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C<sub>2</sub>H<sub>2</sub>-Induced Surface Restructuring of Pd–Ag Catalysts: Insights from Theoretical Modeling

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Supporting Information for:

## **C<sub>2</sub>H<sub>2</sub>-Induced Surface Restructuring of Pd-Ag Catalysts: Insights from Theoretical Modelling**

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As a separate file, the supporting information contain our Fortran code, called SurfaceEquilibrium.f90. It can be compiled by running:

```
gfortran -ffree-line-length-none -o SurfaceEquilibrium.x SurfaceEquilibrium.f90
```

The default version does not account for lateral interactions, but simple instructions in the code are given to turn lateral interactions on. The input file (called fort.10), needs to contain the following three lines:

```
Pressure in Pa
Temperature in K
The silver molar fraction
```

Then, you can run ./SurfaceEquilibrium.x and obtain the output file (fort.11).

## Embedding Energies and Coverage dependent Acetylene adsorption Energies at the PBE level

**SI 1. Adsorption Energies of Acetylene on Different Composition Triangular Sites, in Two Different Embeddings. Energies are in eV. Total energy calculations were performed with the PBE functional.**

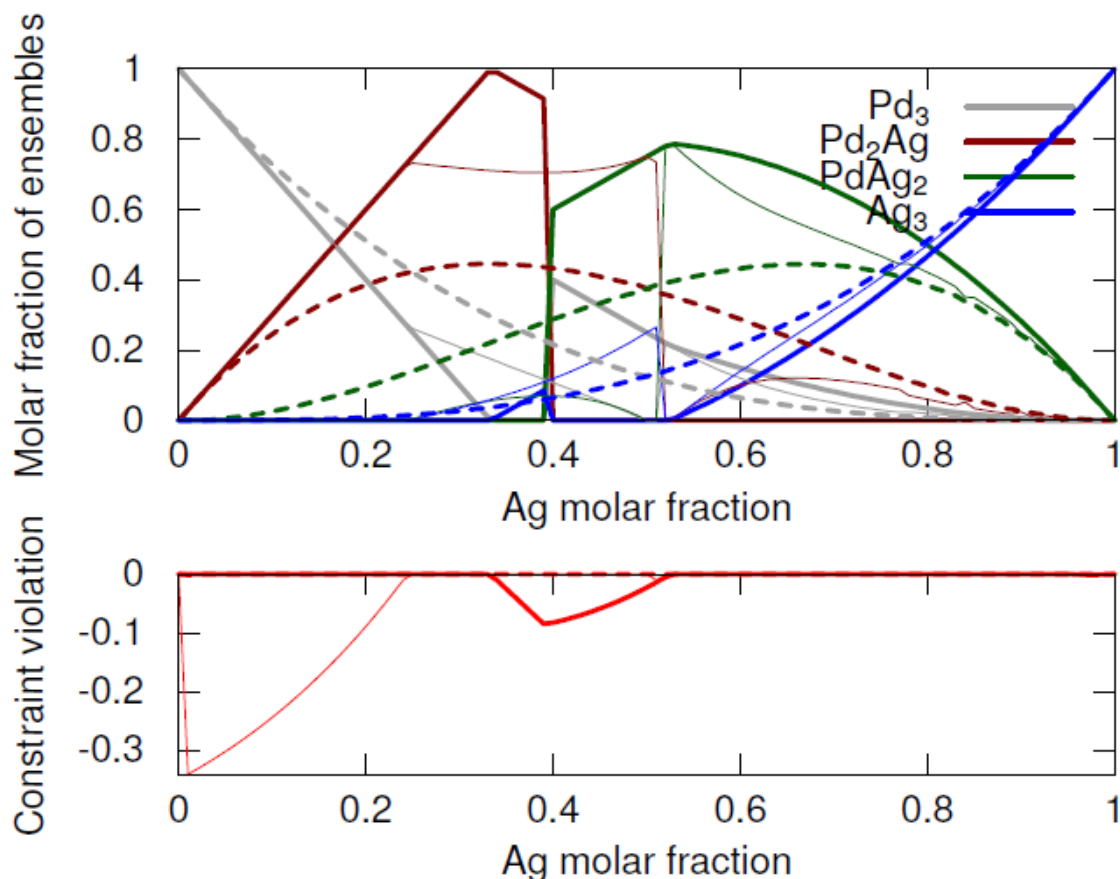
Site	Pd-Bed	Ag-Bed	Average	Error
Pd <sub>3</sub>	-2.08	-1.58	-1.83	-0.25
Pd <sub>2</sub> Ag	-1.51	-1.06	-1.28	-0.23
PdAg <sub>2</sub>	-0.73	-0.48	-0.60	0.13
Ag <sub>3</sub>	1.90	-0.05	0.92	0.98

**SI 2. Coverage dependent acetylene adsorption energy on Pd(111). Total energy calculations were performed with the PBE functional.**

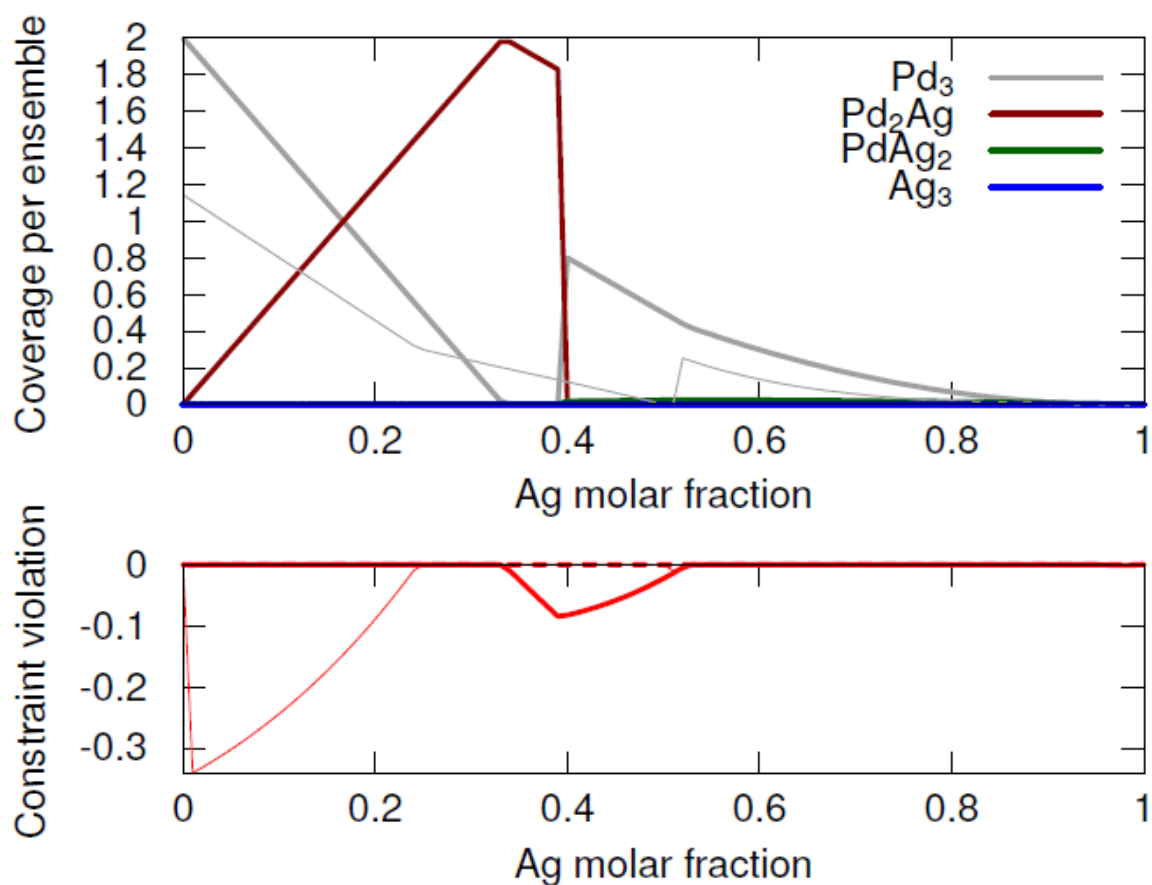
Coverage (ML)	Energy (eV)
0.11	-2.08
0.25	-2.04
0.33	-1.93
0.44	-1.41
0.50	-1.12

