

***Ab initio* Assessment of Bi_{1-x}RE_xCuOS (RE=La, Gd, Y, Lu) Solid Solution as Semiconductor for Photochemical Water Splitting**

Supplementary Information

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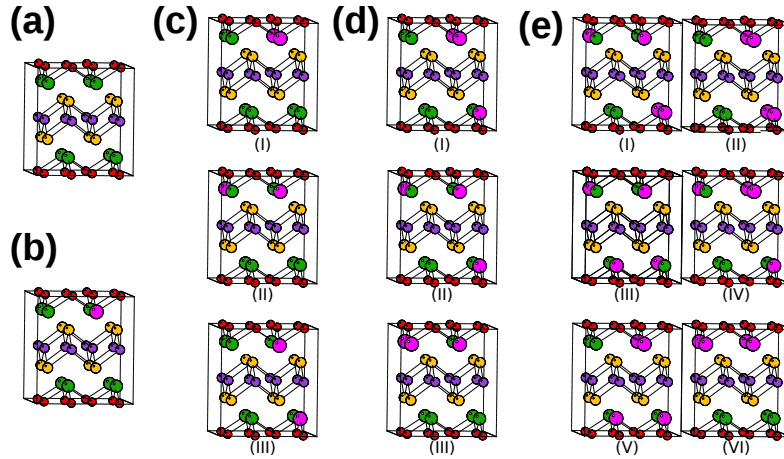


Figure S1 – Overview of all non-equivalent doping configurations for $x=0$ (a), 0.125 (b), 0.25 (c), 0.375 (d), and 0.5 (e). Configurations for $x=0.625$, 0.75 , 0.875 and 1 are the same as (d), (c), (b) and (a) respectively after inverting Bi and RE atoms.

$\text{Bi}_{1-x}\text{La}_x\text{CuOS}$		$\text{Bi}_{1-x}\text{Gd}_x\text{CuOS}$		$\text{Bi}_{1-x}\text{Y}_x\text{CuOS}$		$\text{Bi}_{1-x}\text{Lu}_x\text{CuOS}$	
ΔE	ΔG	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG
-0.177	-0.300	-0.037	-0.160	-0.022	-0.145	0.111	-0.008

Table S1 –Energies and free enthalpies (in eV) of reaction presented in Equation (3), for systems of $x=0.125$ doping. These energies were obtained by DFT calculations with HSE06 functional after geometry optimisation using PBE functional. At $T=200^\circ\text{C}$ the entropic part is $TS= -0.123$ eV.

	$\text{Bi}_{1-x}\text{La}_x\text{CuOS}$		$\text{Bi}_{1-x}\text{Gd}_x\text{CuOS}$		$\text{Bi}_{1-x}\text{Y}_x\text{CuOS}$		$\text{Bi}_{1-x}\text{Lu}_x\text{CuOS}$	
	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG
(I)	-0.234	-0.417	-0.095	-0.279	-0.080	-0.263	0.130	-0.053
(II)	-0.287	-0.470	-0.017	-0.200	0.016	-0.167	0.250	0.067
(III)	-0.373	-0.556	-0.051	-0.234	-0.017	-0.200	0.224	0.040

Table S2 Energies and free enthalpies (in eV) of reaction presented in Equation (3), for systems of $x=0.25$ doping. These energies were obtained by DFT calculations with HSE06 functional after geometry optimisation using PBE functional. At $T=200^\circ\text{C}$ the entropic part is $TS= -0.183$ eV. The most stable geometry is shown in bold with a blue background.

	$\text{Bi}_{1-x}\text{La}_x\text{CuOS}$		$\text{Bi}_{1-x}\text{Gd}_x\text{CuOS}$		$\text{Bi}_{1-x}\text{Y}_x\text{CuOS}$		$\text{Bi}_{1-x}\text{Lu}_x\text{CuOS}$	
	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG
(I)	-0.436	-0.651	-0.097	-0.312	-0.062	-0.277	0.230	0.015
(II)	-0.481	-0.697	-0.016	-0.232	0.033	-0.183	0.356	0.140
(III)	-0.188	-0.404	-0.098	-0.314	-0.079	-0.295	0.177	-0.039

Table S3 – Energies and free enthalpies (in eV) of reaction presented in Equation (3), for systems of $x=0.375$ doping. These energies were obtained by DFT calculations with HSE06 functional after geometry optimisation using PBE functional. At $T=200^\circ\text{C}$ the entropic part is $TS= -0.216$ eV. The most stable geometry is shown in bold with a blue background.

	Bi _{1-x} La _x CuOS		Bi _{1-x} Gd _x CuOS		Bi _{1-x} Y _x CuOS		Bi _{1-x} Lu _x CuOS	
	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG
(I)	-0.541	-0.767	-0.043	-0.269	0.009	-0.217	0.351	0.125
(II)	-0.509	-0.734	-0.126	-0.352	-0.089	-0.314	0.219	-0.007
(III)	-0.578	-0.804	0.041	-0.185	0.106	-0.120	0.482	0.256
(IV)	-0.394	-0.620	-0.079	-0.305	-0.044	-0.270	0.263	0.037
(V)	-0.494	-0.720	-0.124	-0.350	-0.087	-0.313	0.223	-0.003
(VI)	0.035	-0.191	-0.096	-0.322	-0.094	-0.320	0.130	-0.096

Table S4 – Energies and free enthalpies (in eV) of reaction presented in Equation (3), for systems of x=0.5 doping. These energies were obtained by DFT calculations with HSE06 functional after geometry optimisation using PBE functional. At T=200°C the entropic part is TS= -0.226 eV. The most stable geometry is shown in bold with a blue background.

	Bi _{1-x} La _x CuOS		Bi _{1-x} Gd _x CuOS		Bi _{1-x} Y _x CuOS		Bi _{1-x} Lu _x CuOS	
	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG
(I)	-0.457	-0.673	-0.103	-0.319	-0.069	-0.284	0.234	0.018
(II)	-0.486	-0.702	-0.018	-0.234	0.031	-0.184	0.371	0.156
(III)	-0.183	-0.399	-0.075	-0.291	-0.059	-0.275	0.196	-0.019

Table S5 – Energies and free enthalpies (in eV) of reaction presented in Equation (3), for systems of x=0.625 doping. These energies were obtained by DFT calculations with HSE06 functional after geometry optimisation using PBE functional. At T=200°C the entropic part is TS= -0.216 eV. The most stable geometry is shown in bold with a blue background.

	Bi _{1-x} La _x CuOS		Bi _{1-x} Gd _x CuOS		Bi _{1-x} Y _x CuOS		Bi _{1-x} Lu _x CuOS	
	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG
(I)	-0.250	-0.433	-0.088	-0.271	-0.070	-0.254	0.144	-0.039
(II)	-0.274	-0.457	0.002	-0.181	0.035	-0.149	0.292	0.109
(III)	-0.403	-0.586	-0.064	-0.247	-0.030	-0.213	0.233	0.049

Table S6 – Energies and free enthalpies (in eV) of reaction presented in Equation (3), for systems of x=0.75 doping. These energies were obtained by DFT calculations with HSE06 functional after geometry optimisation using PBE functional. At T=200°C the entropic part is TS= -0.183 eV. The most stable geometry is shown in bold with a blue background.

	Bi _{1-x} La _x CuOS		Bi _{1-x} Gd _x CuOS		Bi _{1-x} Y _x CuOS		Bi _{1-x} Lu _x CuOS	
	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG	ΔE	ΔG
	-0.212	-0.335	-0.038	-0.160	-0.023	-0.145	0.126	0.006

Table S7 – Energies and free enthalpies (in eV) of reaction presented in Equation (3), for systems of x=0.875 doping. These energies were obtained by DFT calculations with HSE06 functional after geometry optimisation using PBE functional. At T=200°C the entropic part is TS= -0.123 eV.

	$\text{Bi}_{1-x}\text{La}_x\text{CuOS}$	$\text{Bi}_{1-x}\text{Gd}_x\text{CuOS}$	$\text{Bi}_{1-x}\text{Y}_x\text{CuOS}$	$\text{Bi}_{1-x}\text{Lu}_x\text{CuOS}$
x=0	1.12	1.12	1.12	1.12
x=0.125	1.16	1.21	1.22	1.22
x=0.25	1.73	1.25	1.27	1.30
x=0.375	1.86	1.34	1.36	1.40
x=0.5	2.26	2.15	1.46	1.52
x=0.625	2.44*	2.37	2.39	2.14
x=0.75	2.61	2.45	2.50	2.50*
x=0.875	2.80	2.45	2.85*	2.65
x=1	2.93*	2.70*	2.75*	2.70*

Table S8 – HSE06+Spin Orbit coupling computed bandgap of the most stable structures for each composition. Bandgaps are indirect except the ones marked with an asterisk.

Pure systems				
	$m_e^* <110>$	$m_e^* <001>$	$m_h^* <110>$	$m_h^* <001>$
BiCuOS	0.38	1.48	0.38	2.44
LaCuOS	0.58	2.42	2.68	3.61
GdCuOS	0.66	2.75	1.54	2.75
YCuOS	0.68	7.15	1.31	5.92
LuCuOS	0.53	1.91	1.13	1.75
La-doping				
x=0.125	0.24	0.93	2.10	2.84
x=0.25	0.93	1.28	0.87	3.13
x=0.375	0.74	1.09	0.73	2.40
x=0.5	2.78	1.3	4.23	2.45
x=0.625				
x=0.75				
x=0.875				
Gd-doping				
x=0.125				
x=0.25				
x=0.375				
x=0.5	0.7	2.4	1.01	4.73
x=0.625	0.66	2.75	1.54	9.88
x=0.75				
x=0.875				
Y-doping				
x=0.125				
x=0.25				
x=0.375				
x=0.5				
x=0.625	0.68	7.15	1.31	5.92
x=0.75				
x=0.875				
Lu-doping				
x=0.125	0.28	0.70	0.40	1.62
x=0.25	0.28	0.67	0.65	1.58
x=0.375	0.52	1.13	1.01	8.84
x=0.5	0.37	1.19	0.66	0.92
x=0.625	1.94	0.54	1.13	1.75
x=0.75				
x=0.875				

Table S9 – Computed effective masses of the most stable structure for selected compositions.

	Vibrational contribution of dielectric constant	Electronic contribution of dielectric constant	Total dielectric constant
Pure systems			
BiCuOS	76.68	9.44	86.12
LaCuOS	16.50	5.92	22.42
GdCuOS	15.24	5.99	21.23
LuCuOS	11.70	5.99	17.69
YCuOS	20.26	6.00	26.26
La-doping			
x=0.125	50.76	8.79	59.55
x=0.25	36.42	8.13	44.55
x=0.375	27.29	7.61	34.90
x=0.5	22.41	7.11	29.52
x=0.625	19.89	6.74	26.63
x=0.75	18.34	6.42	24.76
x=0.875	17.52	6.15	23.67
Gd-doping			
x=0.125	52.16	8.85	61.01
x=0.25	41.41	8.35	49.76
x=0.375	33.11	7.93	41.03
x=0.5	26.28	7.36	33.64
x=0.625	21.50	6.97	28.47
x=0.75	18.81	6.64	25.45
x=0.875	16.67	6.29	22.96
Y-doping			
x=0.125	54.01	8.84	62.85
x=0.25	44.92	8.33	53.25
x=0.375	35.49	7.89	43.38
x=0.5	30.78	7.50	38.28
x=0.625	23.99	6.92	30.91
x=0.75	21.13	6.57	27.70
x=0.875	18.66	6.20	24.86
Lu-doping			
x=0.125	61.17	8.88	70.05
x=0.25	58.15	8.40	66.55
x=0.375	40.76	7.96	48.72
x=0.5	33.88	7.57	41.44
x=0.625	31.70	7.08	38.78
x=0.75	27.16	6.66	33.82
x=0.875	23.07	6.27	29.34

Table S10 – Computed electronic and vibrational parts and total dielectric constants of the most stable structure for each composition.

	x=0.00	0.125	0.25	0.375	0.5	0.625	0.75	0.875	1.00
La	1.02	1.81	4.88	6.45	19.76	19.48			11.01
Gd	1.02				12.10	22.03			12.94
Y	1.02					26.76			19.31
Lu	1.02	0.92	1.02	4.05	3.55	5.97			7.61

Table S11 – Computed exciton binding energies (in meV) for selected compositions.

