.8351754411863229	0.5697163966533324	T	T	T
0.1610191644442285	0.5780484975304429	0.5699444599645600	T	T	T
0.4177130309985829	0.5879086236831149	0.5723336302462387	T	T	T
0.4154981816898919	0.8315975619773197	0.5714397329357084	T	T	T
0.9864543730763324	0.5068034068594325	0.5278672014900593	T	T	T
0.4954342108834743	0.7444512869069807	0.5241491105589308	T	T	T
0.2474016655511415	0.7420816370123755	0.5248645718200038	T	T	T
0.2529464769061007	0.5022686989465648	0.5239431274828119	T	T	T
0.3282961270755509	0.6729608878602312	0.6202502855948088	T	T	T
0.3300936807120880	0.9072570472472922	0.6222333937455800	T	T	T
0.0845031560091687	0.9078871111971452	0.6224985541824370	T	T	T
0.1038082464417874	0.6828750595973370	0.6225020552779446	T	T	T
0.9979569726550324	0.4959139453100718	0.3796635475034336	F	F	F
0.5022775938153288	0.2545551876306504	0.3771514688477424	F	F	F
0.7522775938153288	0.2545551876306504	0.3771514688477424	F	F	F
0.7479569726550324	0.4959139453100718	0.3796635475034336	F	F	F
0.8285302450012878	0.1581036779574487	0.4765980910459410	T	T	T
0.8343219777360031	0.4192685034158072	0.4717660113356911	T	T	T
0.5871920008065241	0.4220599045904193	0.4743323907207920	T	T	T
0.5820545250000848	0.1623989291620154	0.4758481127074038	T	T	T
0.6686249435419285	0.3372498870838498	0.4257884655775115	F	F	F
0.6643043223816321	0.0786086447632712	0.4283005442331955	F	F	F
0.9143043223816321	0.0786086447632712	0.4283005442331955	F	F	F
0.9186249435419285	0.3372498870838498	0.4257884655775115	F	F	F

0.6619694349830425	0.3244112988742660	0.5715518935288952	T	T	T
0.6671133306095042	0.0830603910488600	0.5699499398147245	T	T	T
0.9184890030282535	0.0859202783214947	0.5703313635043475	T	T	T
0.9177008112939796	0.3282025303264640	0.5709311219496984	T	T	T
0.5013221741534266	0.0037641925461585	0.5227667823286078	T	T	T
0.9949261222457899	0.2419763469176043	0.5230879780013924	T	T	T
0.7475167982724006	0.2437740484773878	0.5246742746901218	T	T	T
0.7492840315803287	0.9969563218733294	0.5249484591119430	T	T	T
0.8342328391896109	0.1692515881640717	0.6201867806890727	T	T	T
0.8290859311983675	0.3935138040148585	0.6231941571147837	T	T	T
0.5635953338153715	0.3854808457821358	0.6257600873379994	T	T	T
0.5867682603090757	0.1689581927273198	0.6211956977975672	T	T	T
0.9979569726550324	0.9959139453100718	0.3796635475034336	F	F	F
0.5022775938153288	0.7545551876306504	0.3771514688477424	F	F	F
0.7522775938153288	0.7545551876306504	0.3771514688477424	F	F	F
0.7479569726550324	0.9959139453100718	0.3796635475034336	F	F	F
0.8320095748209715	0.6629321445398069	0.4755602632174856	T	T	T
0.8358906415691986	0.9199521152135401	0.4729790854771789	T	T	T
0.5859751910139080	0.9205933184438235	0.4730536240695161	T	T	T
0.5816186922854896	0.6614404453645971	0.4768982981426397	T	T	T
0.6686249435419285	0.8372498870838498	0.4257884655775115	F	F	F
0.6643043223816321	0.5786086447632712	0.4283005442331955	F	F	F
0.9143043223816321	0.5786086447632712	0.4283005442331955	F	F	F
0.9186249435419285	0.8372498870838498	0.4257884655775115	F	F	F
0.6532509210242972	0.8079443940965502	0.5761540156026987	T	T	T
0.6707764125387402	0.5948030434532100	0.5728055932804405	T	T	T
0.9150917931766847	0.6004565771787965	0.5932834806541697	T	T	T
0.9126477506666036	0.8093841876325361	0.5773725578467956	T	T	T