## Ensemble Distributions, Constraint Violations and Coverage at the PBE level

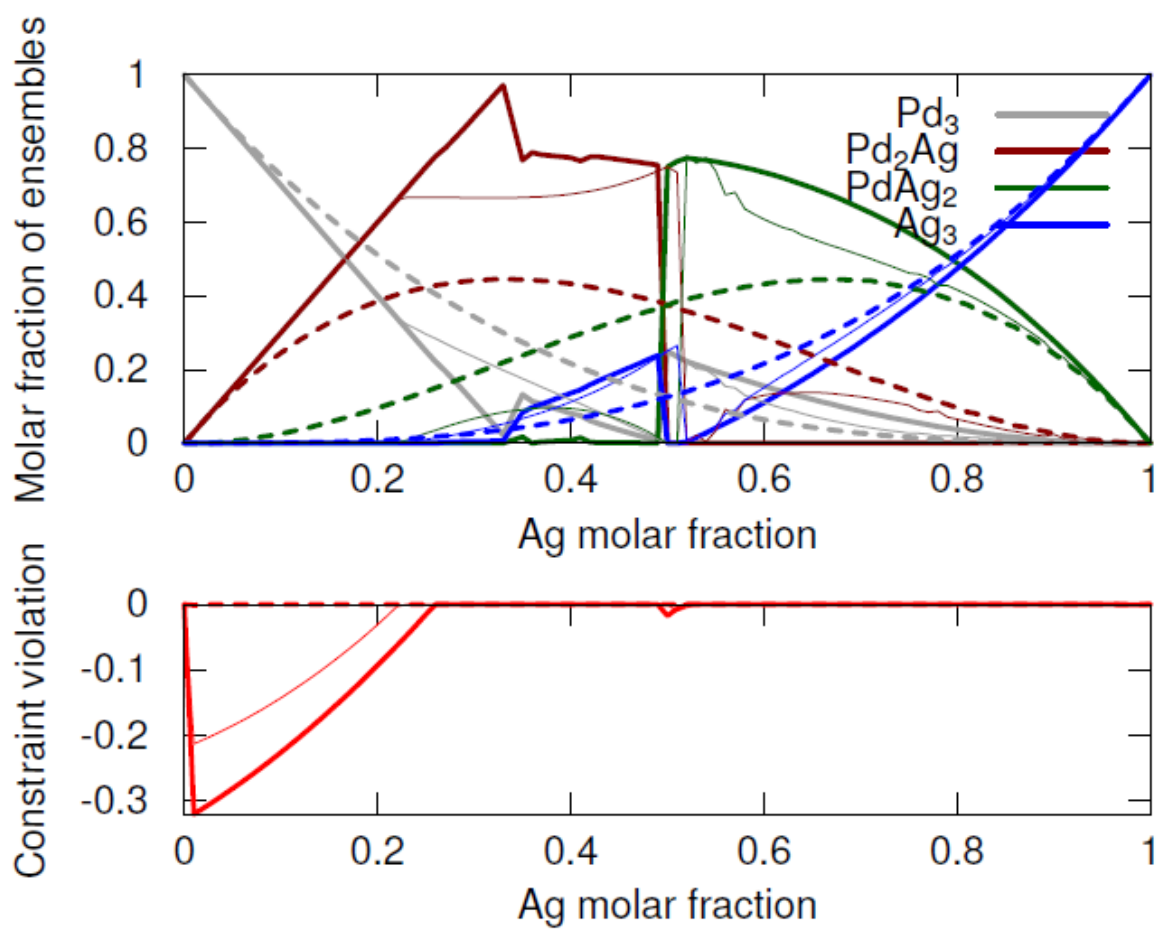
As mentioned in the “Theoretical Background” section of the manuscript, the system of equation requires us to specify the “randomness ansatz” in order to close the system of equations: Mass balance and ensemble equilibrium equations are solved for the molar fractions of three ensembles as a function of the molar fraction of the fourth one. The randomness ansatz suggests that the ensemble distribution of the uncovered part follows Martins’ distribution for the silver molar fraction of this uncovered fraction of the surface, which in general is not the same as for the total surface. Whenever the randomness ansatz is violated (due to stoichiometric constraints and the adsorption equilibrium with acetylene), the algorithm minimizes the deviation.



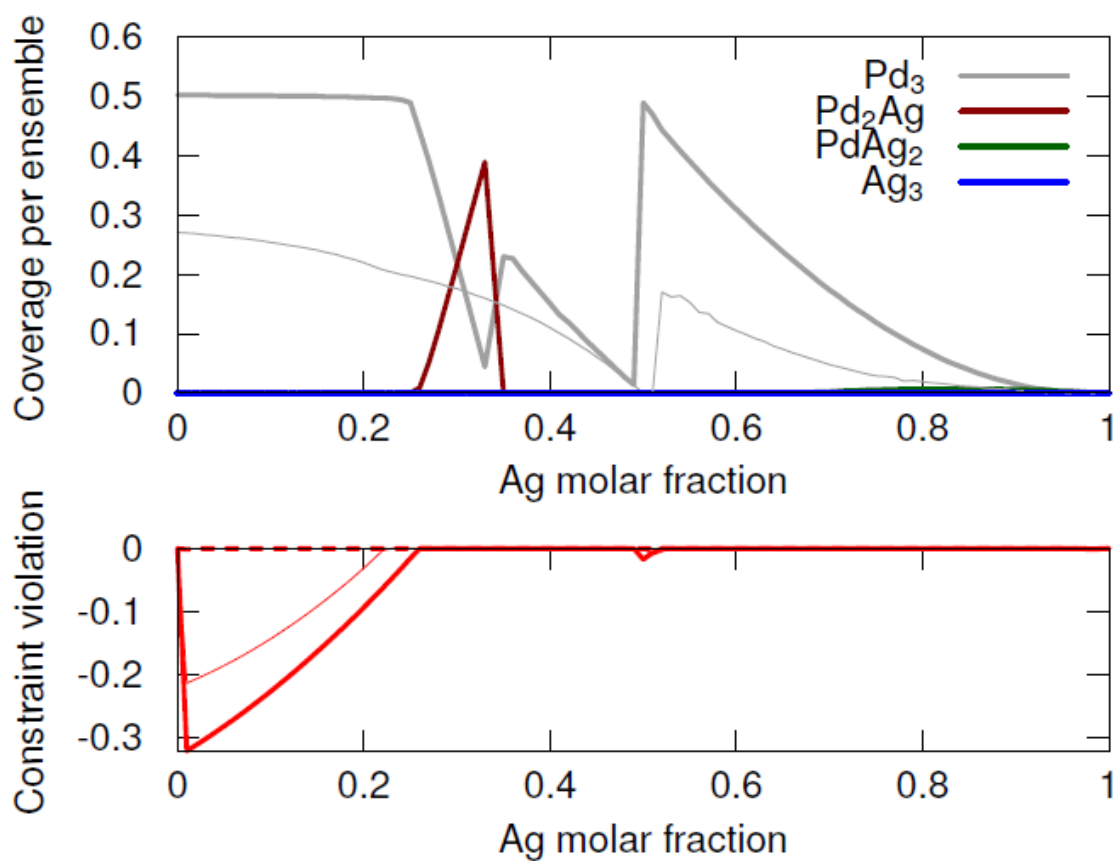
SI 3. Top: Probability presence of Pd<sub>3</sub> (grey) Pd<sub>2</sub>Ag (magenta), PdAg<sub>2</sub> (green) and Ag<sub>3</sub> (blue) triplets on the Pd-Ag surface as a function of the Ag layer concentration in the ideal gas approximation. Total energy calculations were performed with the PBE functional. Thick lines: 300 K; thin lines: 700 K; dashed lines: 900 K. Bottom: Randomness constraint violation as a function of the Ag layer concentration.



SI 4. Top: Acetylene-covered fraction of Pd<sub>3</sub> (grey) Pd<sub>2</sub>Ag (magenta), PdAg<sub>2</sub> (green) and Ag<sub>3</sub> (blue) triplets on the Pd-Ag surface as a function of the Ag layer concentration in the ideal gas approximation. Total energy calculations were performed with the PBE functional. Thick lines: 300 K; thin lines: 700 K; dashed lines: 900 K. Bottom: Randomness constraint violation as a function of the Ag layer concentration.

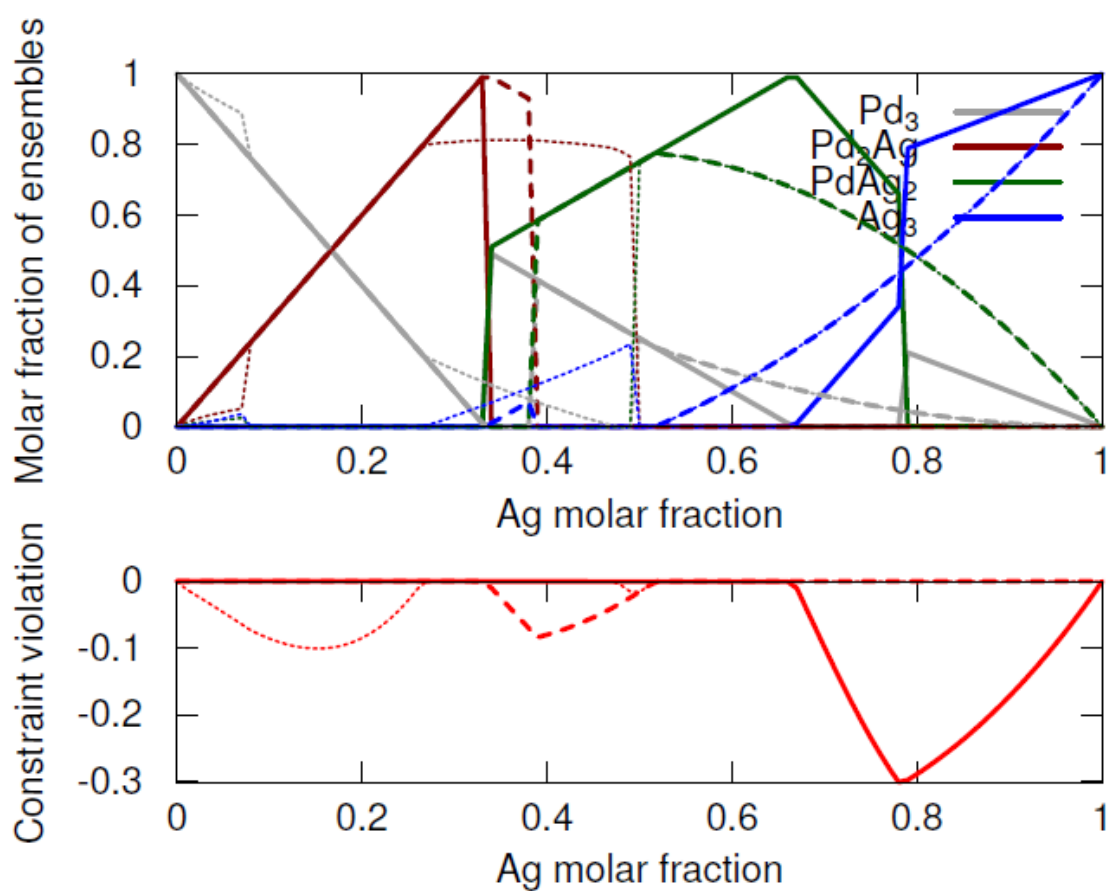


SI 5. Top: Probability presence of  $\text{Pd}_3$  (grey)  $\text{Pd}_2\text{Ag}$  (magenta),  $\text{PdAg}_2$  (green) and  $\text{Ag}_3$  (blue) triplets on the Pd-Ag surface as a function of the Ag layer concentration in the lateral interactions-implemented approximation. Total energy calculations were performed with the PBE functional. Thick lines: 300 K; thin lines: 700 K; dashed lines: 900 K. Bottom: Randomness constraint violation as a function of the Ag layer concentration.