Relaxed structure presented in the POSCAR format of VASP.

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BiCuOS
1.0000000000000000
3.8934916754179980 0.0000000000000000 -0.0000000000000000
-0.0000000000000000 3.8934916754179980 0.0000000000000000
0.0000000000000000 0.0000000000000000 8.6605153658131702
Bi Cu S O
2 2 2 2
Selective dynamics
Direct
0.2500000000000000 0.2500000000000000 0.1487049495444178 T T T
0.7500000000000000 0.7500000000000000 0.8512950504555823 T T T
0.7500000000000000 0.2500000000000000 0.5000000000000000 T T T
0.2500000000000000 0.7500000000000000 0.5000000000000000 T T T
0.2500000000000000 0.2500000000000000 0.6648937464540896 T T T
0.7500000000000000 0.7500000000000000 0.3351062535459102 T T T
0.7500000000000000 0.2500000000000000 -0.0000000000000000 T T T
0.2500000000000000 0.7500000000000000 -0.0000000000000000 T T T

LaCuOS
1.0000000000000000
4.0131267696612127 0.0000000000000000 -0.0000000000000000
0.0000000000000000 4.0131267696612127 -0.0000000000000000
-0.0000000000000000 0.0000000000000000 8.5711381383743390
La Cu S O
2 2 2 2
Selective dynamics
Direct
0.2500000000000000 0.2500000000000000 0.1492666654919752 T T T
0.7500000000000000 0.7500000000000000 0.8507333345080247 T T T
0.7500000000000000 0.2500000000000000 0.5000000000000000 T T T
0.2500000000000000 0.7500000000000000 0.5000000000000000 T T T
0.2500000000000000 0.2500000000000000 0.6586374784537635 T T T
0.7500000000000000 0.7500000000000000 0.3413625215462365 T T T
0.7500000000000000 0.2500000000000000 0.0000000000000000 T T T
0.2500000000000000 0.7500000000000000 0.0000000000000000 T T T

GdCuOS
1.0000000000000000
3.8606896707051792 -0.0000000000000000 0.0000000000000000
0.0000000000000000 3.8606896707051792 -0.0000000000000000
0.0000000000000000 0.0000000000000000 8.3931234652858215
Gd Cu S O
2 2 2 2
Selective dynamics
Direct
0.2500000000000000 0.2500000000000000 0.1396261833560211 T T T
0.7500000000000000 0.7500000000000000 0.8603738166439787 T T T
0.7500000000000000 0.2500000000000000 0.5000000000000000 T T T
0.2500000000000000 0.7500000000000000 0.5000000000000000 T T T
0.2500000000000000 0.2500000000000000 0.6724548661643395 T T T
0.7500000000000000 0.7500000000000000 0.3275451338356609 T T T
0.7500000000000000 0.2500000000000000 0.0000000000000000 T T T
0.2500000000000000 0.7500000000000000 0.0000000000000000 T T T

YCuOS
1.0000000000000000
3.8389669527259440 0.0000000000000000 -0.0000000000000000
-0.0000000000000000 3.8389669527259440 -0.0000000000000000
-0.0000000000000000 0.0000000000000000 8.4611608108579617
Y Cu S O
2 2 2 2

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Selective dynamics

Direct

0.2500000000000000	0.2500000000000000	0.1514965251712465	T	T	T
0.7500000000000000	0.7500000000000000	0.8485034748287534	T	T	T
0.7500000000000000	0.2500000000000000	0.5000000000000000	T	T	T
0.2500000000000000	0.7500000000000000	0.5000000000000000	T	T	T
0.2500000000000000	0.2500000000000000	0.6651830672217468	T	T	T
0.7500000000000000	0.7500000000000000	0.3348169327782531	T	T	T
0.7500000000000000	0.2500000000000000	-0.0000000000000000	T	T	T
0.2500000000000000	0.7500000000000000	-0.0000000000000000	T	T	T

LuCuOS

1.0000000000000000					
3.7036619095582060	0.0000000000000000	-0.0000000000000000			
-0.0000000000000000	3.7036619095582060	0.0000000000000000			
-0.0000000000000000	-0.0000000000000000	8.1417423421297777			

Lu Cu S O
2 2 2 2

Selective dynamics

Direct

0.2500000000000000	0.2500000000000000	0.1341039438631962	T	T	T
0.7500000000000000	0.7500000000000000	0.8658960561368040	T	T	T
0.7500000000000000	0.2500000000000000	0.5000000000000000	T	T	T
0.2500000000000000	0.7500000000000000	0.5000000000000000	T	T	T
0.2500000000000000	0.2500000000000000	0.6813728708114624	T	T	T
0.7500000000000000	0.7500000000000000	0.3186271291885378	T	T	T
0.7500000000000000	0.2500000000000000	-0.0000000000000000	T	T	T
0.2500000000000000	0.7500000000000000	0.0000000000000000	T	T	T

BiLaCuOS (x=12.5)

1.0000000000000000					
7.8134107813422817	0.0000000000000000	0.0000000000000000			
0.0000000000000000	7.8134107813422817	0.0000000000000000			
0.0000000000000000	-0.0000000000000000	8.6595459095883864			

Bi La Cu S O
7 1 8 8 8

Selective dynamics

Direct

0.2510517165905137	0.2510517165905137	0.1477258164000971	T	T	T
0.0000000000000000	0.5000000000000000	0.8565840797050306	T	T	T
0.0000000000000000	0.0000000000000000	0.8538341329527969	T	T	T
0.2510517165905137	0.7489482834094862	0.1477258164000971	T	T	T
0.7489482834094862	0.2510517165905137	0.1477258164000971	T	T	T
0.5000000000000000	0.0000000000000000	0.8565840797050305	T	T	T
0.7489482834094862	0.7489482834094862	0.1477258164000971	T	T	T
0.5000000000000000	0.5000000000000000	0.8315231142332202	T	T	T
0.0000000000000000	0.2494980556454923	0.5000768845833328	T	T	T
0.0000000000000000	0.7505019443545079	0.5000768845833328	T	T	T
0.5000000000000000	0.2492227827561163	0.4984829798279471	T	T	T
0.5000000000000000	0.7507772172438838	0.4984829798279471	T	T	T
0.2494980556454923	0.0000000000000000	0.5000768845833328	T	T	T
0.2492227827561163	0.5000000000000000	0.4984829798279471	T	T	T
0.7505019443545079	0.0000000000000000	0.5000768845833328	T	T	T
0.7507772172438838	0.5000000000000000	0.4984829798279471	T	T	T
0.2518167336394977	0.2518167336394977	0.6646302088068285	T	T	T
0.2518167336394977	0.7481832663605023	0.6646302088068285	T	T	T
0.7481832663605023	0.2518167336394977	0.6646302088068285	T	T	T
0.7481832663605023	0.7481832663605023	0.6646302088068285	T	T	T
0.0000000000000000	0.0000000000000000	0.3378094777675826	T	T	T
0.0000000000000000	0.5000000000000000	0.3382393682628984	T	T	T
0.5000000000000000	0.0000000000000000	0.3382393682628984	T	T	T
0.5000000000000000	0.5000000000000000	0.3342514832097712	T	T	T
0.0000000000000000	0.2477416753798956	0.0001983259364571	T	T	T
0.0000000000000000	0.7522583246201044	0.0001983259364571	T	T	T
0.5000000000000000	0.2452911225110964	0.0021195084205302	T	T	T
0.5000000000000000	0.7547088774889036	0.0021195084205302	T	T	T
0.2477416753798956	0.0000000000000000	0.0001983259364571	T	T	T
0.2452911225110964	0.5000000000000000	0.0021195084205302	T	T	T
0.7522583246201044	0.0000000000000000	0.0001983259364571	T	T	T
0.7547088774889036	0.5000000000000000	0.0021195084205302	T	T	T

BiLaCuOS (x=25%)

1.0000000000000000					
7.8402542206798982	-0.0007895518379023	-0.0076830924237132			
-0.0007895518379023	7.8402542206798973	-0.0076830924237132			

-0.0084210605849972 -0.0084210605849972 8.6584960393107888

Bi La Cu S O
6 2 8 8 8

Selective dynamics

Direct

0.2513526131556866	0.2513526131556866	0.1454277442225148	T	T	T
-0.0012637882608546	0.5002976137209967	0.8574916889606027	T	T	T
-0.0013526131556865	-0.0013526131556865	0.8545722557774852	T	T	T
0.2512637882608545	0.7497023862790033	0.1425083110393971	T	T	T
0.7497023862790033	0.2512637882608545	0.1425083110393971	T	T	T
0.5002976137209967	-0.0012637882608546	0.8574916889606027	T	T	T
0.5006496674268244	0.5006496674268244	0.8330869003542226	T	T	T
0.7493503325731756	0.7493503325731756	0.1669130996457776	T	T	T
0.0002737031268015	0.2497262968731985	0.5000000000000000	T	T	T
0.0010937215040661	0.7504316412043646	0.5026590476722705	T	T	T
0.4995683587956355	0.2489062784959339	0.4973409523277297	T	T	T
0.4992872691807727	0.7507127308192274	0.5000000000000000	T	T	T
0.2497262968731985	0.0002737031268015	0.5000000000000000	T	T	T
0.2489062784959339	0.4995683587956355	0.4973409523277297	T	T	T
0.7504316412043646	0.0010937215040661	0.5026590476722705	T	T	T
0.7507127308192274	0.4992872691807727	0.5000000000000000	T	T	T
0.2524069802612502	0.2524069802612502	0.6614711661027627	T	T	T
0.2524623122304951	0.7479738743507929	0.6617627671165525	T	T	T
0.7479738743507929	0.2524623122304951	0.6617627671165525	T	T	T
0.7483400901535899	0.7483400901535899	0.6658012203128736	T	T	T
-0.0024069802612503	-0.0024069802612503	0.3385288338972370	T	T	T
-0.0024623122304951	0.5020261256492071	0.3382372328834475	T	T	T
0.5020261256492071	-0.0024623122304951	0.3382372328834475	T	T	T
0.5016599098464101	0.5016599098464101	0.3341987796871265	T	T	T
0.0024258286051165	0.2475741713948835	-0.0000000000000000	T	T	T
0.0049361197029828	0.7523187732105895	-0.0020803433696670	T	T	T
0.4976812267894102	0.2450638802970172	0.0020803433696670	T	T	T
0.4951562363287699	0.7548437636712300	-0.0000000000000000	T	T	T
0.2475741713948835	0.0024258286051165	-0.0000000000000000	T	T	T
0.2450638802970172	0.4976812267894102	0.0020803433696670	T	T	T
0.7523187732105895	0.0049361197029828	-0.0020803433696670	T	T	T
0.7548437636712300	0.4951562363287699	-0.0000000000000000	T	T	T

BiLaCuOS (x=37.5%)

1.0000000000000000

7.8664794072418394	-0.0013256660248759	0.0000000000000000
-0.0013218616054771	7.8664590157718575	0.0000000000000000
0.0000000000000000	0.0000000000000000	8.6547874926553767