0.5014369208778725	0.5026205583103774	0.5236702711085440	T	T	T
0.9993116036600658	0.7366454079645990	0.5255937567758800	T	T	T
0.7525234551888813	0.7491840105436099	0.5227355735170067	T	T	T
0.7589733759493335	0.5072981031804438	0.5250185723297454	T	T	T
0.7467563821455406	0.6840608833396680	0.6513542522732659	T	T	T
0.8334329026612423	0.9136146889930147	0.6184652547020725	T	T	T
0.5793749234253496	0.9093887139476914	0.6208036790621138	T	T	T
0.5226617866241490	0.6785171025337057	0.6481901625016956	T	T	T
0.3332909580984804	0.4165819161969608	0.4027260065404690	F	F	F
0.0832909580984804	0.4165819161969608	0.4027260065404690	F	F	F
0.1672003309439053	0.0816736988905542	0.4992702742407882	T	T	T
0.4164253268721576	0.0826185894234664	0.4993589703610916	T	T	T
0.4966762584312772	0.2456382299708878	0.5944532083512410	T	T	T
0.2453158024457325	0.2453042313090684	0.5936372945600908	T	T	T
0.3332909580984804	0.9165819161969608	0.4027260065404690	F	F	F
0.0832909580984804	0.9165819161969608	0.4027260065404690	F	F	F
0.1691431483847796	0.5836892675512189	0.4996790498490317	T	T	T
0.4170076826086990	0.5809920719275125	0.5010875538813656	T	T	T
0.4872137600722857	0.7478136444798623	0.5953812142304661	T	T	T
0.2519450958786192	0.7484302048821625	0.5945515899979704	T	T	T
0.8332909580984804	0.4165819161969608	0.4027260065404690	F	F	F
0.5832909580984804	0.4165819161969608	0.4027260065404690	F	F	F
0.6646145400833783	0.0814239298737800	0.4991300913099398	T	T	T
0.9145531502209738	0.0796340088869138	0.4992941416270464	T	T	T
0.9965088051447332	0.2466924908694513	0.5924597152982278	T	T	T
0.7476389455621903	0.2452330891469394	0.5939840347915464	T	T	T
0.8332909580984804	0.9165819161969608	0.4027260065404690	F	F	F
0.5832909580984804	0.9165819161969608	0.4027260065404690	F	F	F

0.6653017434248981	0.5812901834238485	0.5020867024040790	T	T	T
0.9128449161837900	0.5801825313673742	0.4965954245728925	T	T	T
0.0235414797359608	0.7560176337719922	0.5937152252712752	T	T	T
0.7579432411967679	0.7568081134890854	0.5918217882614983	T	T	T

Ni₄/CZO(111)

Ce Ni O Zr

1.0000000000000000

15.0049857511559779 0.0000000000000000 0.0000000000000000

-7.5024928755779881 13.0447800098917028 0.0000000000000000

0.0000000000000000 0.0000000000000000 31.5474089986390567

Ce Ni O Zr

24 4 96 24

Selective dynamics

Direct

0.3332909580984804	0.1665819161969608	0.4027260065404690	F	F	F
0.0832909580984804	0.1665819161969608	0.4027260065404690	F	F	F
0.1672212167464462	0.3333492893996416	0.4989133339123679	T	T	T
0.4171294109407926	0.3347558237480974	0.5000702157175785	T	T	T
0.4992966789650426	0.4939956076269064	0.6036221169788580	T	T	T
0.2438429242812671	0.4908621567606410	0.5998064414079316	T	T	T
0.3332909580984804	0.6665819161969608	0.4027260065404690	F	F	F
0.0832909580984804	0.6665819161969608	0.4027260065404690	F	F	F
0.1665974005101436	0.8335839722572171	0.4986259095353989	T	T	T
0.4151626151911560	0.8323988459437142	0.4990813411775165	T	T	T
0.4982249243461235	0.0054806382985323	0.5980962330200406	T	T	T
0.2473619413159160	0.9995265726390256	0.5985569378030761	T	T	T
0.8332909580984804	0.1665819161969608	0.4027260065404690	F	F	F

0.5832909580984804	0.1665819161969608	0.4027260065404690	F	F	F
0.6665353176239774	0.3325160479404504	0.4987327441819511	T	T	T
0.9170804312883215	0.3332852648813202	0.4984778598242758	T	T	T
0.9988321181089758	0.4970374501686998	0.5976199661275819	T	T	T
0.7484730700528159	0.4950046844506824	0.5982858733100962	T	T	T
0.8332909580984804	0.6665819161969608	0.4027260065404690	F	F	F
0.5832909580984804	0.6665819161969608	0.4027260065404690	F	F	F
0.6676068188558110	0.8327193216848603	0.4999040361975944	T	T	T
0.9168316500237705	0.8330122687794553	0.4985515355679503	T	T	T
0.0009023010850073	0.9984071801185461	0.5983481436767601	T	T	T
0.7547335185771299	0.0016427536583369	0.6016055569649712	T	T	T
0.3914029900626660	0.6912778020153861	0.6736345745808825	T	T	T
0.4902414827590489	0.7281431432232237	0.7326572078634713	T	T	T
0.5592922899955394	0.6988748190354721	0.6743723874891907	T	T	T
0.5419831966085868	0.8415894635130912	0.6779748394202669	T	T	T
0.4979569726550324	0.4959139453100718	0.3796635475034336	F	F	F
0.0022775938153288	0.2545551876306504	0.3771514688477424	F	F	F
0.2522775938153288	0.2545551876306504	0.3771514688477424	F	F	F
0.2479569726550324	0.4959139453100718	0.3796635475034336	F	F	F
0.3308473378528307	0.1628309882747130	0.4758636035950996	T	T	T
0.3345687084091972	0.4191171271035110	0.4719306775702753	T	T	T
0.0881745383545602	0.4227810757754337	0.4740518110399755	T	T	T
0.0822029311297731	0.1623555637951603	0.4758064218523892	T	T	T
0.1686249435419285	0.3372498870838498	0.4257884655775115	F	F	F
0.1643043223816321	0.0786086447632712	0.4283005442331955	F	F	F
0.4143043223816321	0.0786086447632712	0.4283005442331955	F	F	F
0.4186249435419285	0.3372498870838498	0.4257884655775115	F	F	F
0.1599864342370271	0.3291555430267615	0.5703779077852751	T	T	T