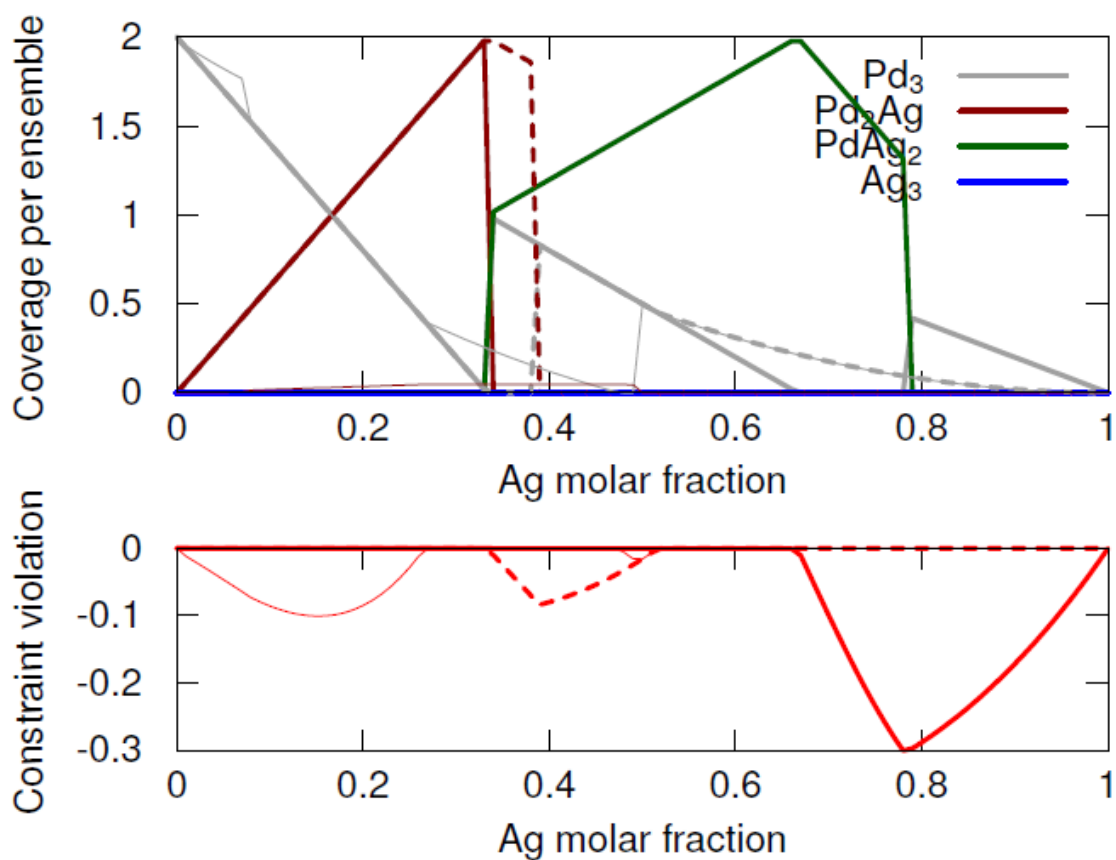
SI 6. Top: Acetylene-covered fraction of  $\text{Pd}_3$  (grey)  $\text{Pd}_2\text{Ag}$  (magenta),  $\text{PdAg}_2$  (green) and  $\text{Ag}_3$  (blue) triplets on the Pd-Ag surface as a function of the Ag layer concentration in the lateral interactions-implemented approximation. Total energy calculations were performed with the PBE functional. Thick lines: 300 K; thin lines: 700 K; dashed lines: 900 K. Bottom: Randomness constraint violation as a function of the Ag layer concentration.

Ensemble Distributions, Constraint Violations and Coverage at the PBE-dDsC level

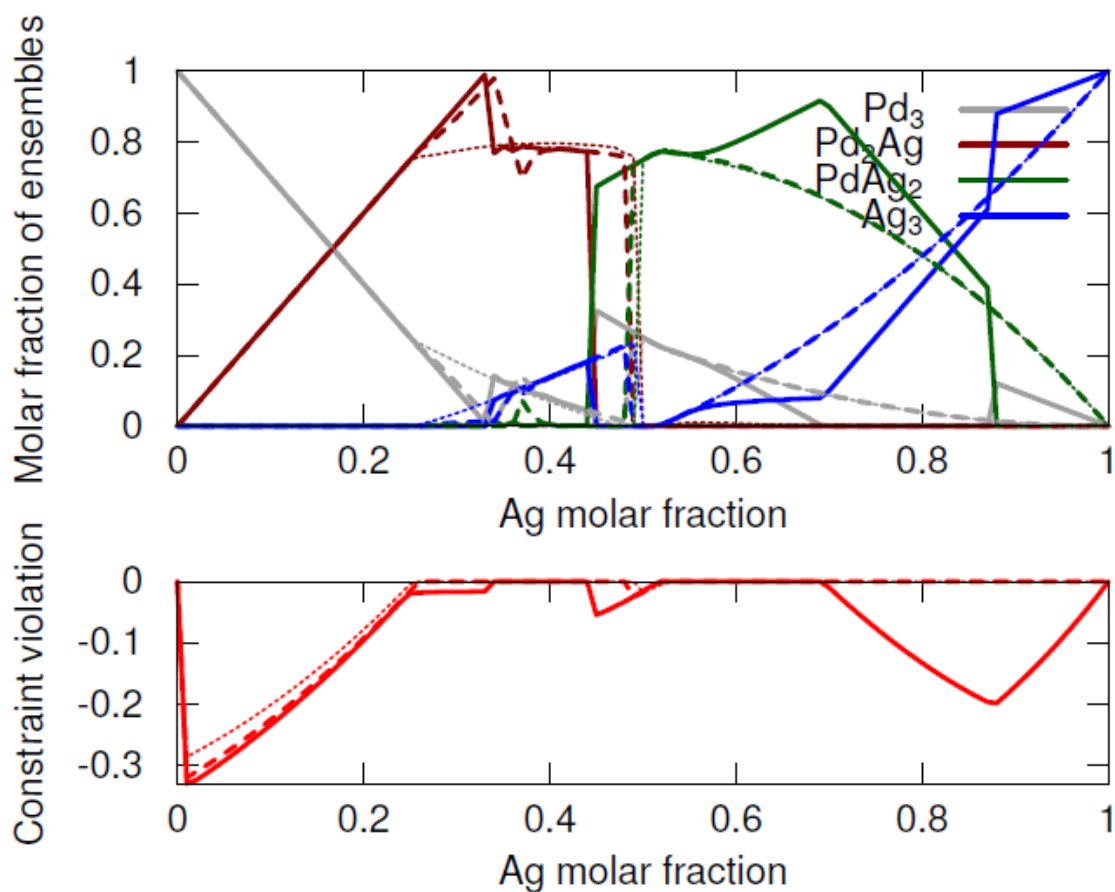


SI 7. Top: Probability presence of Pd<sub>3</sub> (grey) Pd<sub>2</sub>Ag (magenta), PdAg<sub>2</sub> (green) and Ag<sub>3</sub> (blue) triplets on the Pd-Ag surface as a function of the Ag layer concentration in the ideal gas approximation. Total energy calculations were performed with the PBE-dDsC functional. Thick lines: 300 K; dashed lines: 500 K; dotted lines: 700 K. Bottom: Randomness constraint violation as a function of the Ag layer concentration.