Bi La Cu S O
5 3 8 8 8

Selective dynamics

Direct

0.2505637018801886	0.2493864891457107	0.1370860768254534	T	T	T
0.7494362981198117	0.7506135108542891	0.1370860768254534	T	T	T
-0.0000000000000000	0.0000000000000000	0.8591703136655903	T	T	T
-0.0000000000000000	0.5000000000000000	0.8560189890077954	T	T	T
0.5000000000000000	0.5000000000000000	0.8592352484985170	T	T	T
0.7490892079891016	0.2490792389780920	0.1658475436642221	T	T	T
0.5000000000000000	0.0000000000000000	0.8355490976533085	T	T	T
0.2509107920108983	0.7509207610219080	0.1658475436642221	T	T	T
0.0011581197133231	0.2502561252347849	0.5025626289409625	T	T	T
0.9988418802866769	0.7497438747652151	0.5025626289409625	T	T	T
0.4990957931796109	0.2512163017964391	0.4993038027430208	T	T	T
0.5009042068203886	0.7487836982035612	0.4993038027430208	T	T	T
0.2486142205835914	0.0009128431702501	0.4994488662714177	T	T	T
0.2498280700903339	0.4988090436651422	0.5023296927682586	T	T	T
0.7513857794164088	0.9990871568297499	0.4994488662714177	T	T	T
0.7501719299096664	0.5011909563348579	0.5023296927682586	T	T	T
0.2525321765059729	0.2475424986287478	0.6591620701995892	T	T	T
0.2522674684955968	0.7521943337502884	0.6607825563445353	T	T	T
0.7477325315044031	0.2478056662497115	0.6607825563445353	T	T	T
0.7474678234940274	0.7524575013712520	0.6591620701995892	T	T	T
-0.0000000000000000	0.0000000000000000	0.3371054857729439	T	T	T
-0.0000000000000000	0.5000000000000000	0.3379082548980337	T	T	T
0.5000000000000000	0.0000000000000000	0.3333517059743797	T	T	T
0.5000000000000000	0.5000000000000000	0.3370485915486284	T	T	T
0.0022543786898070	0.2524585841685692	0.9978353494669326	T	T	T
0.9977456213101932	0.7475414158314304	0.9978353494669326	T	T	T
0.4977317762111242	0.2550369816394853	0.0000551205049998	T	T	T
0.5022682237888761	0.7449630183605146	0.0000551205049998	T	T	T

0.2449475205765846	0.0022548299840426	0.0000090095076616	T	T	T
0.2475082315739541	0.4977424160809235	-0.0021165607466671	T	T	T
0.7550524794234154	0.9977451700159575	0.0000090095076616	T	T	T
0.7524917684260458	0.5022575839190766	-0.0021165607466671	T	T	T

BiLaCuOS (x=50%)

1.0000000000000000					
7.8949445563465739	-0.0032910648406030	0.0000000000000000			
-0.0032910648406030	7.8949445563465739	0.0000000000000000			
0.0000000000000000	0.0000000000000000	8.6494766774483800			

Bi La Cu S O
4 4 8 8 8

Selective dynamics

Direct

0.2500000000000000	0.2500000000000000	0.1357039665310918	T	T	T
0.7500000000000000	0.7500000000000000	0.1357039665310918	T	T	T
-0.0000000000000000	0.0000000000000000	0.8642960334689085	T	T	T
0.5000000000000000	0.5000000000000000	0.8642960334689085	T	T	T
0.2500000000000000	0.7500000000000000	0.1633372760031325	T	T	T
0.7500000000000000	0.2500000000000000	0.1633372760031325	T	T	T
-0.0000000000000000	0.5000000000000000	0.8366627239968677	T	T	T
0.5000000000000000	0.0000000000000000	0.8366627239968677	T	T	T
0.0013586378512803	0.2486413621487197	0.5000000000000000	T	T	T
-0.0013586378512803	0.7513586378512804	0.5000000000000000	T	T	T
0.4986413621487197	0.2513586378512803	0.5000000000000000	T	T	T
0.5013586378512804	0.7486413621487196	0.5000000000000000	T	T	T
0.2486413621487197	0.0013586378512803	0.5000000000000000	T	T	T
0.2513586378512803	0.4986413621487197	0.5000000000000000	T	T	T
0.7513586378512804	-0.0013586378512803	0.5000000000000000	T	T	T
0.7486413621487196	0.5013586378512804	0.5000000000000000	T	T	T
0.2500000000000000	0.2500000000000000	0.6603588608876407	T	T	T
0.2500000000000000	0.7500000000000000	0.6616055047587575	T	T	T
0.7500000000000000	0.2500000000000000	0.6616055047587575	T	T	T
0.7500000000000000	0.7500000000000000	0.6603588608876407	T	T	T
-0.0000000000000000	0.0000000000000000	0.3396411391123596	T	T	T
-0.0000000000000000	0.5000000000000000	0.3383944952412425	T	T	T
0.5000000000000000	0.0000000000000000	0.3383944952412425	T	T	T
0.5000000000000000	0.5000000000000000	0.3396411391123596	T	T	T
0.0023526081436498	0.2476473918563503	0.0000000000000000	T	T	T
-0.0023526081436498	0.7523526081436498	0.0000000000000000	T	T	T
0.4976473918563504	0.2523526081436496	0.0000000000000000	T	T	T
0.5023526081436499	0.7476473918563502	0.0000000000000000	T	T	T
0.2476473918563503	0.0023526081436498	0.0000000000000000	T	T	T
0.2523526081436496	0.4976473918563504	0.0000000000000000	T	T	T
0.7523526081436499	-0.0023526081436498	0.0000000000000000	T	T	T
0.7476473918563501	0.5023526081436499	0.0000000000000000	T	T	T

BiLaCuOS (x=67.5%)

1.0000000000000000					
7.9307009663115462	-0.0034546494114190	0.0000000000000000			
-0.0034548886714905	7.9303890580847929	0.0000000000000000			
0.0000000000000000	0.0000000000000000	8.6252592521958409			

La Bi Cu S O
5 3 8 8 8

Selective dynamics

Direct

0.2480944357639694	0.2519167438439015	0.1599973167381163	T	T	T
0.7519055642360306	0.7480832561560984	0.1599973167381163	T	T	T
-0.0000000000000000	-0.0000000000000000	0.8405860392119242	T	T	T
-0.0000000000000000	0.5000000000000000	0.8431931812663543	T	T	T
0.5000000000000000	0.0000000000000000	0.8406082706104390	T	T	T
0.7516625475704953	0.2516273232917015	0.1334225243577844	T	T	T
0.5000000000000000	-0.0000000000000000	0.8661800850553207	T	T	T
0.2483374524295047	0.7483726767082982	0.1334225243577844	T	T	T
-0.0014934277791790	0.2509736091492228	0.4991576508377084	T	T	T
0.0014934277791789	0.7490263908507777	0.4991576508377084	T	T	T
0.5023258949990225	0.2491228529926495	0.5000468215386955	T	T	T
0.4976741050009775	0.7508771470073506	0.5000468215386955	T	T	T
0.2509522768905282	-0.0020954126933197	0.5000983477330638	T	T	T
0.2489918048876248	0.5015909236617146	0.4991490019555930	T	T	T
0.7490477231094718	0.0020954126933197	0.5000983477330638	T	T	T
0.7510081951123750	0.4984090763382851	0.4991490019555930	T	T	T

0.2476369692413021	0.2524678305794318	0.6634658667364464	T	T	T
0.2473612896030550	0.7474351765161703	0.6627509633419494	T	T	T
0.7526387103969451	0.2525648234838298	0.6627509633419494	T	T	T
0.7523630307586978	0.7475321694205689	0.6634658667364464	T	T	T
-0.0000000000000000	-0.0000000000000000	0.3426639264558756	T	T	T
-0.0000000000000000	0.5000000000000000	0.3396077207981182	T	T	T
0.5000000000000000	-0.0000000000000000	0.3447951996614629	T	T	T
0.5000000000000000	0.5000000000000000	0.3426217071585690	T	T	T
-0.0021262181354252	0.2477076587992775	0.0004756982626372	T	T	T
0.0021262181354253	0.7522923412007226	0.0004756982626372	T	T	T
0.5024676323671231	0.2455209861931050	0.0004194095336067	T	T	T
0.4975323676328768	0.7544790138068950	0.0004194095336067	T	T	T
0.2544648443448071	-0.0024498382723339	0.0004008400276819	T	T	T
0.2522901075057833	0.5021405316027445	0.0004874938276707	T	T	T
0.7455351556551928	0.0024498382723339	0.0004008400276819	T	T	T
0.7477098924942168	0.4978594683972556	0.0004874938276707	T	T	T

BiLaCuOS (x=75%)

1.0000000000000000					
7.9631344891082216	-0.0021958010530973	-0.0049677783450732			
-0.0021958010530973	7.9631344891082216	-0.0049677783450732			
-0.0053600833501644	-0.0053600833501644	8.6044870657701882			

Bi La Cu S O
2 6 8 8 8

Selective dynamics

Direct

0.4985045529840761	0.4985045529840761	0.8679526984202722	T	T	T
0.7514954470159237	0.7514954470159237	0.1320473015797272	T	T	T
0.2486443479997437	0.2486443479997437	0.1537427609339809	T	T	T
0.0015803293328165	0.4980601775921769	0.8437774492710020	T	T	T
0.0013556520002562	0.0013556520002562	0.8462572390660191	T	T	T
0.2484196706671835	0.7519398224078233	0.1562225507289980	T	T	T
0.7519398224078233	0.2484196706671835	0.1562225507289980	T	T	T
0.4980601775921769	0.0015803293328165	0.8437774492710020	T	T	T
0.0010060340842436	0.2489939659157565	0.5000000000000000	T	T	T
-0.0010687804416718	0.7511004485562826	0.4978784060453065	T	T	T
0.4988995514437174	0.2510687804416717	0.5021215939546934	T	T	T
0.5012969431030561	0.7487030568969439	0.5000000000000000	T	T	T
0.2489939659157565	0.0010060340842436	0.5000000000000000	T	T	T
0.2510687804416717	0.4988995514437174	0.5021215939546934	T	T	T
0.7511004485562826	-0.0010687804416718	0.4978784060453065	T	T	T
0.7487030568969439	0.5012969431030561	0.5000000000000000	T	T	T
0.2474907286147730	0.2474907286147730	0.6628839645699927	T	T	T
0.2474977717789098	0.7527609353579823	0.6594782458286690	T	T	T
0.7527609353579823	0.2474977717789098	0.6594782458286690	T	T	T
0.7528390864948993	0.7528390864948993	0.6571160989504388	T	T	T
0.0025092713852269	0.0025092713852269	0.3371160354300077	T	T	T
0.002502282210903	0.4972390646420176	0.3405217541713309	T	T	T
0.4972390646420176	0.002502282210903	0.3405217541713309	T	T	T
0.4971609135051007	0.4971609135051007	0.3428839010495607	T	T	T
-0.0021041107159294	0.2521041107159294	-0.0000000000000000	T	T	T
-0.0041928671043160	0.7477070191509985	0.0003634125610048	T	T	T
0.5022929808490015	0.2541928671043157	-0.0003634125610048	T	T	T
0.5045660748061103	0.7454339251938897	-0.0000000000000000	T	T	T
0.2521041107159294	-0.0021041107159294	-0.0000000000000000	T	T	T
0.2541928671043157	0.5022929808490015	-0.0003634125610048	T	T	T
0.7477070191509985	-0.0041928671043160	0.0003634125610048	T	T	T
0.7454339251938897	0.5045660748061103	-0.0000000000000000	T	T	T

BiLaCuOS (x=87.5%)

1.0000000000000000					
7.9966005245831573	0.0000000000000000	0.0000000000000000			
0.0000000000000000	7.9966005245831573	0.0000000000000000			
0.0000000000000000	0.0000000000000000	8.5855876609179553			

Bi La Cu S O
1 7 8 8 8

Selective dynamics

Direct

0.5000000000000000	0.5000000000000000	0.8700394998849206	T	T	T
0.2484688761139641	0.2484688761139641	0.1521788419725181	T	T	T
-0.0000000000000000	0.5000000000000000	0.8470649626686411	T	T	T
-0.0000000000000000	0.0000000000000000	0.8492445916906763	T	T	T