0.1654736671564666	0.0819226058610627	0.5702123314694283	T	T	T
0.4162380149292200	0.0860935435304230	0.5716729057991634	T	T	T
0.4163108020907538	0.3265556388417661	0.5722290985054250	T	T	T
0.0007598107467899	0.0027189699977092	0.5225744727042396	T	T	T
0.4967380783547595	0.2424829984665694	0.5241071153787336	T	T	T
0.2469964733457918	0.2441584241710940	0.5253620514491025	T	T	T
0.2528486754176413	0.0040279359810870	0.5229359022813664	T	T	T
0.3305507718716273	0.1703023744364055	0.6215637843024344	T	T	T
0.3149961125531439	0.3956356937046784	0.6228472016560017	T	T	T
0.0764034261777744	0.4045043575869283	0.6223496536776277	T	T	T
0.0888282786282721	0.1738774637349581	0.6208503136732701	T	T	T
0.4979569726550324	0.9959139453100718	0.3796635475034336	F	F	F
0.0022775938153288	0.7545551876306504	0.3771514688477424	F	F	F
0.2522775938153288	0.7545551876306504	0.3771514688477424	F	F	F
0.2479569726550324	0.9959139453100718	0.3796635475034336	F	F	F
0.3289370323161298	0.6622369586575160	0.4754592883024994	T	T	T
0.3349006346946868	0.9194392304854245	0.4726580542315341	T	T	T
0.0854968508609028	0.9202505216369123	0.4729934305614792	T	T	T
0.0836005183067668	0.6625880487724527	0.4755835943346309	T	T	T
0.1686249435419285	0.8372498870838498	0.4257884655775115	F	F	F
0.1643043223816321	0.5786086447632712	0.4283005442331955	F	F	F
0.4143043223816321	0.5786086447632712	0.4283005442331955	F	F	F
0.4186249435419285	0.8372498870838498	0.4257884655775115	F	F	F
0.1625577110277901	0.8303588081213827	0.5711859794696672	T	T	T
0.1673403680129070	0.5821997097943800	0.5703158296978867	T	T	T
0.4207344806892791	0.5992113373187563	0.5859786921647372	T	T	T
0.4132873856696820	0.8218978722646325	0.5746576874773563	T	T	T
0.0018925097613603	0.5052392868002421	0.5226256964592790	T	T	T

0.4940250164011983	0.7394642045915532	0.5234876130398863	T	T	T
0.2473808752326614	0.7453041633935856	0.5258518996582928	T	T	T
0.2626449292240042	0.5068561187016057	0.5252568206255687	T	T	T
0.2940456226791539	0.6633522584070783	0.6354130507743767	T	T	T
0.3257587243255231	0.9059277486030741	0.6207265620053886	T	T	T
0.0790849911599671	0.9059655396456496	0.6226575142736900	T	T	T
0.0855298583964120	0.6737482836730651	0.6204710047101333	T	T	T
0.9979569726550324	0.4959139453100718	0.3796635475034336	F	F	F
0.5022775938153288	0.2545551876306504	0.3771514688477424	F	F	F
0.7522775938153288	0.2545551876306504	0.3771514688477424	F	F	F
0.7479569726550324	0.4959139453100718	0.3796635475034336	F	F	F
0.8288342060160357	0.1596031291325020	0.4759983928201523	T	T	T
0.8348454371190361	0.4192681938408750	0.4726143977262295	T	T	T
0.5848592159946644	0.4221577078160457	0.4744202970490843	T	T	T
0.5806128780233930	0.1594663955960463	0.4762513094413377	T	T	T
0.6686249435419285	0.3372498870838498	0.4257884655775115	F	F	F
0.6643043223816321	0.0786086447632712	0.4283005442331955	F	F	F
0.9143043223816321	0.0786086447632712	0.4283005442331955	F	F	F
0.9186249435419285	0.3372498870838498	0.4257884655775115	F	F	F
0.6647204322075639	0.3282006550708916	0.5703295611214552	T	T	T
0.6634377728242488	0.0832286212098557	0.5709134169331320	T	T	T
0.9222958690887419	0.0870343152234001	0.5712359296430761	T	T	T
0.9177254377976469	0.3326492407515493	0.5700123542443077	T	T	T
0.4971129328915949	0.0004749202865715	0.5243188843891842	T	T	T
0.9952584638479022	0.2422386609399217	0.5235139091883587	T	T	T
0.7478797995728449	0.2426394521051646	0.5247093637879322	T	T	T
0.7517493481143683	0.0002346009551216	0.5239533290273332	T	T	T
0.8411071492248288	0.1826099133232585	0.6207817593310064	T	T	T