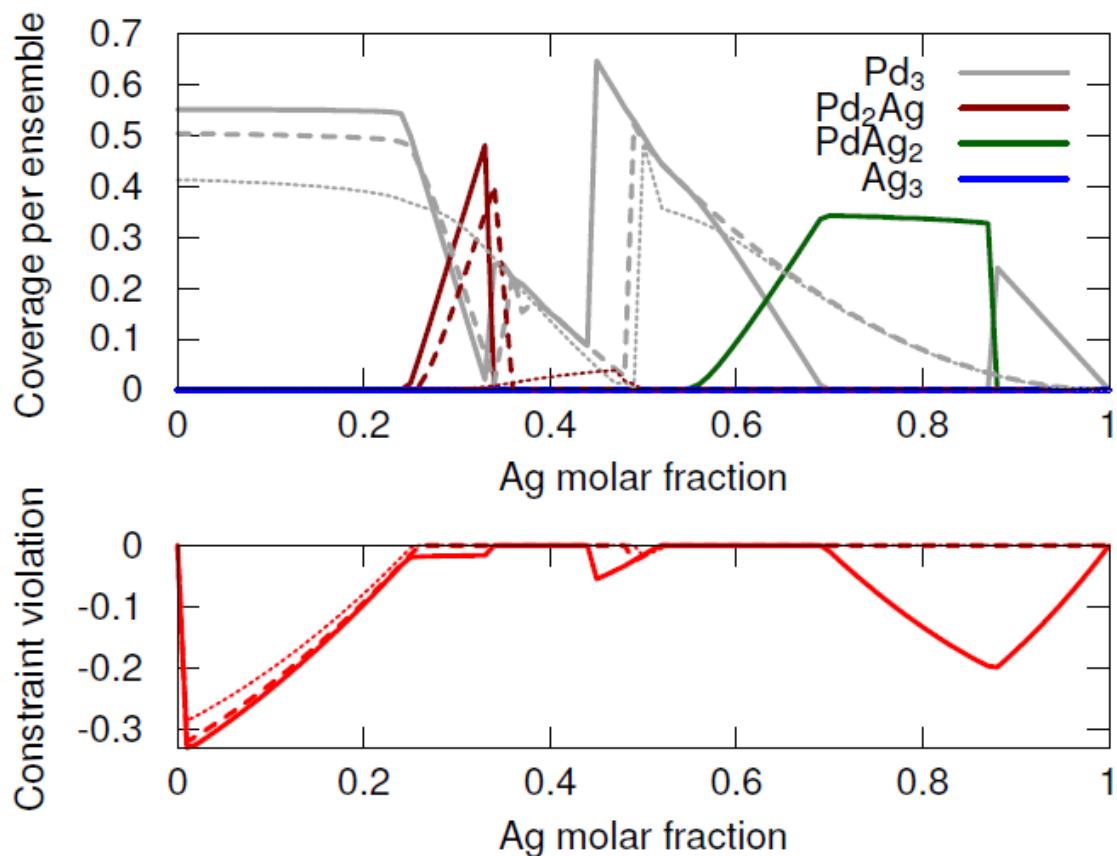




SI 8. Top: Acetylene-covered fraction of  $\text{Pd}_3$  (grey)  $\text{Pd}_2\text{Ag}$  (magenta),  $\text{PdAg}_2$  (green) and  $\text{Ag}_3$  (blue) triplets on the Pd-Ag surface as a function of the Ag layer concentration in the ideal gas approximation. Total energy calculations were performed with the PBE-dDsC functional. Thick lines: 300 K; dashed lines: 500 K; thin lines: 700 K. Bottom: Randomness constraint violation as a function of the Ag layer concentration.

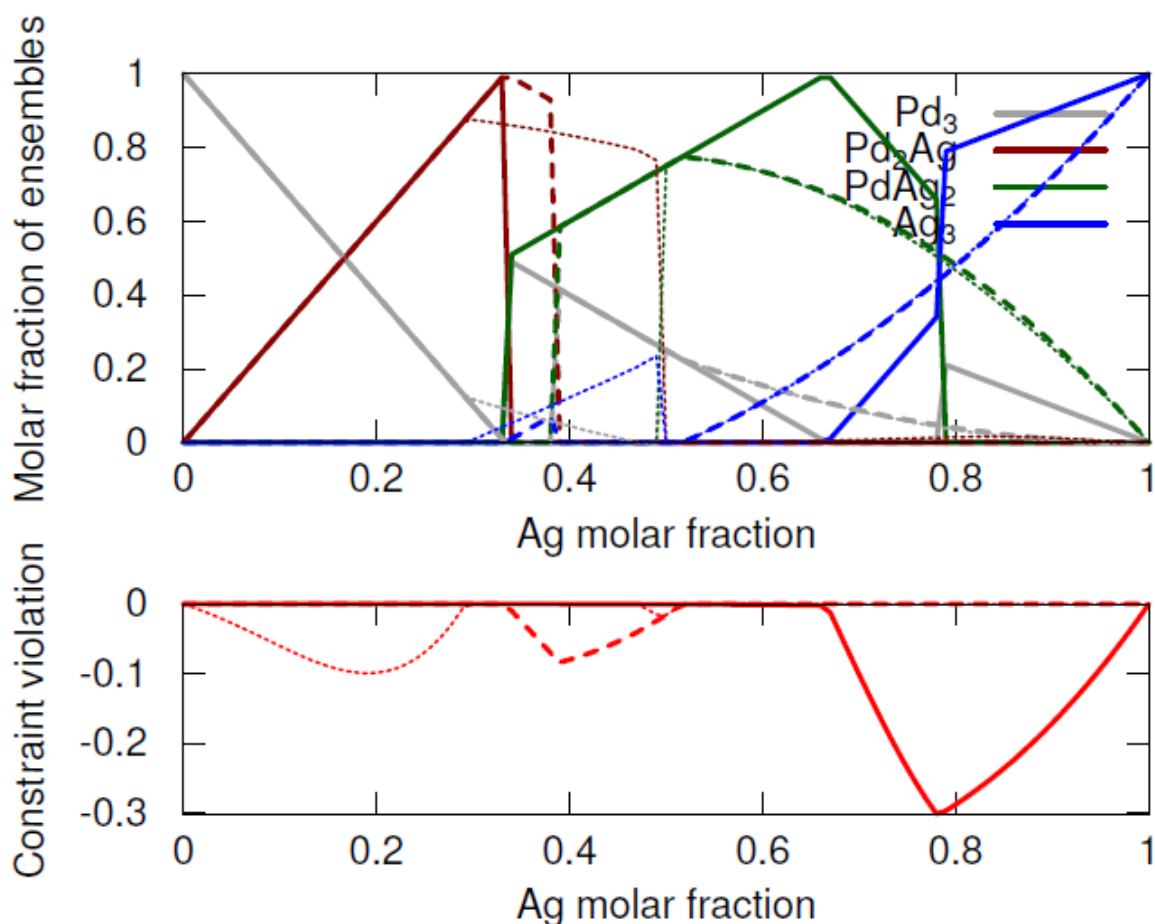


SI 9. Top: Acetylene-covered fraction of  $\text{Pd}_3$  (grey)  $\text{Pd}_2\text{Ag}$  (magenta),  $\text{PdAg}_2$  (green) and  $\text{Ag}_3$  (blue) triplets on the clean Pd-Ag surface as a function of the Ag layer concentration in the lateral interactions-implemented model approximation. Total energy calculations were performed with the PBE-dDsC functional. Thick lines: 300 K; dashed lines: 500 K; dotted lines: 700 K. Bottom: Randomness constraint violation as a function of the Ag layer concentration.

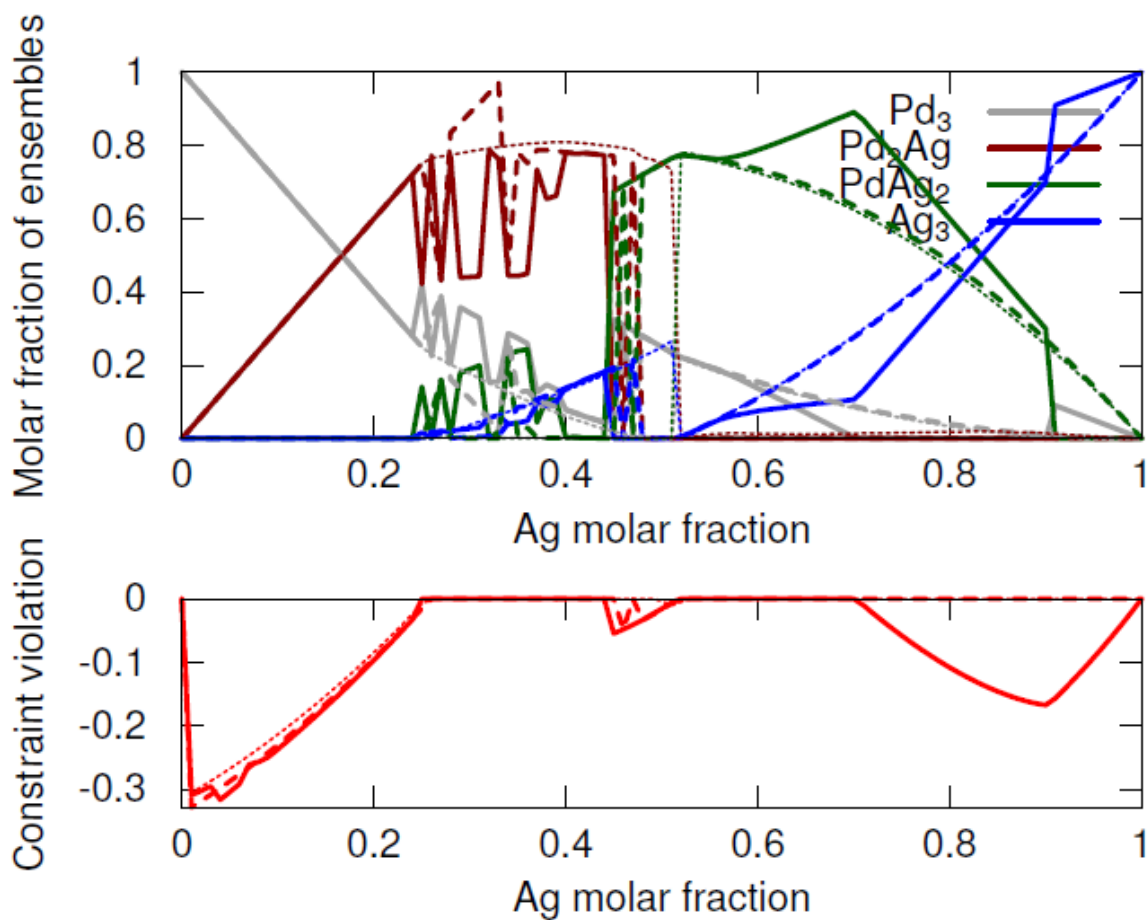


SI 10. Top: Acetylene-covered fraction of  $\text{Pd}_3$  (grey)  $\text{Pd}_2\text{Ag}$  (magenta),  $\text{PdAg}_2$  (green) and  $\text{Ag}_3$  (blue) triplets on the Pd-Ag surface as a function of the Ag layer concentration in the lateral interactions-implemented model approximation. Total energy calculations were performed with the PBE-dDsC functional. Thick lines: 300 K; dashed lines: 500 K; thin lines: 700 K. Bottom: Randomness constraint violation as a function of the Ag layer concentration.