0.2484688761139641	0.7515311238860358	0.1521788419725181	T	T	T
0.7515311238860358	0.2484688761139641	0.1521788419725181	T	T	T
0.5000000000000000	0.0000000000000000	0.8470649626686411	T	T	T
0.7515311238860358	0.7515311238860358	0.1521788419725181	T	T	T
-0.0000000000000000	0.2489025167858267	0.4989736867091326	T	T	T
-0.0000000000000000	0.7510974832141731	0.4989736867091326	T	T	T
0.5000000000000000	0.2515709730728413	0.5018278584549227	T	T	T
0.5000000000000000	0.7484290269271585	0.5018278584549227	T	T	T
0.2489025167858267	0.0000000000000000	0.4989736867091326	T	T	T
0.2515709730728413	0.5000000000000000	0.5018278584549227	T	T	T
0.7510974832141731	0.0000000000000000	0.4989736867091326	T	T	T
0.7484290269271585	0.5000000000000000	0.5018278584549227	T	T	T
0.2472778631147236	0.2472778631147236	0.6563619828315376	T	T	T
0.2472778631147236	0.7527221368852764	0.6563619828315376	T	T	T
0.7527221368852764	0.2472778631147236	0.6563619828315376	T	T	T
0.7527221368852764	0.7527221368852764	0.6563619828315376	T	T	T
-0.0000000000000000	0.0000000000000000	0.3346691656241303	T	T	T
-0.0000000000000000	0.5000000000000000	0.3382190860851570	T	T	T
0.5000000000000000	0.0000000000000000	0.3382190860851570	T	T	T
0.5000000000000000	0.5000000000000000	0.3406588355765947	T	T	T
-0.0000000000000000	0.2520433022209829	-0.0000785445589861	T	T	T
-0.0000000000000000	0.7479566977790170	-0.0000785445589861	T	T	T
0.5000000000000000	0.2542180528701729	-0.0005588729801052	T	T	T
0.5000000000000000	0.7457819471298273	-0.0005588729801052	T	T	T
0.2520433022209829	0.0000000000000000	-0.0000785445589861	T	T	T
0.2542180528701729	0.5000000000000000	-0.0005588729801052	T	T	T
0.7479566977790170	0.0000000000000000	-0.0000785445589861	T	T	T
0.7457819471298273	0.5000000000000000	-0.0005588729801052	T	T	T

BiGdCuOS (x=12.5%)

1.0000000000000000					
7.7766436663365095	0.0000000000000000	0.0000000000000000			
0.0000000000000000	7.7766436663365095	-0.0000000000000000			
0.0000000000000000	-0.0000000000000000	8.6201696323455401			

Bi Gd Cu S O
7 1 8 8 8

Selective dynamics

Direct

0.2521510994583109	0.2521510994583109	0.1461257923757674	T	T	T
0.0000000000000000	0.5000000000000000	0.8512834259186048	T	T	T
0.0000000000000000	-0.0000000000000000	0.8520917491143472	T	T	T
0.2521510994583109	0.7478489005416890	0.1461257923757674	T	T	T
0.7478489005416890	0.2521510994583109	0.1461257923757674	T	T	T
0.5000000000000000	-0.0000000000000000	0.8512834259186048	T	T	T
0.7478489005416890	0.7478489005416890	0.1461257923757674	T	T	T
0.5000000000000000	0.5000000000000000	0.8465480174469182	T	T	T
0.0000000000000000	0.2508531118419769	0.5015344198015814	T	T	T
0.0000000000000000	0.7491468881580231	0.5015344198015814	T	T	T
0.5000000000000000	0.2515954040426265	0.5008519657594497	T	T	T
0.5000000000000000	0.7484045959573739	0.5008519657594497	T	T	T
0.2508531118419769	-0.0000000000000000	0.5015344198015814	T	T	T
0.2515954040426265	0.5000000000000000	0.5008519657594497	T	T	T
0.7491468881580231	-0.0000000000000000	0.5015344198015814	T	T	T
0.7484045959573739	0.5000000000000000	0.5008519657594497	T	T	T
0.2542289383689414	0.2542289383689414	0.6688057991958107	T	T	T
0.2542289383689414	0.7457710616310586	0.6688057991958107	T	T	T
0.7457710616310586	0.2542289383689414	0.6688057991958107	T	T	T
0.7457710616310586	0.7457710616310586	0.6688057991958107	T	T	T
0.0000000000000000	-0.0000000000000000	0.3405291517879169	T	T	T
0.0000000000000000	0.5000000000000000	0.3371467287644348	T	T	T
0.5000000000000000	-0.0000000000000000	0.3371467287644348	T	T	T
0.5000000000000000	0.5000000000000000	0.3317442655489522	T	T	T
0.0000000000000000	0.2492733352108961	0.9996571230337781	T	T	T
0.0000000000000000	0.7507266647891038	0.9996571230337781	T	T	T
0.5000000000000000	0.2511471553940484	0.9960815265175518	T	T	T
0.5000000000000000	0.7488528446059514	0.9960815265175518	T	T	T
0.2492733352108961	-0.0000000000000000	0.9996571230337781	T	T	T
0.2511471553940484	0.5000000000000000	0.9960815265175518	T	T	T
0.7507266647891038	-0.0000000000000000	0.9996571230337781	T	T	T
0.7488528446059514	0.5000000000000000	0.9960815265175518	T	T	T

BiGdCuOS (x=25%)

1.0000000000000000					
7.7562751162745744	0.0000000000000000	0.0000000000000000			

0.0000000000000000 7.7761272183348629 0.0000000000000000
 0.0000000000000000 0.0000000000000000 8.5847003177976902
 Bi Gd Cu S O
 6 2 8 8 8

Selective dynamics

Direct

0.2500000000000000	0.2537844394765629	0.1432034945638914	T	T	T
0.7500000000000000	0.7462155605234371	0.1432034945638914	T	T	T
0.0000000000000000	-0.0000000000000000	0.8510368558292108	T	T	T
0.2500000000000000	0.7462155605234371	0.1432034945638914	T	T	T
0.7500000000000000	0.2537844394765629	0.1432034945638914	T	T	T
0.5000000000000000	-0.0000000000000000	0.8510368558292108	T	T	T
0.5000000000000000	0.5000000000000000	0.8472517626628319	T	T	T
0.0000000000000000	0.5000000000000000	0.8472517626628319	T	T	T
0.0000000000000000	0.2530646698848120	0.5040939379510354	T	T	T
0.0000000000000000	0.7469353301151879	0.5040939379510354	T	T	T
0.5000000000000000	0.2530646698848120	0.5040939379510354	T	T	T
0.5000000000000000	0.7469353301151879	0.5040939379510354	T	T	T
0.2500000000000000	-0.0000000000000000	0.5032625335936163	T	T	T
0.2500000000000000	0.5000000000000000	0.5006049595658441	T	T	T
0.7500000000000000	-0.0000000000000000	0.5032625335936163	T	T	T
0.7500000000000000	0.5000000000000000	0.5006049595658441	T	T	T
0.2500000000000000	0.2589357385279496	0.6724224343645225	T	T	T
0.2500000000000000	0.7410642614720503	0.6724224343645225	T	T	T
0.7500000000000000	0.2589357385279496	0.6724224343645225	T	T	T
0.7500000000000000	0.7410642614720503	0.6724224343645225	T	T	T
0.0000000000000000	-0.0000000000000000	0.3433346497323559	T	T	T
0.0000000000000000	0.5000000000000000	0.3335683628149436	T	T	T
0.5000000000000000	-0.0000000000000000	0.3433346497323559	T	T	T
0.5000000000000000	0.5000000000000000	0.3335683628149436	T	T	T
0.0000000000000000	0.2497359841734478	0.9949154016931333	T	T	T
-0.0000000000000000	0.7502640158265522	0.9949154016931333	T	T	T
0.5000000000000000	0.2497359841734478	0.9949154016931333	T	T	T
0.5000000000000000	0.7502640158265522	0.9949154016931333	T	T	T
0.2500000000000000	-0.0000000000000000	0.9981863222024762	T	T	T
0.2500000000000000	0.5000000000000000	0.9934840164535415	T	T	T
0.7500000000000000	-0.0000000000000000	0.9981863222024762	T	T	T
0.7500000000000000	0.5000000000000000	0.9934840164535415	T	T	T

BiGdCuOS (x=37.5%)

1.0000000000000000
 7.8918347192092613 0.0000000000000000 0.0000000000000000
 0.0000000000000000 7.9053259669378040 0.0000000000000000
 0.0000000000000000 0.0000000000000000 8.6396769660995503

Bi Gd Cu S O
 5 3 8 8 8

Selective dynamics

Direct

0.2522897117983279	0.2500000000000000	0.1354587001027655	T	T	T
0.7477102882016723	0.7500000000000000	0.1354587001027655	T	T	T
0.0000000000000000	0.0000000000000000	0.8609788970077461	T	T	T
0.7472117784641417	0.2500000000000000	0.1631864723343331	T	T	T
0.2527882215358582	0.7500000000000000	0.1631864723343331	T	T	T
0.0000000000000000	0.5000000000000000	0.8609788970077461	T	T	T
0.5000000000000000	0.0000000000000000	0.8392461960655113	T	T	T
0.5000000000000000	0.5000000000000000	0.8392461960655113	T	T	T
0.0018590711866608	0.2500000000000000	0.5019965315570715	T	T	T
-0.0018590711866608	0.7500000000000000	0.5019965315570715	T	T	T
0.4989348557073207	0.2500000000000000	0.4975547839194920	T	T	T
0.5010651442926789	0.7500000000000000	0.4975547839194920	T	T	T
0.2491446094823416	0.0012953199703393	0.5009271049350451	T	T	T
0.2491446094823416	0.4987046800296607	0.5009271049350451	T	T	T
0.7508553905176583	-0.0012953199703393	0.5009271049350451	T	T	T
0.7508553905176583	0.5012953199703390	0.5009271049350451	T	T	T
0.2550644251321894	0.2500000000000000	0.6606383913645393	T	T	T
0.2546664992316462	0.7500000000000000	0.6617549086195509	T	T	T
0.7453335007683538	0.2500000000000000	0.6617549086195509	T	T	T
0.7449355748678109	0.7500000000000000	0.6606383913645393	T	T	T
0.0000000000000000	0.0000000000000000	0.3415940680606144	T	T	T
0.0000000000000000	0.5000000000000000	0.3415940680606144	T	T	T
0.5000000000000000	0.0000000000000000	0.3367381069723284	T	T	T
0.5000000000000000	0.5000000000000000	0.3367381069723284	T	T	T
0.0025999217250203	0.2500000000000000	-0.0020440104382947	T	T	T
-0.0025999217250203	0.7500000000000000	-0.0020440104382947	T	T	T
0.4977106192347439	0.2500000000000000	0.0002448319967602	T	T	T

0.5022893807652562	0.7500000000000000	0.0002448319967602	T	T	T
0.2428311583637137	0.0021053172444596	0.0003989562837464	T	T	T
0.2428311583637137	0.4978946827555404	0.0003989562837464	T	T	T
0.7571688416362863	-0.0021053172444596	0.0003989562837464	T	T	T
0.7571688416362863	0.5021053172444593	0.0003989562837464	T	T	T

BiGdCuOS (x=50%)

1.0000000000000000					
7.7706107569229799	0.0000000000000000	-0.0012764595376440			
0.0000000000000000	7.7334811748836252	0.0000000000000000			
-0.0013771196099461	0.0000000000000000	8.5091916968291770			