0.8276962971671478	0.4033678098610000	0.6210815798466623	T	T	T
0.5831610468211355	0.3973465923336608	0.6243021560301828	T	T	T
0.5864169350391081	0.1732054791773763	0.6210541637282044	T	T	T
0.9979569726550324	0.9959139453100718	0.3796635475034336	F	F	F
0.5022775938153288	0.7545551876306504	0.3771514688477424	F	F	F
0.7522775938153288	0.7545551876306504	0.3771514688477424	F	F	F
0.7479569726550324	0.9959139453100718	0.3796635475034336	F	F	F
0.8292694629306718	0.6612894500289974	0.4759884119786955	T	T	T
0.8343530901725845	0.9192067793376717	0.4727143297179667	T	T	T
0.5845026800742955	0.9196833229751269	0.4740235388544273	T	T	T
0.5836139388410964	0.6629655630373487	0.4755950287691341	T	T	T
0.6686249435419285	0.8372498870838498	0.4257884655775115	F	F	F
0.6643043223816321	0.5786086447632712	0.4283005442331955	F	F	F
0.9143043223816321	0.5786086447632712	0.4283005442331955	F	F	F
0.9186249435419285	0.8372498870838498	0.4257884655775115	F	F	F
0.6535918590112273	0.8150748373938874	0.5763706696056038	T	T	T
0.6699920501940940	0.5839336456697357	0.5706959339124689	T	T	T
0.9170301113094464	0.5819794419545241	0.5716397845700104	T	T	T
0.9207293941679676	0.8291635759807129	0.5706729852530866	T	T	T
0.4959046865204327	0.5078193767641159	0.5248834157011638	T	T	T
0.9960274674575157	0.7399406672889927	0.5239920772730708	T	T	T
0.7490490519631033	0.7464936962882042	0.5258456766160891	T	T	T
0.7534926458579826	0.5029084283502961	0.5230861606707634	T	T	T
0.8436734996719264	0.6739989652643951	0.6211975125650080	T	T	T
0.8358548393303984	0.9011272211089117	0.6220656902309278	T	T	T
0.5748201928251618	0.9164655272820399	0.6300592604845495	T	T	T
0.6314909506359891	0.6679174313424194	0.6397564520826554	T	T	T
0.3332909580984804	0.4165819161969608	0.4027260065404690	F	F	F

0.0832909580984804	0.4165819161969608	0.4027260065404690	F	F	F
0.1658664907813616	0.0822183232074116	0.4990377392360574	T	T	T
0.4150271071357379	0.0820821034364556	0.4991424156460945	T	T	T
0.5008954631698889	0.2496446033439489	0.5936664850794678	T	T	T
0.2471354759130905	0.2450608025691182	0.5947981195205171	T	T	T
0.3332909580984804	0.9165819161969608	0.4027260065404690	F	F	F
0.0832909580984804	0.9165819161969608	0.4027260065404690	F	F	F
0.1663440334103027	0.5831752536695403	0.4995472308413765	T	T	T
0.4164124584181791	0.5801930737887397	0.4972441976633447	T	T	T
0.5006954421537856	0.7556936004583832	0.5914908447199092	T	T	T
0.2398227664455908	0.7480724976835927	0.5951310355845563	T	T	T
0.8332909580984804	0.4165819161969608	0.4027260065404690	F	F	F
0.5832909580984804	0.4165819161969608	0.4027260065404690	F	F	F
0.6666164108978213	0.0807317611726885	0.5000063104263035	T	T	T
0.9152308919873695	0.0806151936429070	0.4997613891239405	T	T	T
0.9979996997668654	0.2467755819898062	0.5929954350216369	T	T	T
0.7506522955783835	0.2469447877155588	0.5934351496312587	T	T	T
0.8332909580984804	0.9165819161969608	0.4027260065404690	F	F	F
0.5832909580984804	0.9165819161969608	0.4027260065404690	F	F	F
0.6663320539734390	0.5828483314860609	0.5007626799054083	T	T	T
0.9150153240181205	0.5806879089701393	0.4993833250340307	T	T	T
0.9990541564889760	0.7467078705102583	0.5933993130422710	T	T	T
0.7616175533221926	0.7473604640377489	0.5961864729781485	T	T	T

Ni/CeO₂^{vac} – CZO(111)

Ce Ni O Zr

1.0000000000000000

15.0049857511559779 0.0000000000000000 0.0000000000000000

-7.5024928755779881 13.0447800098917028 0.0000000000000000
0.0000000000000000 0.0000000000000000 31.5474089986390567

Ce Ni O Zr
23 1 94 24

Selective dynamics

Direct

0.3332909580984804	0.1665819161969608	0.4027260065404690	F	F	F
0.0832909580984804	0.1665819161969608	0.4027260065404690	F	F	F
0.1683962907728462	0.3334929341065530	0.4977802708403584	T	T	T
0.4173120413473951	0.3340159033322376	0.4989763944394224	T	T	T
0.2521125651785108	0.4994379960995847	0.5988053457804744	T	T	T
0.3332909580984804	0.6665819161969608	0.4027260065404690	F	F	F
0.0832909580984804	0.6665819161969608	0.4027260065404690	F	F	F
0.1652623910302603	0.8317749189957571	0.4981628263321918	T	T	T
0.4151436330270549	0.8333497076968611	0.4982174684981451	T	T	T
0.4980603341698462	0.9972628236574405	0.6002986150924728	T	T	T
0.2453568339146213	0.9927423309226663	0.5985598035563722	T	T	T
0.8332909580984804	0.1665819161969608	0.4027260065404690	F	F	F
0.5832909580984804	0.1665819161969608	0.4027260065404690	F	F	F
0.6655291977358738	0.3367273626881090	0.5002802341344654	T	T	T
0.9143239603085149	0.3306002430291947	0.5010665969674364	T	T	T
0.9978630794784480	0.4928134146766938	0.6014624916170513	T	T	T
0.7579466034108411	0.5097047685997312	0.5957028008001217	T	T	T
0.8332909580984804	0.6665819161969608	0.4027260065404690	F	F	F
0.5832909580984804	0.6665819161969608	0.4027260065404690	F	F	F
0.6663681114159465	0.8301668515815459	0.4999476105346192	T	T	T
0.9194343724597975	0.8350860551799120	0.4972385312630552	T	T	T
0.0026364661145453	0.0017323884401105	0.5984437860352346	T	T	T