Ensemble Distributions, Constraint Violations and Coverage at the PBE-dDsC level, Accounting for the Embedding Effect Through Linear Interpolation between Pd and Ag Embedding



SI 11. Top: Probability presence of Pd<sub>3</sub> (grey) Pd<sub>2</sub>Ag (magenta), PdAg<sub>2</sub> (green) and Ag<sub>3</sub> (blue) triplets on the Pd-Ag surface as a function of the Ag layer concentration in the ideal gas approximation. Total energy calculations were performed with the PBE-dDsC functional. Here, energies of adsorption are interpolated in a linear construction from one embedding to the other one. Thick lines: 300 K; dashed lines: 500 K; dotted lines: 700 K. Bottom: Randomness constraint violation as a function of the Ag layer concentration.



SI 12. Top: Probability presence of  $\text{Pd}_3$  (grey)  $\text{Pd}_2\text{Ag}$  (magenta),  $\text{PdAg}_2$  (green) and  $\text{Ag}_3$  (blue) triplets on the Pd-Ag surface as a function of the Ag layer concentration in the lateral interactions-implemented approximation. Total energy calculations were performed with the PBE-dDsC functional. Here, energies of adsorption are interpolated in a linear construction from one embedding to the other one. Thick lines: 300 K; dashed lines: 500 K; dotted lines: 700 K. Bottom: Randomness constraint violation as a function of the Ag layer concentration.



## PBE Geometries

```

2x2_0.25ML_PBE
 2.80166844800000
 2.0000000000000000 0.0000000000000000 0.0000000000000000
 1.0000000000000000 1.7320508079999999 0.0000000000000000
 0.0000000000000000 0.0000000000000000 9.3825138849999998
 Pd   C   H
 24   2   2
Selective dynamics
Direct
 0.0000000000000000 0.0000000000000000 0.0000000000000000 F F F
 0.6666666670000012 0.6666666670000012 0.0870232210000026 F F F
 0.3321679087030786 0.3321679087030786 0.1734683193668690 T T T
-0.0020482821257293 -0.0020482821257293 0.2610964549314602 T T T
 0.6660059179749832 0.6660059179749832 0.3462450012092086 T T T
 0.8353743511871657 0.8353743511871657 0.4374220904839186 T T T
 0.5000000000000000 0.0000000000000000 0.0000000000000000 F F F
 0.0000000000000000 0.5000000000000000 0.0000000000000000 F F F
 0.5000000000000000 0.5000000000000000 0.0000000000000000 F F F
 0.1666666670000012 0.1666666670000012 0.0870232210000026 F F F
 0.6666666670000012 0.1666666670000012 0.0870232210000026 F F F
 0.1666666670000012 0.6666666670000012 0.0870232210000026 F F F
 0.8322650019117384 0.3313125318914861 0.1734682031764224 T T T
 0.3313125318914861 0.8322650019117455 0.1734682031764224 T T T
 0.8321245640311894 0.8321245640311894 0.1735298028984940 T T T
 0.4979619035748740 -0.0013485676601067 0.2597964728092105 T T T
-0.0013485676601067 0.4979619035748740 0.2597964728092105 T T T
 0.4978257832430732 0.4978257832430803 0.2601778084543792 T T T
 0.1649455766254360 0.1649455766254360 0.3468626209176550 T T T
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 0.6671438837579839 0.1639831742627702 0.3479524917099414 T T T
 0.3321590217913316 0.3321590217913316 0.4325801988469195 T T T
 0.8306273998331097 0.3314518960116161 0.4354009112066054 T T T
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 0.8120212043408775 0.5673002252195672 0.4944759581180903 T T T
 0.5673002252195672 0.8120212043408775 0.4944759581180903 T T T
 0.9530085536624558 0.4702392877843469 0.5265413807109375 T T T
 0.4702392877843469 0.9530085536624558 0.5265413807109375 T T T
2x2_0.5ML_PBE
 2.80166844800000
 2.0000000000000000 0.0000000000000000 0.0000000000000000
 1.0000000000000000 1.7320508079999999 0.0000000000000000
 0.0000000000000000 0.0000000000000000 9.3825138849999998
 Pd   C   H
 24   4   4
Selective dynamics
Direct
 0.0000000000000000 0.0000000000000000 0.0000000000000000 F F F
 0.6666666670000012 0.6666666670000012 0.0870232210000026 F F F
 0.3323292403602982 0.3332265512247770 0.1736917733402403 T T T
-0.0017057671627498 0.0007819763566005 0.2601446968373119 T T T
 0.6611845133379267 0.6753895423435367 0.3479788778352061 T T T
 0.8368474211873951 0.8300634964964698 0.4413937434611583 T T T
 0.5000000000000000 0.0000000000000000 0.0000000000000000 F F F
 0.0000000000000000 0.5000000000000000 0.0000000000000000 F F F
 0.5000000000000000 0.5000000000000000 0.0000000000000000 F F F

```

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0.6666666670000012	0.1666666670000012	0.0870232210000026	F	F	F
0.1666666670000012	0.6666666670000012	0.0870232210000026	F	F	F
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0.4983385297158586	0.0006834935067302	0.2600953651296770	T	T	T
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0.0000000000000000	0.0000000000000000	9.3825138849999998			
Pd					
24					
Selective dynamics					
Direct					
0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666670000012	0.6666666670000012	0.0870232210000026	F	F	F
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0.3333333329999988	0.3333333329999988	0.4333816090338239	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.1666666670000012	0.1666666670000012	0.0870232210000026	F	F	F
0.6666666670000012	0.1666666670000012	0.0870232210000026	F	F	F
0.1666666670000012	0.6666666670000012	0.0870232210000026	F	F	F
0.8333333329999988	0.3333333329999988	0.1734936405688727	T	T	T
0.3333333329999988	0.8333333329999988	0.1734936405688727	T	T	T
0.8333333329999988	0.8333333329999988	0.1734936405688727	T	T	T
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0.1666666670000012	0.1666666670000012	0.3463453834628618	T	T	T
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0.6666666670000012	0.1666666670000012	0.3463453834628618	T	T	T
0.8333333329999988	0.3333333329999988	0.4333816090338239	T	T	T
0.3333333329999988	0.8333333329999988	0.4333816090338239	T	T	T
0.8333333329999988	0.8333333329999988	0.4333816090338239	T	T	T
3x3_0.11ML_PBE					
2.80166844800000					



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	1.4999999999999998	2.5980762110000000	0.0000000000000000			
	0.0000000000000000	0.0000000000000000	11.4687304500000007			
Pd	C	H				
54	2	2				
Selective dynamics						
Direct						
	0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
	0.3333333329999988	0.0000000000000000	0.0000000000000000	F	F	F
	0.6666666659999976	0.0000000000000000	0.0000000000000000	F	F	F
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	0.0000000000000000	0.6666666659999976	0.0000000000000000	F	F	F
	0.3333333329999988	0.6666666659999976	0.0000000000000000	F	F	F
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	0.8861678664155527	0.2243054874174288	0.1417208206475286	T	T	T
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	0.3284464299353275	0.0036905963739791	0.2121447350726786	T	T	T
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0.6615796561964410	0.3363616631981789	0.2129493117531045	0.2129493117531045	T	T	T
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0.4404477802121622	0.1128424395184272	0.2840086587002046	0.2840086587002046	T	T	T
0.7720884706070028	0.1130034426566179	0.2841278498315107	0.2841278498315107	T	T	T
0.1057678884601966	0.4472637752912743	0.2836933861285197	0.2836933861285197	T	T	T
0.4390301832810046	0.4466772557562477	0.2837083205785026	0.2837083205785026	T	T	T
0.7716756974155013	0.4474542313344401	0.2837406890903555	0.2837406890903555	T	T	T
0.1052910818483318	0.7802193902097314	0.2839993526102654	0.2839993526102654	T	T	T
0.4393773586683583	0.7802198571022939	0.2839582440215945	0.2839582440215945	T	T	T
0.7726549361038899	0.7800590136055118	0.2835093404349889	0.2835093404349889	T	T	T
0.2154253102404106	0.2217685982228845	0.3542690569023880	0.3542690569023880	T	T	T
0.5540603239377359	0.2173180326513493	0.3571256392621859	0.3571256392621859	T	T	T
0.8885271026785345	0.2218407980326328	0.3543458140941756	0.3543458140941756	T	T	T
0.2151664330422152	0.5590879631484400	0.3568733198212879	0.3568733198212879	T	T	T
0.5507817731188751	0.5588311738069376	0.3569108687972856	0.3569108687972856	T	T	T
0.8834988329142461	0.5581976880549878	0.3546864506678900	0.3546864506678900	T	T	T