Bi Gd Cu S O
4 4 8 8 8

Selective dynamics

Direct

0.2539202058523222	0.2500000000000000	0.1428004162378541	T	T	T
0.2539202058523222	0.7500000000000000	0.1428004162378541	T	T	T
0.9960797941476776	0.0000000000000000	0.8571995837621458	T	T	T
0.9960797941476776	0.5000000000000000	0.8571995837621458	T	T	T
0.7454594806741595	0.2500000000000000	0.1469933399890569	T	T	T
0.7454594806741595	0.7500000000000000	0.1469933399890569	T	T	T
0.5045405193258405	0.0000000000000000	0.8530066600109433	T	T	T
0.5045405193258405	0.5000000000000000	0.8530066600109433	T	T	T
0.9978988011761234	0.2500000000000000	0.4991639669480322	T	T	T
0.9978988011761234	0.7500000000000000	0.4991639669480322	T	T	T
0.5026394498136025	0.2500000000000000	0.4974225162804021	T	T	T
0.5026394498136025	0.7500000000000000	0.4974225162804021	T	T	T
0.2521011988238763	0.0000000000000000	0.5008360330519677	T	T	T
0.2521011988238763	0.5000000000000000	0.5008360330519677	T	T	T
0.7473605501863975	-0.0000000000000000	0.5025774837195982	T	T	T
0.7473605501863975	0.5000000000000000	0.5025774837195982	T	T	T
0.2578145792071779	0.2500000000000000	0.6652893843881318	T	T	T
0.2578145792071779	0.7500000000000000	0.6652893843881318	T	T	T
0.7419954911312309	0.2500000000000000	0.6732839047001149	T	T	T
0.7419954911312309	0.7500000000000000	0.6732839047001149	T	T	T
0.9921854207928222	0.0000000000000000	0.3347106156118683	T	T	T
0.9921854207928222	0.5000000000000000	0.3347106156118683	T	T	T
0.5080045088687691	-0.0000000000000000	0.3267160952998855	T	T	T
0.5080045088687691	0.5000000000000000	0.3267160952998855	T	T	T
0.9998354729960225	0.2500000000000000	0.0042873260148412	T	T	T
0.9998354729960225	0.7500000000000000	0.0042873260148412	T	T	T
0.4996972959151002	0.2500000000000000	0.9971076858119934	T	T	T
0.4996972959151002	0.7500000000000000	0.9971076858119934	T	T	T
0.2501645270039777	0.0000000000000000	0.9957126739851586	T	T	T
0.2501645270039777	0.5000000000000000	0.9957126739851586	T	T	T
0.7503027040848995	0.0000000000000000	0.0028923141880064	T	T	T
0.7503027040848995	0.5000000000000000	0.0028923141880064	T	T	T

BiGdCuOS (x=62.5%)

1.0000000000000000					
7.7507483939861910	0.0000000000000000	0.0000148117938091			
0.0000000000000000	7.7341511561518148	0.0000000000000000			
-0.0000174292166611	0.0000000000000000	8.4772896285277142			

Gd Bi Cu S O
5 3 8 8 8

Selective dynamics

Direct

0.2452176608472921	0.2500000000000000	0.1464409170083866	T	T	T
0.7546948108453132	0.7500000000000000	0.1463751224753427	T	T	T
0.0024080753660807	-0.0021938166027965	0.8561044276571922	T	T	T
0.0024080753660807	0.5021938166027967	0.8561044276571922	T	T	T
0.2461097448714348	0.7500000000000000	0.1461993230572231	T	T	T
0.7531038808852464	0.2500000000000000	0.1423248998747220	T	T	T
0.4981480162620198	-0.0019931674112581	0.8596414570952475	T	T	T
0.4981480162620198	0.5019931674112580	0.8596414570952475	T	T	T
0.0019483356437096	0.2500000000000000	0.4958150599905087	T	T	T
0.0009052381579691	0.7500000000000000	0.4967430643936493	T	T	T
0.4978805343928267	0.2500000000000000	0.4983097369698025	T	T	T
0.4992516581660209	0.7500000000000000	0.4998042389953092	T	T	T
0.2474069281291919	-0.0009184242989318	0.5001127525038015	T	T	T
0.2474069281291919	0.5009184242989316	0.5001127525038015	T	T	T
0.7523858158694218	0.9979439995255004	0.4987999147409376	T	T	T
0.7523858158694218	0.5020560004744996	0.4987999147409376	T	T	T

0.2423249212449451	0.2500000000000000	0.6685850836651154	T	T	T
0.2421188682162252	0.7500000000000000	0.6716276401647880	T	T	T
0.7570563644088973	0.2500000000000000	0.6630074855858969	T	T	T
0.7579723694681189	0.7500000000000000	0.6686094761480124	T	T	T
0.0040796913737320	-0.0040145416375499	0.3237242233628994	T	T	T
0.0040796913737320	0.5040145416375497	0.3237242233628994	T	T	T
0.4960768655271414	-0.0036536749021161	0.3317238248920759	T	T	T
0.4960768655271414	0.5036536749021159	0.3317238248920759	T	T	T
0.0002589512620705	0.2500000000000000	-0.0027356018789349	T	T	T
-0.0006555027684075	0.7500000000000000	0.0004669935857545	T	T	T
0.4991664869810109	0.2500000000000000	0.0042427048892438	T	T	T
0.5010403568093034	0.7500000000000000	0.0072876847711206	T	T	T
0.2503877415920719	0.0008221886066962	0.0032756185070947	T	T	T
0.2503877415920719	0.4991778113933037	0.0032756185070947	T	T	T
0.7499095261643524	-0.0004387218333476	0.0000658663927663	T	T	T
0.7499095261643524	0.5004387218333478	0.0000658663927663	T	T	T

BiGdCuOS (x=75%)

1.0000000000000000					
7.7255282199670638	0.0000000000000000	0.0000000000000000			
0.0000000000000000	7.7404937494008488	0.0000000000000000			
0.0000000000000000	0.0000000000000000	8.4507047198219549			

Bi Gd Cu S O
2 6 8 8 8

Selective dynamics

Direct

0.5000000000000000	0.5000000000000000	0.8623218636892676	T	T	T
-0.0000000000000000	0.5000000000000000	0.8623218636892676	T	T	T
0.2500000000000000	0.2458348657013666	0.1456201182534282	T	T	T
0.7500000000000000	0.7541651342986333	0.1456201182534282	T	T	T
0.0000000000000000	0.0000000000000000	0.8591566733573045	T	T	T
0.2500000000000000	0.7541651342986333	0.1456201182534282	T	T	T
0.7500000000000000	0.2458348657013666	0.1456201182534282	T	T	T
0.5000000000000000	0.0000000000000000	0.8591566733573045	T	T	T
0.0000000000000000	0.2473838120769171	0.4980038593963755	T	T	T
-0.0000000000000000	0.7526161879230830	0.4980038593963755	T	T	T
0.5000000000000000	0.2473838120769171	0.4980038593963755	T	T	T
0.5000000000000000	0.7526161879230830	0.4980038593963755	T	T	T
0.2500000000000000	0.0000000000000000	0.4946932140794609	T	T	T
0.2500000000000000	0.5000000000000000	0.4982672778365300	T	T	T
0.7500000000000000	0.0000000000000000	0.4946932140794609	T	T	T
0.7500000000000000	0.5000000000000000	0.4982672778365300	T	T	T
0.2500000000000000	0.2424582304222920	0.6665296558169638	T	T	T
0.2500000000000000	0.7575417695777079	0.6665296558169638	T	T	T
0.7500000000000000	0.2424582304222920	0.6665296558169638	T	T	T
0.7500000000000000	0.7575417695777079	0.6665296558169638	T	T	T
0.0000000000000000	0.0000000000000000	0.3208632975348579	T	T	T
-0.0000000000000000	0.5000000000000000	0.3289010573196988	T	T	T
0.5000000000000000	0.0000000000000000	0.3208632975348579	T	T	T
0.5000000000000000	0.5000000000000000	0.3289010573196988	T	T	T
-0.0000000000000000	0.2502957988783407	0.0035875088881764	T	T	T
0.0000000000000000	0.7497042011216589	0.0035875088881764	T	T	T
0.5000000000000000	0.2502957988783407	0.0035875088881764	T	T	T
0.5000000000000000	0.7497042011216589	0.0035875088881764	T	T	T
0.2500000000000000	0.0000000000000000	0.0007704554238954	T	T	T
0.2500000000000000	0.5000000000000000	0.0075438760490814	T	T	T
0.7500000000000000	0.0000000000000000	0.0007704554238954	T	T	T
0.7500000000000000	0.5000000000000000	0.0075438760490814	T	T	T

BiGdCuOS (x=87.5%)

1.0000000000000000					
7.7277665557456752	0.0000000000000000	0.0000000000000000			
0.0000000000000000	7.7277665557456752	-0.0000000000000000			
0.0000000000000000	-0.0000000000000000	8.4177121984426257			

Bi Gd Cu S O
1 7 8 8 8

Selective dynamics

Direct

0.5000000000000000	0.5000000000000000	0.8627914293699791	T	T	T
0.2479626158372282	0.2479626158372282	0.1427417093185468	T	T	T
0.0000000000000000	0.5000000000000000	0.8597119693177773	T	T	T
0.0000000000000000	-0.0000000000000000	0.8599116791082232	T	T	T
0.2479626158372282	0.7520373841627715	0.1427417093185468	T	T	T
0.7520373841627715	0.2479626158372282	0.1427417093185468	T	T	T

0.5000000000000000	-0.0000000000000000	0.8597119693177773	T	T	T
0.7520373841627715	0.7520373841627715	0.1427417093185468	T	T	T
0.0000000000000000	0.2488237805225059	0.4970206825065692	T	T	T
0.0000000000000000	0.7511762194774939	0.4970206825065692	T	T	T
0.5000000000000000	0.2476933100781811	0.5002043953475177	T	T	T
0.5000000000000000	0.7523066899218190	0.5002043953475177	T	T	T
0.2488237805225059	-0.0000000000000000	0.4970206825065692	T	T	T
0.2476933100781811	0.5000000000000000	0.5002043953475177	T	T	T
0.7511762194774939	-0.0000000000000000	0.4970206825065692	T	T	T
0.7523066899218190	0.5000000000000000	0.5002043953475177	T	T	T
0.2459855788014940	0.2459855788014940	0.6694568380418738	T	T	T
0.2459855788014940	0.7540144211985060	0.6694568380418738	T	T	T
0.7540144211985060	0.2459855788014940	0.6694568380418738	T	T	T
0.7540144211985060	0.7540144211985060	0.6694568380418738	T	T	T
0.0000000000000000	-0.0000000000000000	0.3219994995751780	T	T	T
0.0000000000000000	0.5000000000000000	0.3255103108866498	T	T	T
0.5000000000000000	-0.0000000000000000	0.3255103108866498	T	T	T
0.5000000000000000	0.5000000000000000	0.3313657985487823	T	T	T
0.0000000000000000	0.2508596986511801	0.0004644790899760	T	T	T
0.0000000000000000	0.7491403013488199	0.0004644790899760	T	T	T
0.5000000000000000	0.2497229591799640	0.0034836539427675	T	T	T
0.5000000000000000	0.7502770408200361	0.0034836539427675	T	T	T
0.2508596986511801	-0.0000000000000000	0.0004644790899760	T	T	T
0.2497229591799640	0.5000000000000000	0.0034836539427675	T	T	T
0.7491403013488199	-0.0000000000000000	0.0004644790899760	T	T	T
0.7502770408200361	0.5000000000000000	0.0034836539427675	T	T	T

BiYCuOS (x=12.5%)

1.0000000000000000					
7.7706707332808787	0.0000000000000000	0.0000000000000000			
0.0000000000000000	7.7706707332808787	-0.0000000000000000			
0.0000000000000000	-0.0000000000000000	8.6163490734496619			