0.7465125617675760	0.9941637253256184	0.6019290316134164	T	T	T
0.4269840579518233	0.4607107185248134	0.5760193558621408	T	T	T
0.4979569726550324	0.4959139453100718	0.3796635475034336	F	F	F
0.0022775938153288	0.2545551876306504	0.3771514688477424	F	F	F
0.2522775938153288	0.2545551876306504	0.3771514688477424	F	F	F
0.2479569726550324	0.4959139453100718	0.3796635475034336	F	F	F
0.3291416494257821	0.1623164558545164	0.4750587336065854	T	T	T
0.3364572747716730	0.4203610514332830	0.4724313381800412	T	T	T
0.0848337399867568	0.4194794414127884	0.4738032926791269	T	T	T
0.0834327740328008	0.1619022403699033	0.4753273035000902	T	T	T
0.1686249435419285	0.3372498870838498	0.4257884655775115	F	F	F
0.1643043223816321	0.0786086447632712	0.4283005442331955	F	F	F
0.4143043223816321	0.0786086447632712	0.4283005442331955	F	F	F
0.4186249435419285	0.3372498870838498	0.4257884655775115	F	F	F
0.1678951579709305	0.3293194843211356	0.5694729304815053	T	T	T
0.1662899270942426	0.0811863959630617	0.5704045044312173	T	T	T
0.4089187194873975	0.0788683559185661	0.5702509864390067	T	T	T
0.4200619996601024	0.3337059449966999	0.5735813269368975	T	T	T
0.9988711786302786	0.0066249946904433	0.5241603648925801	T	T	T
0.4916642431633719	0.2349843041767471	0.5221009485373219	T	T	T
0.2492704556152309	0.2419429132717300	0.5250406798182079	T	T	T
0.2506914495889608	0.0024579334817998	0.5216519416233969	T	T	T
0.3350269802162421	0.1715717451930998	0.6201566776684336	T	T	T
0.3284539111095482	0.4031151406292834	0.6194093227398036	T	T	T
0.0878979547760304	0.4004943839489953	0.6239708891936508	T	T	T
0.0972086545935181	0.1763915616630565	0.6217168854440971	T	T	T
0.4979569726550324	0.9959139453100718	0.3796635475034336	F	F	F
0.0022775938153288	0.7545551876306504	0.3771514688477424	F	F	F

0.2522775938153288	0.7545551876306504	0.3771514688477424	F	F	F
0.2479569726550324	0.9959139453100718	0.3796635475034336	F	F	F
0.3304880086425636	0.6618708892884925	0.4756055585516109	T	T	T
0.3328955358794555	0.9179131574232441	0.4718862033247596	T	T	T
0.0852854091072667	0.9218881678300154	0.4726368595447702	T	T	T
0.0806308928218542	0.6588572036624233	0.4758070566987588	T	T	T
0.1686249435419285	0.8372498870838498	0.4257884655775115	F	F	F
0.1643043223816321	0.5786086447632712	0.4283005442331955	F	F	F
0.4143043223816321	0.5786086447632712	0.4283005442331955	F	F	F
0.4186249435419285	0.8372498870838498	0.4257884655775115	F	F	F
0.1634773709284054	0.8304666423350173	0.5697458005859518	T	T	T
0.1689207290379944	0.5828891619217067	0.5709675866141363	T	T	T
0.4259282649347102	0.5851474291296916	0.5749361726397161	T	T	T
0.4105174813333917	0.8272923405063601	0.5701196408749066	T	T	T
0.9984023054511639	0.4980578696212711	0.5238032381486423	T	T	T
0.4952656290752072	0.7435631629523222	0.5239355597860784	T	T	T
0.2444284468928289	0.7423914729900011	0.5243856163413173	T	T	T
0.2566926206998146	0.5053447683601722	0.5235510755710818	T	T	T
0.3358759386425573	0.6738187448093155	0.6214329127025029	T	T	T
0.3167292698689522	0.8978824681972269	0.6229595903551104	T	T	T
0.0787047188294962	0.9062111102168207	0.6226213193431592	T	T	T
0.0908778097614037	0.6806236240443155	0.6215148493727191	T	T	T
0.9979569726550324	0.4959139453100718	0.3796635475034336	F	F	F
0.5022775938153288	0.2545551876306504	0.3771514688477424	F	F	F
0.7522775938153288	0.2545551876306504	0.3771514688477424	F	F	F
0.7479569726550324	0.4959139453100718	0.3796635475034336	F	F	F
0.8232271941041281	0.1559642900205038	0.4798597390675641	T	T	T
0.8339185376076954	0.4177101068324227	0.4730022866920007	T	T	T