0.2167130656504608	0.8922756242181992	0.3545809042066618	T	T	T
0.5511929443100566	0.8883844306818399	0.3549118814801761	T	T	T
0.8854729809013601	0.8886096460556041	0.3550211102339796	T	T	T
0.5397552279922602	0.4084106363185789	0.4041949771098000	T	T	T
0.3764823527450708	0.4083491107201980	0.4041258845616776	T	T	T
0.6349255166221788	0.3777123741876027	0.4302413009152111	T	T	T
0.3118393558894495	0.3774020628391124	0.4300956814191628	T	T	T
3x3 0.44ML_PBE					
2.80166844800000					
2.9999999999999996	0.0000000000000000	0.0000000000000000			
1.4999999999999998	2.5980762110000000	0.0000000000000000			
0.0000000000000000	0.0000000000000000	11.4687304500000007			
Pd	C	H			
54	8	8			
Selective dynamics					
Direct					
0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3333333329999988	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666659999976	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333329999988	0.0000000000000000	F	F	F
0.3333333329999988	0.3333333329999988	0.0000000000000000	F	F	F
0.6666666659999976	0.3333333329999988	0.0000000000000000	F	F	F
0.0000000000000000	0.6666666659999976	0.0000000000000000	F	F	F
0.3333333329999988	0.6666666659999976	0.0000000000000000	F	F	F
0.6666666659999976	0.6666666659999976	0.0000000000000000	F	F	F
0.1111111109999996	0.1111111109999996	0.0711932869999998	F	F	F
0.4444444439999984	0.1111111109999996	0.0711932869999998	F	F	F
0.7777777769999972	0.1111111109999996	0.0711932869999998	F	F	F
0.1111111109999996	0.4444444439999984	0.0711932869999998	F	F	F
0.4444444439999984	0.4444444439999984	0.0711932869999998	F	F	F
0.7777777769999972	0.4444444439999984	0.0711932869999998	F	F	F
0.1111111109999996	0.7777777769999972	0.0711932869999998	F	F	F
0.4444444439999984	0.7777777769999972	0.0711932869999998	F	F	F
0.7777777769999972	0.7777777769999972	0.0711932869999998	F	F	F
0.2221487813065969	0.2226084454380435	0.1419969876638102	T	T	T
0.5560191099697569	0.2226311864906916	0.1418063509535914	T	T	T
0.8893025821194337	0.2227391935200747	0.1421340796278488	T	T	T
0.2227182580347833	0.5561249894887688	0.1419765445142625	T	T	T
0.5559855844805118	0.5569126472041710	0.1420588196341619	T	T	T
0.8890238687540230	0.5560536389022700	0.1422888124646182	T	T	T
0.2225907032030422	0.8887876061991347	0.1419322674681446	T	T	T
0.5564532012362223	0.8885393870730448	0.1418525806623434	T	T	T
0.8894371031690589	0.8888615970704472	0.1420764655387141	T	T	T
0.0018926081374786	0.0007872325750589	0.2131855411845051	T	T	T
0.3341870409977190	-0.0008024898053109	0.2123822207025537	T	T	T
0.6691357621512674	0.0006568418417704	0.2127550927070895	T	T	T
0.0008725743958289	0.3335481545248237	0.2136436451739830	T	T	T
0.3332765677080834	0.3350105280023823	0.2125002847263367	T	T	T
0.6669773938127692	0.3345646915315666	0.2129053165155312	T	T	T
0.0016056686132512	0.6681185179886984	0.2135734756231258	T	T	T
0.3336017400666408	0.6676519158057986	0.2135557583020251	T	T	T
0.6677977176489254	0.6672773876426604	0.2138214403947470	T	T	T
0.1155388363908840	0.1122975492497648	0.2858087817485042	T	T	T
0.4432517939225467	0.1125191542714807	0.2818426828352367	T	T	T
0.7828722880524082	0.1125886724335412	0.2838134374196658	T	T	T
0.1099494591170847	0.4484304223196781	0.2845802069059152	T	T	T
0.4414900310887384	0.4513171763136541	0.2843990383250457	T	T	T
0.7765451457906232	0.4475479368615648	0.2852651690999679	T	T	T

0.1126920560991445	0.7817009301183340	0.2857356236808439	T	T	T
0.4454335118936844	0.7762611133330438	0.2848610114858745	T	T	T
0.7774404167872881	0.7789952742890618	0.2849083546042846	T	T	T
0.2224755038556530	0.2342501929950630	0.3584327893701860	T	T	T
0.5549777017177581	0.2212558895966403	0.3501797694888596	T	T	T
0.8906315189141499	0.2210322322334716	0.3553712884714978	T	T	T
0.1936597225028840	0.5763640210876640	0.3597949431539221	T	T	T
0.5449316496689912	0.5289051230364898	0.3815374129871759	T	T	T
0.8646233072894136	0.5675983512824742	0.3601855320973416	T	T	T
0.2283550295066150	0.8860394375030923	0.3586165336555474	T	T	T
0.5483046387679478	0.8956394161400314	0.3546684069452198	T	T	T
0.8727791849018094	0.9106150151189887	0.3556262647911634	T	T	T
0.4056504561144801	0.9143908753022514	0.4064979157972879	T	T	T
0.3870361432810278	0.7657432684434350	0.4143237696273055	T	T	T
0.9237284197815019	0.3802221802811663	0.4061953419687427	T	T	T
0.7810188854437679	0.3506917229231244	0.4128279197699145	T	T	T
0.4709364099860928	0.3254053816417886	0.4072251387906021	T	T	T
0.2884584507974927	0.3768920562225381	0.4046103281660964	T	T	T
0.0190324799693301	0.7426255124486645	0.4059031891724885	T	T	T
0.8568310577314334	0.7427093272523148	0.4054397325687994	T	T	T
0.3810905194329530	0.0228186725845121	0.4288644206441438	T	T	T
0.3281919452545168	0.7437324798824680	0.4427308069614347	T	T	T
0.0291732162704113	0.3503161010673957	0.4296244270579158	T	T	T
0.7665273339441145	0.2789093536645496	0.4396854974371357	T	T	T
0.5556784012244267	0.2607088880661154	0.4347913526755384	T	T	T
0.2044699864125660	0.4010750410586165	0.4326343108352421	T	T	T
0.0777224789536615	0.7811504813187720	0.4316664701562989	T	T	T
0.7573116988820001	0.7832233827200558	0.4307855041838145	T	T	T
3x3_PBE_bare					
2.80166844800000					
2.9999999999999996	0.0000000000000000	0.0000000000000000			
1.4999999999999998	2.5980762110000000	0.0000000000000000			
0.0000000000000000	0.0000000000000000	11.4687304500000007			
Pd					
54					
Selective dynamics					
Direct					
0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3333333299999988	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666599999976	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333299999988	0.0000000000000000	F	F	F
0.3333333299999988	0.3333333299999988	0.0000000000000000	F	F	F
0.6666666599999976	0.3333333299999988	0.0000000000000000	F	F	F
0.0000000000000000	0.6666666599999976	0.0000000000000000	F	F	F
0.3333333299999988	0.6666666599999976	0.0000000000000000	F	F	F
0.6666666599999976	0.6666666599999976	0.0000000000000000	F	F	F
0.1111111099999996	0.1111111099999996	0.0711932869999998	F	F	F
0.4444444399999984	0.1111111099999996	0.0711932869999998	F	F	F
0.7777777699999972	0.1111111099999996	0.0711932869999998	F	F	F
0.1111111099999996	0.4444444399999984	0.0711932869999998	F	F	F
0.4444444399999984	0.4444444399999984	0.0711932869999998	F	F	F
0.7777777699999972	0.4444444399999984	0.0711932869999998	F	F	F
0.1111111099999996	0.7777777699999972	0.0711932869999998	F	F	F
0.4444444399999984	0.7777777699999972	0.0711932869999998	F	F	F
0.7777777699999972	0.7777777699999972	0.0711932869999998	F	F	F
0.2222222199999992	0.2222222199999992	0.1418432811439177	T	T	T
0.5555555499999980	0.2222222199999992	0.1418432811439177	T	T	T
0.8888888799999968	0.2222222199999992	0.1418432811439177	T	T	T

0.222222219999992	0.555555549999980	0.1418432811439177	T	T	T
0.555555549999980	0.555555549999980	0.1418432811439177	T	T	T
0.888888879999968	0.555555549999980	0.1418432811439177	T	T	T
0.222222219999992	0.888888879999968	0.1418432811439177	T	T	T
0.555555549999980	0.888888879999968	0.1418432811439177	T	T	T
0.888888879999968	0.888888879999968	0.1418432811439177	T	T	T
-0.000000000000000	-0.000000000000000	0.2126047287731679	T	T	T
0.333333329999988	0.000000000000000	0.2126047287731679	T	T	T
0.666666659999976	-0.000000000000000	0.2126047287731679	T	T	T
-0.000000000000000	0.333333329999988	0.2126047287731679	T	T	T
0.333333329999988	0.333333329999988	0.2126047287731679	T	T	T
0.666666659999976	0.333333329999988	0.2126047287731679	T	T	T
-0.000000000000000	0.666666659999976	0.2126047287731679	T	T	T
0.333333329999988	0.666666659999976	0.2126047287731679	T	T	T
0.666666659999976	0.666666659999976	0.2126047287731679	T	T	T
0.111111109999996	0.111111109999996	0.2831538900484000	T	T	T
0.444444439999984	0.111111109999996	0.2831538900484000	T	T	T
0.777777769999972	0.111111109999996	0.2831538900484000	T	T	T
0.111111109999996	0.444444439999984	0.2831538900484000	T	T	T
0.444444439999984	0.444444439999984	0.2831538900484000	T	T	T
0.777777769999972	0.444444439999984	0.2831538900484000	T	T	T
0.111111109999996	0.777777769999972	0.2831538900484000	T	T	T
0.444444439999984	0.777777769999972	0.2831538900484000	T	T	T
0.777777769999972	0.777777769999972	0.2831538900484000	T	T	T
0.222222219999992	0.222222219999992	0.3543985364233493	T	T	T
0.555555549999980	0.222222219999992	0.3543985364233493	T	T	T
0.888888879999968	0.222222219999992	0.3543985364233493	T	T	T
0.222222219999992	0.555555549999980	0.3543985364233493	T	T	T
0.555555549999980	0.555555549999980	0.3543985364233493	T	T	T
0.888888879999968	0.555555549999980	0.3543985364233493	T	T	T
0.222222219999992	0.888888879999968	0.3543985364233493	T	T	T
0.555555549999980	0.888888879999968	0.3543985364233493	T	T	T
0.888888879999968	0.888888879999968	0.3543985364233493	T	T	T
Ag3_AgEmb_0.11ML_PBE					
2.92418893300000					
2.999999999999996	0.000000000000000	0.000000000000000			
1.499999999999998	2.598076211000000	0.000000000000000			
0.000000000000000	0.000000000000000	11.468730450000007			
Ag	C	H			
54	2	2			
Selective dynamics					
Direct					
0.000000000000000	0.000000000000000	0.000000000000000	F	F	F
0.333333329999988	0.000000000000000	0.000000000000000	F	F	F
0.666666659999976	0.000000000000000	0.000000000000000	F	F	F
0.000000000000000	0.333333329999988	0.000000000000000	F	F	F
0.333333329999988	0.333333329999988	0.000000000000000	F	F	F
0.666666659999976	0.333333329999988	0.000000000000000	F	F	F
0.000000000000000	0.666666659999976	0.000000000000000	F	F	F
0.333333329999988	0.666666659999976	0.000000000000000	F	F	F
0.666666659999976	0.666666659999976	0.000000000000000	F	F	F
0.111111109999996	0.111111109999996	0.071193286999998	F	F	F
0.444444439999984	0.111111109999996	0.071193286999998	F	F	F
0.777777769999972	0.111111109999996	0.071193286999998	F	F	F
0.111111109999996	0.444444439999984	0.071193286999998	F	F	F
0.444444439999984	0.444444439999984	0.071193286999998	F	F	F
0.777777769999972	0.444444439999984	0.071193286999998	F	F	F
0.111111109999996	0.777777769999972	0.071193286999998	F	F	F