Bi Y Cu S O
7 1 8 8 8

Selective dynamics

Direct

0.2522142519570921	0.2522142519570921	0.1458660436928658	T	T	T
-0.0000000000000000	0.5000000000000000	0.8503681494428842	T	T	T
-0.0000000000000000	-0.0000000000000000	0.8515952215089571	T	T	T
0.2522142519570921	0.7477857480429074	0.1458660436928658	T	T	T
0.7477857480429074	0.2522142519570921	0.1458660436928658	T	T	T
0.5000000000000000	-0.0000000000000000	0.8503681494428842	T	T	T
0.7477857480429074	0.7477857480429074	0.1458660436928658	T	T	T
0.5000000000000000	0.5000000000000000	0.8512400475713932	T	T	T
-0.0000000000000000	0.2509731978579173	0.5017479251351330	T	T	T
-0.0000000000000000	0.7490268021420829	0.5017479251351330	T	T	T
0.5000000000000000	0.2516466035639608	0.5010282154941701	T	T	T
0.5000000000000000	0.7483533964360389	0.5010282154941701	T	T	T
0.2509731978579173	-0.0000000000000000	0.5017479251351330	T	T	T
0.2516466035639608	0.5000000000000000	0.5010282154941701	T	T	T
0.7490268021420829	-0.0000000000000000	0.5017479251351330	T	T	T
0.7483533964360389	0.5000000000000000	0.5010282154941701	T	T	T
0.2545836531388068	0.2545836531388068	0.6693154472908863	T	T	T
0.2545836531388068	0.7454163468611932	0.6693154472908863	T	T	T
0.7454163468611932	0.2545836531388068	0.6693154472908863	T	T	T
0.7454163468611932	0.7454163468611932	0.6693154472908863	T	T	T
-0.0000000000000000	-0.0000000000000000	0.3407090699833998	T	T	T
-0.0000000000000000	0.5000000000000000	0.3367899695329135	T	T	T
0.5000000000000000	-0.0000000000000000	0.3367899695329135	T	T	T
0.5000000000000000	0.5000000000000000	0.3315538322715709	T	T	T
-0.0000000000000000	0.2495274104756010	-0.0005229847319041	T	T	T
-0.0000000000000000	0.7504725895243988	-0.0005229847319041	T	T	T
0.5000000000000000	0.2520575351465611	-0.0047882492028805	T	T	T
0.5000000000000000	0.7479424648534391	-0.0047882492028805	T	T	T
0.2495274104756010	-0.0000000000000000	-0.0005229847319041	T	T	T
0.2520575351465611	0.5000000000000000	-0.0047882492028805	T	T	T
0.7504725895243988	-0.0000000000000000	-0.0005229847319041	T	T	T
0.7479424648534391	0.5000000000000000	-0.0047882492028805	T	T	T

BiYCuOS (x=25%)

1.0000000000000000					
7.7387427035316305	0.0000000000000000	0.0000000000000000			
0.0000000000000000	7.7665477030346670	0.0000000000000000			
0.0000000000000000	0.0000000000000000	8.5812338686389467			

Bi Y Cu S O
6 2 8 8 8

Selective dynamics

Direct

0.2500000000000000	0.2543635971877349	0.1430975185315131	T	T	T
0.7500000000000000	0.7456364028122651	0.1430975185315131	T	T	T
-0.0000000000000000	-0.0000000000000000	0.8507644369583637	T	T	T
0.2500000000000000	0.7456364028122651	0.1430975185315131	T	T	T
0.7500000000000000	0.2543635971877349	0.1430975185315131	T	T	T
0.5000000000000000	-0.0000000000000000	0.8507644369583637	T	T	T
0.5000000000000000	0.5000000000000000	0.8508923392782396	T	T	T
-0.0000000000000000	0.5000000000000000	0.8508923392782396	T	T	T
-0.0000000000000000	0.2531594566260163	0.5038787042239784	T	T	T
0.0000000000000000	0.7468405433739833	0.5038787042239784	T	T	T
0.5000000000000000	0.2531594566260163	0.5038787042239784	T	T	T
0.5000000000000000	0.7468405433739833	0.5038787042239784	T	T	T
0.2500000000000000	-0.0000000000000000	0.5024112741634373	T	T	T
0.2500000000000000	0.5000000000000000	0.5010430678114269	T	T	T
0.7500000000000000	-0.0000000000000000	0.5024112741634373	T	T	T
0.7500000000000000	0.5000000000000000	0.5010430678114269	T	T	T
0.2500000000000000	0.2594120595429436	0.6732047374995798	T	T	T
0.2500000000000000	0.7405879404570567	0.6732047374995798	T	T	T
0.7500000000000000	0.2594120595429436	0.6732047374995798	T	T	T
0.7500000000000000	0.7405879404570567	0.6732047374995798	T	T	T
-0.0000000000000000	-0.0000000000000000	0.3424708515457294	T	T	T
-0.0000000000000000	0.5000000000000000	0.3328440710311600	T	T	T
0.5000000000000000	-0.0000000000000000	0.3424708515457294	T	T	T
0.5000000000000000	0.5000000000000000	0.3328440710311600	T	T	T
-0.0000000000000000	0.2512976292228516	-0.0057365743879387	T	T	T
-0.0000000000000000	0.7487023707771484	-0.0057365743879387	T	T	T
0.5000000000000000	0.2512976292228516	-0.0057365743879387	T	T	T
0.5000000000000000	0.7487023707771484	-0.0057365743879387	T	T	T
0.2500000000000000	-0.0000000000000000	-0.0008226195316125	T	T	T
0.2500000000000000	0.5000000000000000	-0.0084921929910106	T	T	T
0.7500000000000000	-0.0000000000000000	-0.0008226195316125	T	T	T
0.7500000000000000	0.5000000000000000	-0.0084921929910106	T	T	T

BiYCuOS (x=37.5%)

1.0000000000000000

7.7344140092438023	0.0000691652697330	0.0000000000000000
0.0000699930792712	7.7344938975619559	0.0000000000000000
0.0000000000000000	0.0000000000000000	8.5470891706684267

Bi Y Cu S O
5 3 8 8 8

Selective dynamics

Direct

0.2521706203161514	0.2521812966108960	0.1404006032948944	T	T	T
0.7478293796838490	0.7478187033891043	0.1404006032948944	T	T	T
0.0000000000000000	0.0000000000000000	0.8507629548208175	T	T	T
0.7478277366629867	0.2521786873879782	0.1404047849005261	T	T	T
0.2521722633370135	0.7478213126120220	0.1404047849005261	T	T	T
0.0000000000000000	0.5000000000000000	0.8512584692421471	T	T	T
0.5000000000000000	0.0000000000000000	0.8512929615979496	T	T	T
0.5000000000000000	0.5000000000000000	0.8510387996954113	T	T	T
0.0000175731857956	0.2526152971119932	0.5050706174519001	T	T	T
0.9999824268142047	0.7473847028880066	0.5050706174519001	T	T	T
0.5000004878082639	0.2508379519639294	0.5039146140594131	T	T	T
0.4999995121917363	0.7491620480360707	0.5039146140594131	T	T	T
0.2526347053455014	-0.0000089154218430	0.5049989807346210	T	T	T
0.2508329834606864	0.5000069505149323	0.5039860462399660	T	T	T
0.7473652946544983	0.0000089154218431	0.5049989807346210	T	T	T
0.7491670165393139	0.4999930494850682	0.5039860462399660	T	T	T
0.2547072178004666	0.2546634124372724	0.6762128780092083	T	T	T
0.2547005740599963	0.7453359923219841	0.6762115805176557	T	T	T
0.7452994259400036	0.2546640076780158	0.6762115805176557	T	T	T
0.7452927821995334	0.7453365875627274	0.6762128780092083	T	T	T
0.0000000000000000	0.0000000000000000	0.3445603027491063	T	T	T
0.0000000000000000	0.5000000000000000	0.3377959719403560	T	T	T
0.5000000000000000	0.0000000000000000	0.3377365727224646	T	T	T
0.5000000000000000	0.5000000000000000	0.3344345560873582	T	T	T
0.0000064752006070	0.2515686456843549	0.9940874809134439	T	T	T
-0.0000064752006071	0.7484313543156450	0.9940874809134439	T	T	T
0.5000095889776325	0.2494424261574271	-0.0094085186206157	T	T	T
0.4999904110223674	0.7505575738425727	-0.0094085186206157	T	T	T
0.2515597181988024	-0.0000050660246284	-0.0058999751881395	T	T	T

0.2494385580303031	0.4999977945545910	-0.0094193867406928	T	T	T
0.7484402818011976	0.0000050660246285	-0.0058999751881395	T	T	T
0.7505614419696971	0.5000022054454091	-0.0094193867406928	T	T	T

BiYCuOS (x=50%)

1.000000000000000		
3.8581377832256019	-0.000000000000000	0.000000000000000
0.000000000000000	3.8581377832256019	-0.000000000000000
-0.000000000000000	0.000000000000000	8.5246972626122268

Bi Y Cu S O
1 1 2 2 2

Selective dynamics

Direct

0.250000000000000	0.250000000000000	0.1375345145001615	T	T	T
0.750000000000000	0.750000000000000	0.8514691873463412	T	T	T
0.750000000000000	0.250000000000000	0.5060588097408604	T	T	T
0.250000000000000	0.750000000000000	0.5060588097408604	T	T	T
0.250000000000000	0.250000000000000	0.6791264874398125	T	T	T
0.750000000000000	0.750000000000000	0.3397509609114165	T	T	T
0.750000000000000	0.250000000000000	-0.0099993848397261	T	T	T
0.250000000000000	0.750000000000000	-0.0099993848397261	T	T	T

BiYCuOS (x=62.5%)

1.000000000000000		
7.7187319809562682	0.000000000000000	0.0056650666285793
0.000000000000000	7.6972077939567489	0.000000000000000
0.0061875468039614	0.000000000000000	8.4637687803429404

Y Bi Cu S O
5 3 8 8 8

Selective dynamics

Direct

0.2443287706053151	0.250000000000000	0.1422848995412368	T	T	T
0.7549520967716455	0.750000000000000	0.1422869758758611	T	T	T
0.0028668997590249	-0.0023062665042362	0.8603405712768319	T	T	T
0.0028668997590249	0.5023062665042359	0.8603405712768319	T	T	T
0.2456999082756770	0.750000000000000	0.1427339465183427	T	T	T
0.7528113695000075	0.250000000000000	0.1439773933649220	T	T	T
0.4984881350769148	-0.0020261013240044	0.8589311109840535	T	T	T
0.4984881350769148	0.5020261013240047	0.8589311109840535	T	T	T
0.0021136911999861	0.250000000000000	0.4949611022841666	T	T	T
0.0010032302140057	0.750000000000000	0.4962644871897949	T	T	T
0.4974016680877015	0.250000000000000	0.4980512464144461	T	T	T
0.4994690726543722	0.750000000000000	0.5000939615733911	T	T	T
0.2471954313342285	-0.0009920532203874	0.5001197024557416	T	T	T
0.2471954313342285	0.5009920532203871	0.5001197024557416	T	T	T
0.7524788672337405	0.9977018972932336	0.4982390635025986	T	T	T
0.7524788672337405	0.5022981027067664	0.4982390635025986	T	T	T
0.2411656762042999	0.250000000000000	0.6703641869596861	T	T	T
0.2409703709085323	0.750000000000000	0.6737393054635041	T	T	T
0.7573548296008664	0.250000000000000	0.6643326674549785	T	T	T
0.7588380193155905	0.750000000000000	0.6704322000799988	T	T	T
0.0047145851148966	-0.0044515210609176	0.3219506114027549	T	T	T
0.0047145851148966	0.5044515210609176	0.3219506114027549	T	T	T
0.4959079818597776	-0.0040081148780067	0.3305976304612477	T	T	T
0.4959079818597776	0.5040081148780070	0.3305976304612477	T	T	T
0.0009731304848907	0.250000000000000	0.9964365894873239	T	T	T
-0.0003216410860896	0.750000000000000	0.0006051033013621	T	T	T
0.4981520009090903	0.250000000000000	0.0053689490302752	T	T	T
0.5008592790975697	0.750000000000000	0.0091329508900056	T	T	T
0.2492823716158431	0.0005290982253110	0.0041933633535276	T	T	T
0.2492823716158431	0.4994709017746890	0.0041933633535276	T	T	T
0.7511799916338436	-0.0013025923194994	0.0000949638485826	T	T	T
0.7511799916338436	0.5013025923194996	0.0000949638485826	T	T	T

BiYCuOS (x=75%)

1.000000000000000		
7.6809341948171017	0.000000000000000	0.000000000000000
0.000000000000000	7.7006313517296361	0.000000000000000
0.000000000000000	0.000000000000000	8.4344381723208972