0.5856596481740652	0.4225782356511200	0.4739792813157838	T	T	T
0.5848708202757255	0.1646132835179105	0.4755432992402451	T	T	T
0.6686249435419285	0.3372498870838498	0.4257884655775115	F	F	F
0.6643043223816321	0.0786086447632712	0.4283005442331955	F	F	F
0.9143043223816321	0.0786086447632712	0.4283005442331955	F	F	F
0.9186249435419285	0.3372498870838498	0.4257884655775115	F	F	F
0.6255223180684676	0.3655044262794888	0.5750568022647115	T	T	T
0.6704552730077976	0.0788323082547196	0.5671176590497983	T	T	T
0.9195965466760322	0.0928295946667353	0.5766046553819668	T	T	T
0.9131332379774268	0.3086145664199002	0.5755963527555638	T	T	T
0.4975558671588647	0.0040746105373383	0.5212021333068775	T	T	T
0.0001971467465651	0.2416594642784944	0.5230093020803277	T	T	T
0.7420222031899931	0.2528156677211854	0.5294578868481961	T	T	T
0.7584876089582377	0.9861889734939294	0.5290199772390903	T	T	T
0.7959180526679838	0.1466699987345679	0.6316670662359540	T	T	T
0.8095242564741768	0.3936131196411648	0.6154558109905445	T	T	T
0.5911652144055218	0.1872446423041683	0.6141695428453253	T	T	T
0.9979569726550324	0.9959139453100718	0.3796635475034336	F	F	F
0.5022775938153288	0.7545551876306504	0.3771514688477424	F	F	F
0.7522775938153288	0.7545551876306504	0.3771514688477424	F	F	F
0.7479569726550324	0.9959139453100718	0.3796635475034336	F	F	F
0.8311685072988916	0.6629443585997218	0.4755057417654098	T	T	T
0.8352051245121314	0.9199648971523333	0.4715335288168233	T	T	T
0.5884795001861153	0.9224650586826162	0.4746160721200247	T	T	T
0.5816110768327047	0.6604606246020340	0.4766708006400931	T	T	T
0.6686249435419285	0.8372498870838498	0.4257884655775115	F	F	F
0.6643043223816321	0.5786086447632712	0.4283005442331955	F	F	F
0.9143043223816321	0.5786086447632712	0.4283005442331955	F	F	F

0.9186249435419285	0.8372498870838498	0.4257884655775115	F	F	F
0.6457267933509304	0.7848878995735915	0.5823563504463969	T	T	T
0.6797723349242889	0.5952952058520585	0.5721355871631050	T	T	T
0.9190498811855792	0.5877805626624351	0.5708351367879210	T	T	T
0.9234810671375242	0.8327880867135957	0.5696258734655271	T	T	T
0.5016994022225266	0.5046309571065538	0.5245897149047893	T	T	T
0.9972837656856046	0.7424159631676505	0.5233116715592010	T	T	T
0.7533399088141097	0.7497292012755948	0.5229893887724898	T	T	T
0.7573889630019797	0.5067162673369890	0.5218254294160309	T	T	T
0.8478428595493309	0.6811498032828441	0.6229349932967557	T	T	T
0.8338955893734938	0.9060454810407403	0.6202510421667414	T	T	T
0.5769753937523399	0.8959483257224379	0.6211660415607371	T	T	T
0.3332909580984804	0.4165819161969608	0.4027260065404690	F	F	F
0.0832909580984804	0.4165819161969608	0.4027260065404690	F	F	F
0.1672621937406421	0.0829400573486978	0.4986938401736556	T	T	T
0.4112188964586216	0.0771723498548206	0.4982947589688097	T	T	T
0.4861883213561994	0.2331737130404968	0.5896002013855405	T	T	T
0.2516060958210368	0.2457933035376439	0.5937147872216209	T	T	T
0.3332909580984804	0.9165819161969608	0.4027260065404690	F	F	F
0.0832909580984804	0.9165819161969608	0.4027260065404690	F	F	F
0.1653047244730268	0.5804194282844471	0.5003109405647119	T	T	T
0.4160230213633100	0.5811221556080841	0.4993515767569213	T	T	T
0.4865776009715679	0.7497733723324300	0.5917142417115944	T	T	T
0.2438731720055729	0.7463424828495381	0.5941386685484878	T	T	T
0.8332909580984804	0.4165819161969608	0.4027260065404690	F	F	F
0.5832909580984804	0.4165819161969608	0.4027260065404690	F	F	F
0.6585866706207388	0.0825369299079103	0.4992761291230746	T	T	T
0.9139688858759701	0.0793635673924134	0.5005798900583154	T	T	T

0.0177824064529768	0.2534132148393001	0.5925737960646843	T	T	T
0.7503092820776771	0.2352934168886252	0.5975472395302763	T	T	T
0.8332909580984804	0.9165819161969608	0.4027260065404690	F	F	F
0.5832909580984804	0.9165819161969608	0.4027260065404690	F	F	F
0.6673165245508428	0.5833631019082169	0.5015101532505651	T	T	T
0.9183122218297000	0.5813010513572209	0.4989148073548185	T	T	T
0.0045215407468362	0.7477717911863807	0.5938619723144078	T	T	T
0.7697209720848179	0.7532027000052947	0.5907166106052691	T	T	T

Ni₄/CeO₂^{vac} – CZO(111)