0.4444444439999984	0.7777777769999972	0.0711932869999998	F	F	F
0.7777777769999972	0.7777777769999972	0.0711932869999998	F	F	F
0.2213375224124568	0.2221729871806307	0.1428590949758566	T	T	T
0.5547418409779803	0.2221345803968276	0.1427557225332475	T	T	T
0.8880250786830690	0.2220878354301370	0.1427466970948250	T	T	T
0.2214544733041158	0.5554090194002743	0.1427561158916746	T	T	T
0.5548122631657857	0.5553787328722442	0.1427465823908897	T	T	T
0.8880196779761581	0.5554243994994461	0.1427347819461051	T	T	T
0.2214948276447233	0.8886577199400588	0.1427408017552392	T	T	T
0.5547483594536615	0.8887183812690264	0.1427274337946564	T	T	T
0.8880213554955950	0.8887090645433867	0.1427348204423297	T	T	T
-0.0017016614703132	-0.0002696378090539	0.2143647824514388	T	T	T
0.3319992280508125	-0.0008249772270402	0.2144979894355590	T	T	T
0.6649227429535315	-0.0001893520300334	0.2143995340874396	T	T	T
-0.0021381651173939	0.3332938531406708	0.2144824779789210	T	T	T
0.3319615001661384	0.3331642434645995	0.2145506745393720	T	T	T
0.6649076005526823	0.3333465176840202	0.2145790795141673	T	T	T
-0.0017391613658361	0.6663082273553657	0.2143710514459272	T	T	T
0.3318863401448322	0.6661997589791107	0.2145406367720709	T	T	T
0.6648835957295052	0.6663685864668792	0.2145582071351304	T	T	T
0.1089209313907841	0.1109286534655492	0.2857445763087368	T	T	T
0.4422690484024508	0.1106651230005592	0.2858940038471558	T	T	T
0.7756941668641264	0.1105708823784752	0.2859125620078641	T	T	T
0.1089744855085173	0.4439412290681978	0.2858147335472322	T	T	T
0.4427406091426841	0.4444568629865626	0.2864062126671968	T	T	T
0.7746665108049011	0.4447709225733701	0.2863823947037152	T	T	T
0.1088515044065808	0.7774098566793171	0.2858218583629782	T	T	T
0.4426518494369210	0.7767092270690871	0.2863732563096744	T	T	T
0.7756540977181600	0.7774463089168052	0.2859349100806216	T	T	T
0.2194267635133208	0.2221442390552208	0.3577228024285727	T	T	T
0.8868194341433452	0.2214286852573367	0.3575112188472956	T	T	T
0.8869658346828007	0.5554155049321401	0.3576520044476324	T	T	T
0.2189718425831171	0.8895074455177137	0.3574551359272793	T	T	T
0.5531773464912175	0.8893088833137520	0.3577116514081470	T	T	T
0.8866061370088484	0.8885720171923901	0.3578727459606572	T	T	T
0.5533149534940097	0.5554747378709273	0.3592671813815432	T	T	T
0.2190397276917826	0.5556747814147459	0.3574883715443091	T	T	T
0.5531569433829890	0.2213923067361381	0.3576306895023244	T	T	T
0.4635217739467386	0.5955639518676902	0.4564537317558321	T	T	T
0.6224501297085286	0.5073879580340165	0.4567809845908292	T	T	T
0.3227737222729180	0.6736942951303033	0.4564492883017754	T	T	T
0.7631587647232378	0.4292999213604912	0.4573540419105663	T	T	T

Ag3\_AgEmb\_PBE\_bare

2.92418893300000

3.0000000000000000	0.0000000000000000	0.0000000000000000
1.5000000000000000	2.5980762110000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	11.4687304500000007

Ag

54

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3333333299999988	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666599999976	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333299999988	0.0000000000000000	F	F	F
0.3333333299999988	0.3333333299999988	0.0000000000000000	F	F	F
0.6666666599999976	0.3333333299999988	0.0000000000000000	F	F	F
0.0000000000000000	0.6666666599999976	0.0000000000000000	F	F	F

0.333333329999988	0.666666659999976	0.000000000000000	F	F	F
0.666666659999976	0.666666659999976	0.000000000000000	F	F	F
0.1111111109999996	0.1111111109999996	0.0711932869999998	F	F	F
0.4444444439999984	0.1111111109999996	0.0711932869999998	F	F	F
0.777777769999972	0.1111111109999996	0.0711932869999998	F	F	F
0.1111111109999996	0.4444444439999984	0.0711932869999998	F	F	F
0.4444444439999984	0.4444444439999984	0.0711932869999998	F	F	F
0.777777769999972	0.4444444439999984	0.0711932869999998	F	F	F
0.1111111109999996	0.777777769999972	0.0711932869999998	F	F	F
0.4444444439999984	0.777777769999972	0.0711932869999998	F	F	F
0.777777769999972	0.777777769999972	0.0711932869999998	F	F	F
0.222222219999992	0.222222219999992	0.1428140523614924	T	T	T
0.555555549999980	0.222222219999992	0.1428140523614924	T	T	T
0.888888879999968	0.222222219999992	0.1428140523614924	T	T	T
0.222222219999992	0.555555549999980	0.1428140523614924	T	T	T
0.555555549999980	0.555555549999980	0.1428140523614924	T	T	T
0.888888879999968	0.555555549999980	0.1428140523614924	T	T	T
0.222222219999992	0.888888879999968	0.1428140523614924	T	T	T
0.555555549999980	0.888888879999968	0.1428140523614924	T	T	T
0.888888879999968	0.888888879999968	0.1428140523614924	T	T	T
-0.000000000000000	0.000000000000000	0.2144934383918506	T	T	T
0.333333329999988	0.000000000000000	0.2144934383918506	T	T	T
0.666666659999976	0.000000000000000	0.2144934383918506	T	T	T
0.000000000000000	0.333333329999988	0.2144934383918506	T	T	T
0.333333329999988	0.333333329999988	0.2144934383918506	T	T	T
0.666666659999976	0.333333329999988	0.2144934383918506	T	T	T
-0.000000000000000	0.666666659999976	0.2144934383918506	T	T	T
0.333333329999988	0.666666659999976	0.2144934383918506	T	T	T
0.666666659999976	0.666666659999976	0.2144934383918506	T	T	T
0.1111111109999996	0.1111111109999996	0.2860014918010663	T	T	T
0.4444444439999984	0.1111111109999996	0.2860014918010663	T	T	T
0.777777769999972	0.1111111109999996	0.2860014918010663	T	T	T
0.1111111109999996	0.4444444439999984	0.2860014918010663	T	T	T
0.4444444439999984	0.4444444439999984	0.2860014918010663	T	T	T
0.777777769999972	0.4444444439999984	0.2860014918010663	T	T	T
0.1111111109999996	0.777777769999972	0.2860014918010663	T	T	T
0.4444444439999984	0.777777769999972	0.2860014918010663	T	T	T
0.777777769999972	0.777777769999972	0.2860014918010663	T	T	T
0.222222219999992	0.222222219999992	0.3578211817381153	T	T	T
0.888888879999968	0.222222219999992	0.3578211817381153	T	T	T
0.888888879999968	0.555555549999980	0.3578211817381153	T	T	T
0.222222219999992	0.888888879999968	0.3578211817381153	T	T	T
0.555555549999980	0.888888879999968	0.3578211817381153	T	T	T
0.888888879999968	0.888888879999968	0.3578211817381153	T	T	T
0.555555549999980	0.555555549999980	0.3578211817381153	T	T	T
0.222222219999992	0.555555549999980	0.3578211817381153	T	T	T
0.555555549999980	0.222222219999992	0.3578211817381153	T	T	T
Ag3_PdEmb_0.11ML_PBE					
2.80166844800000					
2.999999999999996	0.000000000000000	0.000000000000000			
1.499999999999998	2.598076211000000	0.000000000000000			
0.000000000000000	0.000000000000000	11.468730450000007			
Pd	Ag	C	H		
51	3	2	2		
Selective dynamics					
Direct					
0.000000000000000	0.000000000000000	0.000000000000000	F	F	F
0.333333329999988	0.000000000000000	0.000000000000000	F	F	F