Bi Y Cu S O
2 6 8 8 8

Selective dynamics

Direct

0.5000000000000000	0.5000000000000000	0.8617223009349304	T	T	T
0.0000000000000000	0.5000000000000000	0.8617223009349304	T	T	T
0.2500000000000000	0.2454557631625615	0.1423111456862920	T	T	T
0.7500000000000000	0.7545442368374385	0.1423111456862920	T	T	T
0.0000000000000000	-0.0000000000000000	0.8633644841040912	T	T	T
0.2500000000000000	0.7545442368374384	0.1423111456862920	T	T	T
0.7500000000000000	0.2454557631625615	0.1423111456862920	T	T	T
0.5000000000000000	-0.0000000000000000	0.8633644841040912	T	T	T
-0.0000000000000000	0.2473471876014576	0.4973660482499537	T	T	T
0.0000000000000000	0.7526528123985424	0.4973660482499537	T	T	T
0.5000000000000000	0.2473471876014576	0.4973660482499537	T	T	T
0.5000000000000000	0.7526528123985424	0.4973660482499537	T	T	T
0.2500000000000000	-0.0000000000000000	0.4935310313242146	T	T	T
0.2500000000000000	0.5000000000000000	0.4980728490900610	T	T	T
0.7500000000000000	-0.0000000000000000	0.4935310313242146	T	T	T
0.7500000000000000	0.5000000000000000	0.4980728490900610	T	T	T
0.2500000000000000	0.2414635193124325	0.6687688624752798	T	T	T
0.2500000000000000	0.7585364806875678	0.6687688624752798	T	T	T
0.7500000000000000	0.2414635193124325	0.6687688624752798	T	T	T
0.7500000000000000	0.7585364806875678	0.6687688624752798	T	T	T
-0.0000000000000000	-0.0000000000000000	0.3189903307652655	T	T	T
0.0000000000000000	0.5000000000000000	0.3276720244510919	T	T	T
0.5000000000000000	-0.0000000000000000	0.3189903307652655	T	T	T
0.5000000000000000	0.5000000000000000	0.3276720244510919	T	T	T
-0.0000000000000000	0.2491154741807597	0.0046162408592047	T	T	T
-0.0000000000000000	0.7508845258192404	0.0046162408592047	T	T	T
0.5000000000000000	0.2491154741807597	0.0046162408592047	T	T	T
0.5000000000000000	0.7508845258192404	0.0046162408592047	T	T	T
0.2500000000000000	-0.0000000000000000	0.0009249568745162	T	T	T
0.2500000000000000	0.5000000000000000	0.0095974279143550	T	T	T
0.7500000000000000	-0.0000000000000000	0.0009249568745162	T	T	T
0.7500000000000000	0.5000000000000000	0.0095974279143550	T	T	T

BiYCuOS (x=87.5%)

1.0000000000000000					
7.6776367005028101	0.0000000000000000	0.0000000000000000			
0.0000000000000000	7.6776367005028101	-0.0000000000000000			
0.0000000000000000	0.0000000000000000	8.4019429687004088			

Bi Y Cu S O
1 7 8 8 8

Selective dynamics

Direct

0.5000000000000000	0.5000000000000000	0.8613482868426392	T	T	T
0.2477201268978833	0.2477201268978833	0.1392599654632132	T	T	T
0.0000000000000000	0.5000000000000000	0.8639004003354848	T	T	T
0.0000000000000000	0.0000000000000000	0.8631749551380734	T	T	T
0.2477201268978833	0.7522798731021167	0.1392599654632132	T	T	T
0.7522798731021167	0.2477201268978833	0.1392599654632132	T	T	T
0.5000000000000000	0.0000000000000000	0.8639004003354848	T	T	T
0.7522798731021167	0.7522798731021167	0.1392599654632132	T	T	T
0.0000000000000000	0.2490049866625925	0.4971821250567672	T	T	T
0.0000000000000000	0.7509950133374078	0.4971821250567672	T	T	T
0.5000000000000000	0.2480303759611513	0.4994461596621467	T	T	T
0.5000000000000000	0.7519696240388489	0.4994461596621467	T	T	T
0.2490049866625925	0.0000000000000000	0.4971821250567672	T	T	T
0.2480303759611513	0.5000000000000000	0.4994461596621467	T	T	T
0.7509950133374078	0.0000000000000000	0.4971821250567672	T	T	T
0.7519696240388489	0.5000000000000000	0.4994461596621467	T	T	T
0.2457597223627820	0.2457597223627820	0.6719582884397438	T	T	T
0.2457597223627820	0.7542402776372181	0.6719582884397438	T	T	T
0.7542402776372181	0.2457597223627820	0.6719582884397438	T	T	T
0.7542402776372181	0.7542402776372181	0.6719582884397438	T	T	T
0.0000000000000000	0.0000000000000000	0.3201570407195666	T	T	T
0.0000000000000000	0.5000000000000000	0.3237360827260300	T	T	T
0.5000000000000000	0.0000000000000000	0.3237360827260300	T	T	T
0.5000000000000000	0.5000000000000000	0.3291991084089689	T	T	T
0.0000000000000000	0.2505043124689618	0.0003829987388079	T	T	T
0.0000000000000000	0.7494956875310387	0.0003829987388079	T	T	T
0.5000000000000000	0.2488170899553643	0.0044823733312517	T	T	T
0.5000000000000000	0.7511829100446361	0.0044823733312517	T	T	T
0.2505043124689618	0.0000000000000000	0.0003829987388079	T	T	T
0.2488170899553643	0.5000000000000000	0.0044823733312517	T	T	T
0.7494956875310387	0.0000000000000000	0.0003829987388079	T	T	T
0.7511829100446361	0.5000000000000000	0.0044823733312517	T	T	T

BiLuCuOS (x=12.5%)

1.0000000000000000
 7.7546232448390402 0.0000000000000000 0.0000000000000000
 0.0000000000000000 7.7546232448390402 -0.0000000000000000
 0.0000000000000000 -0.0000000000000000 8.6128831030355943

Bi Lu Cu S O
 7 1 8 8 8

Selective dynamics

Direct

0.2522013575102968	0.2522013575102968	0.1455399872977403	T	T	T
-0.0000000000000000	0.5000000000000000	0.8483538613805853	T	T	T
-0.0000000000000000	0.0000000000000000	0.8504376463040463	T	T	T
0.2522013575102968	0.7477986424897035	0.1455399872977403	T	T	T
0.7477986424897035	0.2522013575102968	0.1455399872977403	T	T	T
0.5000000000000000	0.0000000000000000	0.8483538613805853	T	T	T
0.7477986424897035	0.7477986424897035	0.1455399872977403	T	T	T
0.5000000000000000	0.5000000000000000	0.8616261212032107	T	T	T
-0.0000000000000000	0.2509078676593529	0.5024973132857240	T	T	T
-0.0000000000000000	0.7490921323406469	0.5024973132857240	T	T	T
0.5000000000000000	0.2518877669137767	0.5011428945147953	T	T	T
0.5000000000000000	0.7481122330862233	0.5011428945147953	T	T	T
0.2509078676593529	0.0000000000000000	0.5024973132857240	T	T	T
0.2518877669137767	0.5000000000000000	0.5011428945147953	T	T	T
0.7490921323406469	0.0000000000000000	0.5024973132857240	T	T	T
0.7481122330862233	0.5000000000000000	0.5011428945147953	T	T	T
0.2550595657482257	0.2550595657482257	0.6701740871078913	T	T	T
0.2550595657482257	0.7449404342517741	0.6701740871078913	T	T	T
0.7449404342517741	0.2550595657482257	0.6701740871078913	T	T	T
0.7449404342517741	0.7449404342517741	0.6701740871078913	T	T	T
-0.0000000000000000	0.0000000000000000	0.3400884332359416	T	T	T
-0.0000000000000000	0.5000000000000000	0.3361354960756523	T	T	T
0.5000000000000000	0.0000000000000000	0.3361354960756523	T	T	T
0.5000000000000000	0.5000000000000000	0.3312342693296572	T	T	T
-0.0000000000000000	0.2503294071778457	-0.0008151667585620	T	T	T
-0.0000000000000000	0.7496705928221544	-0.0008151667585620	T	T	T
0.5000000000000000	0.2548703669436232	-0.0066304116939216	T	T	T
0.5000000000000000	0.7451296330563765	-0.0066304116939216	T	T	T
0.2503294071778457	0.0000000000000000	-0.0008151667585620	T	T	T
0.2548703669436232	0.5000000000000000	-0.0066304116939216	T	T	T
0.7496705928221544	0.0000000000000000	-0.0008151667585620	T	T	T
0.7451296330563765	0.5000000000000000	-0.0066304116939216	T	T	T

BiLuCuOS (x=25%)

1.0000000000000000
 7.6996544902180704 0.0000000000000000 0.0000000000000000
 0.0000000000000000 7.7344769744840232 0.0000000000000000
 0.0000000000000000 0.0000000000000000 8.5729582901950252

Bi Lu Cu S O
 6 2 8 8 8

Selective dynamics

Direct

0.2500000000000000	0.2542748503632122	0.1426378728359788	T	T	T
0.7500000000000000	0.7457251496367875	0.1426378728359788	T	T	T
-0.0000000000000000	0.0000000000000000	0.8475772730475601	T	T	T
0.2500000000000000	0.7457251496367875	0.1426378728359788	T	T	T
0.7500000000000000	0.2542748503632122	0.1426378728359788	T	T	T
0.5000000000000000	0.0000000000000000	0.8475772730475601	T	T	T
0.5000000000000000	0.5000000000000000	0.8588177260786486	T	T	T
-0.0000000000000000	0.5000000000000000	0.8588177260786486	T	T	T
0.0000000000000000	0.2534989664962183	0.5050284652100793	T	T	T
-0.0000000000000000	0.7465010335037813	0.5050284652100793	T	T	T
0.5000000000000000	0.2534989664962183	0.5050284652100793	T	T	T
0.5000000000000000	0.7465010335037813	0.5050284652100793	T	T	T
0.2500000000000000	0.0000000000000000	0.5042122479326213	T	T	T
0.2500000000000000	0.5000000000000000	0.5012926097706404	T	T	T
0.7500000000000000	0.0000000000000000	0.5042122479326213	T	T	T
0.7500000000000000	0.5000000000000000	0.5012926097706404	T	T	T
0.2500000000000000	0.2606144460162866	0.6749158684711061	T	T	T
0.2500000000000000	0.7393855539837132	0.6749158684711061	T	T	T
0.7500000000000000	0.2606144460162866	0.6749158684711061	T	T	T
0.7500000000000000	0.7393855539837132	0.6749158684711061	T	T	T
-0.0000000000000000	0.0000000000000000	0.3412031805900174	T	T	T
-0.0000000000000000	0.5000000000000000	0.3315703088473170	T	T	T
0.5000000000000000	0.0000000000000000	0.3412031805900174	T	T	T
0.5000000000000000	0.5000000000000000	0.3315703088473170	T	T	T

-0.0000000000000000	0.2550167624283265	-0.0080978544775827	T	T	T
0.0000000000000000	0.7449832375716734	-0.0080978544775827	T	T	T
0.5000000000000000	0.2550167624283265	-0.0080978544775827	T	T	T
0.5000000000000000	0.7449832375716734	-0.0080978544775827	T	T	T
0.2500000000000000	0.0000000000000000	-0.0013292422378844	T	T	T
0.2500000000000000	0.5000000000000000	-0.0123128081080827	T	T	T
0.7500000000000000	0.0000000000000000	-0.0013292422378844	T	T	T
0.7500000000000000	0.5000000000000000	-0.0123128081080827	T	T	T

BiLuCuOS (x=37.5%)

1.0000000000000000			
7.8918347192092613	0.0000000000000000	0.0000000000000000	
0.0000000000000000	0.5000000000000000	7.9053259669378040	0.0000000000000000
0.0000000000000000	0.0000000000000000	8.6396769660995503	