Ce Ni O Zr

1.0000000000000000

15.0049857511559779 0.0000000000000000 0.0000000000000000

-7.5024928755779881 13.0447800098917028 0.0000000000000000

0.0000000000000000 0.0000000000000000 31.5474089986390567

Ce Ni O Zr

23 4 94 24

Selective dynamics

Direct

0.3332909580984804	0.1665819161969608	0.4027260065404690	F	F	F
0.0832909580984804	0.1665819161969608	0.4027260065404690	F	F	F
0.1689216165329629	0.3348862378374640	0.4989493548607812	T	T	T
0.4183017271010143	0.3356195358521570	0.5011475865982402	T	T	T
0.2589830668113048	0.4905357459307346	0.6075115768830157	T	T	T
0.3332909580984804	0.6665819161969608	0.4027260065404690	F	F	F
0.0832909580984804	0.6665819161969608	0.4027260065404690	F	F	F
0.1636547437919679	0.8306464854450190	0.4978585036059929	T	T	T

0.4125028825239994	0.8296563584882309	0.5003735481248801	T	T	T
0.4960680741103287	0.9954844691500827	0.6014613642832782	T	T	T
0.2432200541096306	0.9938361346423368	0.5993660059722064	T	T	T
0.8332909580984804	0.1665819161969608	0.4027260065404690	F	F	F
0.5832909580984804	0.1665819161969608	0.4027260065404690	F	F	F
0.6648507968581950	0.3347970309932465	0.5007445762521349	T	T	T
0.9167377973204874	0.3334044831757282	0.5028300981853492	T	T	T
0.0070178258219441	0.4952800876033544	0.6055383028085417	T	T	T
0.7583860362727709	0.5041457149471290	0.5955919530832092	T	T	T
0.8332909580984804	0.6665819161969608	0.4027260065404690	F	F	F
0.5832909580984804	0.6665819161969608	0.4027260065404690	F	F	F
0.6660969826293323	0.8314303492331361	0.4994632833789425	T	T	T
0.9188487063749887	0.8367852719899698	0.4971424033732885	T	T	T
-0.0009674548531838	-0.0001671881873300	0.5986113490879125	T	T	T
0.7480354509791559	-0.0006534140897110	0.6008254758539481	T	T	T
0.4869603276230798	0.5896796170738300	0.6525538328766151	T	T	T
0.5972130306861909	0.5319475837915734	0.6533573792435090	T	T	T
0.4415334112849061	0.4184903742816570	0.6252823277107855	T	T	T
0.5350982231886512	0.5603764858872436	0.5837243191126338	T	T	T
0.4979569726550324	0.4959139453100718	0.3796635475034336	F	F	F
0.0022775938153288	0.2545551876306504	0.3771514688477424	F	F	F
0.2522775938153288	0.2545551876306504	0.3771514688477424	F	F	F
0.2479569726550324	0.4959139453100718	0.3796635475034336	F	F	F
0.3302708524050119	0.1622199860693462	0.4751830434909194	T	T	T
0.3361049727987077	0.4219755776413171	0.4743922615217772	T	T	T
0.0836268761819532	0.4179599204561509	0.4718705402729537	T	T	T
0.0828148517646005	0.1625898592649142	0.4755417520234100	T	T	T
0.1686249435419285	0.3372498870838498	0.4257884655775115	F	F	F

0.1643043223816321	0.0786086447632712	0.4283005442331955	F	F	F
0.4143043223816321	0.0786086447632712	0.4283005442331955	F	F	F
0.4186249435419285	0.3372498870838498	0.4257884655775115	F	F	F
0.1707283689754973	0.3248553122177816	0.5711382442483096	T	T	T
0.1638311197745193	0.0781950895338984	0.5699351768499705	T	T	T
0.4079253347820317	0.0767722488218367	0.5697428811717175	T	T	T
0.4139944550862844	0.3250164520231719	0.5765102601947513	T	T	T
0.9981468104353323	0.0064440960980126	0.5237122906381880	T	T	T
0.4912761929823339	0.2347359313628536	0.5227613928785961	T	T	T
0.2496457887845553	0.2413042039863815	0.5246876332784077	T	T	T
0.2499240862042247	0.0012492686312955	0.5209513504140560	T	T	T
0.3308376733326469	0.1611226082986984	0.6223891403448297	T	T	T
0.3021236547489113	0.3617510754785380	0.6360510038477983	T	T	T
0.0775859506014680	0.3885572831475100	0.6263140493624573	T	T	T
0.0876333425987557	0.1666173345494918	0.6218233398925588	T	T	T
0.4979569726550324	0.9959139453100718	0.3796635475034336	F	F	F
0.0022775938153288	0.7545551876306504	0.3771514688477424	F	F	F
0.2522775938153288	0.7545551876306504	0.3771514688477424	F	F	F
0.2479569726550324	0.9959139453100718	0.3796635475034336	F	F	F
0.3317383744223879	0.6627840544800275	0.4753130408640592	T	T	T
0.3321151609657896	0.9153388392634026	0.4724268444932057	T	T	T
0.0847486439792405	0.9209435302159674	0.4724384307283872	T	T	T
0.0760842190712740	0.6568175412592551	0.4753996415328385	T	T	T
0.1686249435419285	0.8372498870838498	0.4257884655775115	F	F	F
0.1643043223816321	0.5786086447632712	0.4283005442331955	F	F	F
0.4143043223816321	0.5786086447632712	0.4283005442331955	F	F	F
0.4186249435419285	0.8372498870838498	0.4257884655775115	F	F	F
0.1595466698636258	0.8318318484273787	0.5694173192718235	T	T	T