Bi Lu Cu S O
5 3 8 8 8

Selective dynamics

Direct

0.2522897117983279	0.2500000000000000	0.1354587001027655	T	T	T
0.7477102882016723	0.7500000000000000	0.1354587001027655	T	T	T
0.0000000000000000	0.0000000000000000	0.8609788970077461	T	T	T
0.7472117784641417	0.2500000000000000	0.1631864723343331	T	T	T
0.2527882215358582	0.7500000000000000	0.1631864723343331	T	T	T
0.0000000000000000	0.5000000000000000	0.8609788970077461	T	T	T
0.5000000000000000	0.0000000000000000	0.8392461960655113	T	T	T
0.5000000000000000	0.5000000000000000	0.8392461960655113	T	T	T
0.0018590711866608	0.2500000000000000	0.5019965315570715	T	T	T
-0.0018590711866608	0.7500000000000000	0.5019965315570715	T	T	T
0.4989348557073207	0.2500000000000000	0.4975547839194920	T	T	T
0.5010651442926789	0.7500000000000000	0.4975547839194920	T	T	T
0.2491446094823416	0.0012953199703393	0.5009271049350451	T	T	T
0.2491446094823416	0.4987046800296607	0.5009271049350451	T	T	T
0.7508553905176583	-0.0012953199703393	0.5009271049350451	T	T	T
0.7508553905176583	0.5012953199703393	0.5009271049350451	T	T	T
0.2550644251321894	0.2500000000000000	0.6606383913645393	T	T	T
0.2546664992316462	0.7500000000000000	0.6617549086195509	T	T	T
0.7453335007683538	0.2500000000000000	0.6617549086195509	T	T	T
0.7449355748678109	0.7500000000000000	0.6606383913645393	T	T	T
0.0000000000000000	0.0000000000000000	0.3415940680606144	T	T	T
0.0000000000000000	0.5000000000000000	0.3415940680606144	T	T	T
0.5000000000000000	0.0000000000000000	0.3367381069723284	T	T	T
0.5000000000000000	0.5000000000000000	0.3367381069723284	T	T	T
0.0025999217250203	0.2500000000000000	-0.0020440104382947	T	T	T
-0.0025999217250203	0.7500000000000000	-0.0020440104382947	T	T	T
0.4977106192347439	0.2500000000000000	0.0002448319967602	T	T	T
0.5022893807652562	0.7500000000000000	0.0002448319967602	T	T	T
0.2428311583637137	0.0021053172444596	0.0003989562837464	T	T	T
0.2428311583637137	0.4978946827555404	0.0003989562837464	T	T	T
0.7571688416362863	-0.0021053172444596	0.0003989562837464	T	T	T
0.7571688416362863	0.5021053172444593	0.0003989562837464	T	T	T

BiLuCuOS (x=50%)

1.0000000000000000			
3.8220364887663889	0.0000000000000000	0.0000000000000000	
-0.0000000000000000	3.8220364887663889	0.0000000000000000	
-0.0000000000000000	-0.0000000000000000	8.4913847090862422	

Bi Lu Cu S O
1 1 2 2 2

Selective dynamics

Direct

0.2500000000000000	0.2500000000000000	0.1375019001062802	T	T	T
0.7500000000000000	0.7500000000000000	0.8560696779316539	T	T	T
0.7500000000000000	0.2500000000000000	0.5090049856360319	T	T	T
0.2500000000000000	0.7500000000000000	0.5090049856360319	T	T	T
0.2500000000000000	0.2500000000000000	0.6815191439173834	T	T	T
0.7500000000000000	0.7500000000000000	0.3362679019772909	T	T	T
0.7500000000000000	0.2500000000000000	-0.0146842976023360	T	T	T
0.2500000000000000	0.7500000000000000	-0.0146842976023360	T	T	T

BiLuCuOS (x=62.5%)

1.0000000000000000			
7.6150061948151633	-0.0001152597756899	0.0000000000000000	

-0.0001152642792064 7.6149304505599185 0.0000000000000000
0.0000000000000000 0.0000000000000000 8.4425176476493142

Lu Bi Cu S O
5 3 8 8 8

Selective dynamics

Direct

0.2474456068193768	0.2474452615839328	0.1407146431359256	T	T	T
0.7525543931806233	0.7525547384160677	0.1407146431359256	T	T	T
0.0000000000000000	-0.0000000000000000	0.8741289321968562	T	T	T
0.7525562013751524	0.2474440101681520	0.1407101316485831	T	T	T
0.2474437986248477	0.7525559898318483	0.1407101316485831	T	T	T
0.0000000000000000	0.5000000000000000	0.8594297841169796	T	T	T
0.5000000000000000	-0.0000000000000000	0.8594330982917999	T	T	T
0.5000000000000000	0.5000000000000000	0.8624635827817945	T	T	T
0.0000012534338712	0.2492476824224723	0.4905984254827530	T	T	T
-0.0000012534338712	0.7507523175775278	0.4905984254827530	T	T	T
0.4999980632583186	0.2491865641461431	0.4946971503740711	T	T	T
0.5000019367416816	0.7508134358538567	0.4946971503740711	T	T	T
0.2492466181725756	0.0000053464101753	0.4905808254171421	T	T	T
0.2491885448588228	0.5000008782981600	0.4946738739767593	T	T	T
0.7507533818274243	-0.0000053464101753	0.4905808254171421	T	T	T
0.7508114551411771	0.4999991217018397	0.4946738739767593	T	T	T
0.2446075266904435	0.2446041696224670	0.6688735582539296	T	T	T
0.2446091246076469	0.7553969935149969	0.6688716901202250	T	T	T
0.7553908753923532	0.2446030064850026	0.6688716901202250	T	T	T
0.7553924733095566	0.7553958303775328	0.6688735582539296	T	T	T
0.0000000000000000	-0.0000000000000000	0.3150036235250202	T	T	T
0.0000000000000000	0.5000000000000000	0.3187728253720231	T	T	T
0.5000000000000000	-0.0000000000000000	0.3187752754520336	T	T	T
0.5000000000000000	0.5000000000000000	0.3236708533636092	T	T	T
0.0000026062875251	0.2460456526932595	0.0080190808213296	T	T	T
-0.0000026062875250	0.7539543473067407	0.0080190808213296	T	T	T
0.5000001316137017	0.2496272524572730	0.0141994791529291	T	T	T
0.4999998683862976	0.7503727475427274	0.0141994791529291	T	T	T
0.2460470158050861	0.0000015991492108	0.0080192061399323	T	T	T
0.2496305709633359	0.5000006302194293	0.0142029479263477	T	T	T
0.7539529841949136	-0.0000015991492110	0.0080192061399323	T	T	T
0.7503694290366640	0.4999993697805709	0.0142029479263477	T	T	T

BiLuCuOS (x=75%)

1.0000000000000000

7.5682372041202317	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.5951204066112767	0.0000000000000000
0.0000000000000000	0.0000000000000000	8.4010472842008088

Bi Lu Cu S O
2 6 8 8 8

Selective dynamics

Direct

0.5000000000000000	0.5000000000000000	0.8593279815582731	T	T	T
-0.0000000000000000	0.5000000000000000	0.8593279815582731	T	T	T
0.2500000000000000	0.2450164906343386	0.1375615415178678	T	T	T
0.7500000000000000	0.7549835093656614	0.1375615415178678	T	T	T
-0.0000000000000000	-0.0000000000000000	0.8710480432301451	T	T	T
0.2500000000000000	0.7549835093656614	0.1375615415178678	T	T	T
0.7500000000000000	0.2450164906343386	0.1375615415178678	T	T	T
0.5000000000000000	-0.0000000000000000	0.8710480432301451	T	T	T
-0.0000000000000000	0.2478427989020127	0.4958165916866513	T	T	T
-0.0000000000000000	0.7521572010979872	0.4958165916866513	T	T	T
0.5000000000000000	0.2478427989020127	0.4958165916866513	T	T	T
0.5000000000000000	0.7521572010979872	0.4958165916866513	T	T	T
0.2500000000000000	-0.0000000000000000	0.4895960764936135	T	T	T
0.2500000000000000	0.5000000000000000	0.4976266601758527	T	T	T
0.7500000000000000	-0.0000000000000000	0.4895960764936135	T	T	T
0.7500000000000000	0.5000000000000000	0.4976266601758527	T	T	T
0.2500000000000000	0.2388913748672940	0.6736913167201272	T	T	T
0.2500000000000000	0.7611086251327061	0.6736913167201272	T	T	T
0.7500000000000000	0.2388913748672940	0.6736913167201272	T	T	T
0.7500000000000000	0.7611086251327061	0.6736913167201272	T	T	T
0.0000000000000000	-0.0000000000000000	0.3147149649388215	T	T	T
-0.0000000000000000	0.5000000000000000	0.3239134616271207	T	T	T
0.5000000000000000	-0.0000000000000000	0.3147149649388215	T	T	T
0.5000000000000000	0.5000000000000000	0.3239134616271207	T	T	T
0.0000000000000000	0.2458415300762723	0.0069110023636973	T	T	T
-0.0000000000000000	0.7541584699237274	0.0069110023636973	T	T	T

0.5000000000000000	0.2458415300762723	0.0069110023636973	T	T	T
0.5000000000000000	0.7541584699237274	0.0069110023636973	T	T	T
0.2500000000000000	-0.0000000000000000	0.0018482386078343	T	T	T
0.2500000000000000	0.5000000000000000	0.0139636687916523	T	T	T
0.7500000000000000	-0.0000000000000000	0.0018482386078343	T	T	T
0.7500000000000000	0.5000000000000000	0.0139636687916523	T	T	T

BiLuCuOS (x=87.5%)

1.0000000000000000					
7.5489894439022667	0.0000000000000000	0.0000000000000000			
0.0000000000000000	7.5489894439022667	-0.0000000000000000			
0.0000000000000000	-0.0000000000000000	8.3620088549305631			

Bi Lu Cu S O
1 7 8 8 8

Selective dynamics

Direct

0.5000000000000000	0.5000000000000000	0.8569877500998956	T	T	T
0.2476218395999087	0.2476218395999087	0.1346555692589075	T	T	T
-0.0000000000000000	0.5000000000000000	0.8708191267253694	T	T	T
-0.0000000000000000	-0.0000000000000000	0.8688191449532956	T	T	T
0.2476218395999087	0.7523781604000909	0.1346555692589075	T	T	T
0.7523781604000909	0.2476218395999087	0.1346555692589075	T	T	T
0.5000000000000000	-0.0000000000000000	0.8708191267253694	T	T	T
0.7523781604000909	0.7523781604000909	0.1346555692589075	T	T	T
-0.0000000000000000	0.2491877301562400	0.4948670731702932	T	T	T
-0.0000000000000000	0.7508122698437605	0.4948670731702932	T	T	T
0.5000000000000000	0.2479180863171079	0.4995416017666433	T	T	T
0.5000000000000000	0.7520819136828922	0.4995416017666433	T	T	T
0.2491877301562400	-0.0000000000000000	0.4948670731702932	T	T	T
0.2479180863171079	0.5000000000000000	0.4995416017666433	T	T	T
0.7508122698437605	-0.0000000000000000	0.4948670731702932	T	T	T
0.7520819136828922	0.5000000000000000	0.4995416017666433	T	T	T
0.2444157396503880	0.2444157396503880	0.6773987098101291	T	T	T
0.2444157396503880	0.7555842603496119	0.6773987098101291	T	T	T
0.7555842603496119	0.2444157396503880	0.6773987098101291	T	T	T
0.7555842603496119	0.7555842603496119	0.6773987098101291	T	T	T
-0.0000000000000000	-0.0000000000000000	0.3145722762488714	T	T	T
-0.0000000000000000	0.5000000000000000	0.3188261337680577	T	T	T
0.5000000000000000	-0.0000000000000000	0.3188261337680577	T	T	T
0.5000000000000000	0.5000000000000000	0.3244754177965988	T	T	T
-0.0000000000000000	0.2497618015269667	0.0008674923191001	T	T	T
-0.0000000000000000	0.7502381984730332	0.0008674923191001	T	T	T
0.5000000000000000	0.2463461591768646	0.0066332761535477	T	T	T
0.5000000000000000	0.7536538408231354	0.0066332761535477	T	T	T
0.2497618015269667	-0.0000000000000000	0.0008674923191001	T	T	T
0.2463461591768646	0.5000000000000000	0.0066332761535477	T	T	T
0.7502381984730332	-0.0000000000000000	0.0008674923191001	T	T	T
0.7536538408231354	0.5000000000000000	0.0066332761535477	T	T	T