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0.3966082112000216	0.8066351378132148	0.5783849028920783	T	T	T
0.0222818151914170	0.5018715855058489	0.5302267722169747	T	T	T
0.4979273695482324	0.7498955003747660	0.5236872805676670	T	T	T
0.2349108244747371	0.7311607890195089	0.5269470383106613	T	T	T
0.2484265347563737	0.5080114556097223	0.5251420207455930	T	T	T
0.4245007554229028	0.6638262897982737	0.6469430555852539	T	T	T
0.3132953194828077	0.9011935764172283	0.6248385669334579	T	T	T
0.0738537837817432	0.9049905059558435	0.6228197612899853	T	T	T
0.0789072078356405	0.6857666166266617	0.6236453947041055	T	T	T
0.9979569726550324	0.4959139453100718	0.3796635475034336	F	F	F
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0.7479569726550324	0.4959139453100718	0.3796635475034336	F	F	F
0.8252901190243903	0.1602162790997639	0.4798123087842605	T	T	T
0.8399906775506210	0.4230680018174802	0.4752736620242433	T	T	T
0.5852414280144690	0.4197866613126544	0.4731257255553242	T	T	T
0.5831469351149843	0.1599077526443061	0.4770611151529564	T	T	T
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0.9143043223816321	0.0786086447632712	0.4283005442331955	F	F	F
0.9186249435419285	0.3372498870838498	0.4257884655775115	F	F	F
0.6268622127771241	0.3604879494928608	0.5748874816783855	T	T	T
0.6694114077164169	0.0831487642108490	0.5675325347945902	T	T	T
0.9152884077885013	0.0906720470491619	0.5745072147100619	T	T	T
0.9108602427390725	0.3081326797496657	0.5757376423050485	T	T	T
0.4940188483139364	0.9954376297231293	0.5235997207893477	T	T	T

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0.7446724431803062	0.2584371642941918	0.5303564940506380	T	T	T
0.7523144572529057	0.9921546620131546	0.5260912877081092	T	T	T
0.7968142664988438	0.1489996984299748	0.6318096766979907	T	T	T
0.8109650523560352	0.3950424298669408	0.6185031357598791	T	T	T
0.5882013870659982	0.1836241856028698	0.6161815188737660	T	T	T
0.9979569726550324	0.9959139453100718	0.3796635475034336	F	F	F
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0.7522775938153288	0.7545551876306504	0.3771514688477424	F	F	F
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0.8330479430675984	0.6630834549933324	0.4749423563999031	T	T	T
0.8350029014709979	0.9209077151917525	0.4718828099646797	T	T	T
0.5853961499704482	0.9213842216383954	0.4737835099125737	T	T	T
0.5816643980933768	0.6638499907002483	0.4758958317537658	T	T	T
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0.9186249435419285	0.8372498870838498	0.4257884655775115	F	F	F
0.6518127054550713	0.7934540137920407	0.5792632827607141	T	T	T
0.6734039207021463	0.5938126752486430	0.5711749647776780	T	T	T
0.9170545153217192	0.5835955583114089	0.5695242116306694	T	T	T
0.9196824578644875	0.8330060107510255	0.5696686454156938	T	T	T
0.5067604779755212	0.5066753517215987	0.5217152699184513	T	T	T
0.9956348634357265	0.7434490120189023	0.5235768441392261	T	T	T
0.7527251986604228	0.7473860689687472	0.5226049191885814	T	T	T
0.7537119457679413	0.5074003990223274	0.5216700195398465	T	T	T
0.8416270451250729	0.6779666342952889	0.6218909343516004	T	T	T
0.8316236779987514	0.9052628158654510	0.6208560245478343	T	T	T

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0.3332909580984804	0.4165819161969608	0.4027260065404690	F	F	F
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0.1683627067883170	0.0836952506029704	0.4983975939852440	T	T	T
0.4112645979833159	0.0763569028885598	0.4986941967045909	T	T	T
0.4839707678503533	0.2292457751990551	0.5907614868221552	T	T	T
0.2445756295705096	0.2359502443069324	0.5950708657132218	T	T	T
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0.1655907787590472	0.5773349126176925	0.4966150823344145	T	T	T
0.4146652051621314	0.5821197039468594	0.5002486900834019	T	T	T
0.4977594272658312	0.7528128320829802	0.5943957258084928	T	T	T
0.2328560318825309	0.7530603615560090	0.5955462497520781	T	T	T
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0.6601345846502795	0.0779278503511146	0.4997281787286872	T	T	T
0.9148437083554214	0.0817117778068664	0.5003757143205138	T	T	T
0.0168144838556034	0.2527390510286481	0.5934017223278308	T	T	T
0.7498266915281319	0.2373732819627735	0.5984570380942940	T	T	T
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0.6649791739537816	0.5819793990758066	0.4984920809906180	T	T	T
0.9150501724367063	0.5852230070106698	0.4988316140495234	T	T	T
-0.0011391686184543	0.7480517897492841	0.5942568482036861	T	T	T
0.7692224252336377	0.7553852363965076	0.5912178328682574	T	T	T