0.6666666659999976	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333329999988	0.0000000000000000	F	F	F
0.3333333329999988	0.3333333329999988	0.0000000000000000	F	F	F
0.6666666659999976	0.3333333329999988	0.0000000000000000	F	F	F
0.0000000000000000	0.6666666659999976	0.0000000000000000	F	F	F
0.3333333329999988	0.6666666659999976	0.0000000000000000	F	F	F
0.6666666659999976	0.6666666659999976	0.0000000000000000	F	F	F
0.1111111109999996	0.1111111109999996	0.0711932869999998	F	F	F
0.4444444439999984	0.1111111109999996	0.0711932869999998	F	F	F
0.7777777769999972	0.1111111109999996	0.0711932869999998	F	F	F
0.1111111109999996	0.4444444439999984	0.0711932869999998	F	F	F
0.4444444439999984	0.4444444439999984	0.0711932869999998	F	F	F
0.7777777769999972	0.4444444439999984	0.0711932869999998	F	F	F
0.1111111109999996	0.7777777769999972	0.0711932869999998	F	F	F
0.4444444439999984	0.7777777769999972	0.0711932869999998	F	F	F
0.7777777769999972	0.7777777769999972	0.0711932869999998	F	F	F
0.2223177324660046	0.2222727256714377	0.1417256792598086	T	T	T
0.5552701036406028	0.2224705287114931	0.1422335911547389	T	T	T
0.8881991796758077	0.2224838744746526	0.1416737434091774	T	T	T
0.2222796937783302	0.5553894504787914	0.1422356299735321	T	T	T
0.5553252971622441	0.5553302941727768	0.14227444404814031	T	T	T
0.8885290263379051	0.5554717733041086	0.1418542832739178	T	T	T
0.2224689393760571	0.8882270121804072	0.1416466431155244	T	T	T
0.5554204524642101	0.8886253905075285	0.1418629460777937	T	T	T
0.8885758141787071	0.8887803977083981	0.1417903084685043	T	T	T
0.9990758549429118	0.9995224249040442	0.2121117422480541	T	T	T
0.3333993681765743	0.9990847357765047	0.2122967286929420	T	T	T
0.6659006666588300	-0.0001940077103415	0.2127275401445400	T	T	T
0.9987399876983606	0.3337091353248002	0.2122944122290035	T	T	T
0.3329706828552466	0.3336264186886813	0.2135119187350104	T	T	T
0.6653940088352976	0.3335201584903450	0.2135100529002553	T	T	T
-0.0007045423615191	0.6664743633221807	0.2127502131544564	T	T	T
0.3330618090303961	0.6658344018376002	0.2134790808119387	T	T	T
0.6659056184055461	0.6661866606674099	0.2129435188947783	T	T	T
0.1100483533610144	0.1106468469793317	0.2819588083714111	T	T	T
0.4438111879033790	0.1111750577567594	0.2836509166884728	T	T	T
0.7753207260803034	0.1113934630302916	0.2837317636186030	T	T	T
0.1105646139624785	0.4443559565311289	0.2836328717138216	T	T	T
0.4438457747102353	0.4442338719837879	0.2864167170656949	T	T	T
0.7741530257802152	0.4448632161123411	0.2843079309732975	T	T	T
0.1104869425702722	0.7761754984863997	0.2836851682973239	T	T	T
0.4442617297732679	0.7747516602803792	0.2842413932564252	T	T	T
0.7763927593791400	0.7773681908261696	0.2828986337099644	T	T	T
0.2177787374928414	0.2186870005426640	0.3539337320935942	T	T	T
0.8923216126215977	0.2179805391987805	0.3538970215613754	T	T	T
0.8864324823018999	0.5561210924100659	0.3538344601332732	T	T	T
0.2172004584650675	0.8932813215853426	0.3538654103830980	T	T	T
0.5549868873808361	0.8875688291542068	0.3538099994545572	T	T	T
0.8865938983083758	0.8871753978313953	0.3539145684531717	T	T	T
0.5547628735305401	0.5558359214884930	0.3625687179319056	T	T	T
0.2165379301779208	0.5560205267427381	0.3594881398698348	T	T	T
0.5551505414907772	0.2175785165292976	0.3597941723397143	T	T	T
0.4764003119835321	0.6127031288095898	0.4511996365018177	T	T	T
0.6408878297278285	0.5075398142965936	0.4501846319656087	T	T	T
0.3311857571270028	0.7057172404730299	0.4529562222641104	T	T	T
0.7864131603586088	0.4148308613743391	0.4503146201913775	T	T	T

Ag3\_PdEmb\_PBE\_bare  
2.80166844800000

2.9999999999999996	0.0000000000000000	0.0000000000000000
1.4999999999999998	2.5980762110000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	11.4687304500000007

Pd Ag  
51 3

Selective dynamics  
Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3333333329999988	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666659999976	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333329999988	0.0000000000000000	F	F	F
0.3333333329999988	0.3333333329999988	0.0000000000000000	F	F	F
0.6666666659999976	0.3333333329999988	0.0000000000000000	F	F	F
0.0000000000000000	0.6666666659999976	0.0000000000000000	F	F	F
0.3333333329999988	0.6666666659999976	0.0000000000000000	F	F	F
0.6666666659999976	0.6666666659999976	0.0000000000000000	F	F	F
0.1111111109999996	0.1111111109999996	0.0711932869999998	F	F	F
0.4444444439999984	0.1111111109999996	0.0711932869999998	F	F	F
0.777777769999972	0.1111111109999996	0.0711932869999998	F	F	F
0.1111111109999996	0.4444444439999984	0.0711932869999998	F	F	F
0.4444444439999984	0.4444444439999984	0.0711932869999998	F	F	F
0.777777769999972	0.4444444439999984	0.0711932869999998	F	F	F
0.1111111109999996	0.777777769999972	0.0711932869999998	F	F	F
0.4444444439999984	0.777777769999972	0.0711932869999998	F	F	F
0.777777769999972	0.777777769999972	0.0711932869999998	F	F	F
0.2224201859461861	0.2224201859461861	0.1417762889557049	T	T	T
0.5554160174772822	0.2225012970454303	0.1423078284561064	T	T	T
0.8884929601076232	0.2224201859461861	0.1417762889557049	T	T	T
0.2225012970454303	0.5554160174772822	0.1423078284561064	T	T	T
0.5554160174772822	0.5554160174772822	0.1423078284561064	T	T	T
0.8887886871878572	0.5557559566242770	0.1418805008885224	T	T	T
0.2224201859461861	0.8884929601076232	0.1417762889557049	T	T	T
0.5557559566242770	0.8887886871878572	0.1418805008885224	T	T	T
0.8887886871878572	0.8887886871878572	0.1418805008885224	T	T	T
-0.0003195241416669	-0.0003195241416669	0.2123787055240895	T	T	T
0.3339723812833326	-0.0003195241416669	0.2123787055240895	T	T	T
0.6665425314665158	0.0002482690669638	0.2129855882765079	T	T	T
-0.0003195241416669	0.3339723812833326	0.2123787055240895	T	T	T
0.3335866875047659	0.3335866875047659	0.2136486868733963	T	T	T
0.6661599569904633	0.3335866875047659	0.2136486868733963	T	T	T
0.0002482690669638	0.6665425314665158	0.2129855882765079	T	T	T
0.3335866875047659	0.6661599569904633	0.2136486868733963	T	T	T
0.6665425314665158	0.6665425314665158	0.2129855882765079	T	T	T
0.1111111109999996	0.1111111109999996	0.2823431092217170	T	T	T
0.4450449493166512	0.1118700079021070	0.2840886730515415	T	T	T
0.7764183747812369	0.1118700079021070	0.2840886730515415	T	T	T
0.1118700079021070	0.4450449493166512	0.2840886730515415	T	T	T
0.4444444439999984	0.4444444439999984	0.2862556467375746	T	T	T
0.7764183747812369	0.4450449493166512	0.2840886730515415	T	T	T
0.1118700079021070	0.7764183747812369	0.2840886730515415	T	T	T
0.4450449493166512	0.7764183747812369	0.2840886730515415	T	T	T
0.777777769999972	0.777777769999972	0.2831640285251343	T	T	T
0.2198234733616756	0.2198234733616756	0.3542856686399649	T	T	T
0.8936863852766441	0.2198234733616756	0.3542856686399649	T	T	T
0.8883675010988726	0.5565983288022458	0.3541874384143346	T	T	T
0.2198234733616756	0.8936863852766441	0.3542856686399649	T	T	T
0.5565983288022458	0.8883675010988726	0.3541874384143346	T	T	T
0.8883675010988726	0.8883675010988726	0.3541874384143346	T	T	T



0.5569666217430012	0.5569666217430012	0.3604826734630067	T	T	T
0.2194000885139931	0.5569666217430012	0.3604826734630067	T	T	T
0.5569666217430012	0.2194000885139931	0.3604826734630067	T	T	T
C2H2_PBE					
1.0000000000000000					
25.0000000000000000	0.0000000000000000	0.0000000000000000			
0.0000000000000000	26.0000000000000000	0.0000000000000000			
0.0000000000000000	0.0000000000000000	27.0000000000000000			
C	H				
2	2				
Selective dynamics					
Direct					
0.4938296576381868	0.4550472350126736	0.5000000000000000	T	T	T
0.5060325190674312	0.4999864252944644	0.5000000000000000	T	T	T
0.4830308038094647	0.4151859165496251	0.5000000000000000	T	T	T
0.5171070194849173	0.5397804231432335	0.5000000000000000	T	T	T
Pd2Ag_AgEmb_0.11ML_PBE					
2.92418893300000					
3.0000000000000000	0.0000000000000000	0.0000000000000000			
1.5000000000000000	2.5980762110000000	0.0000000000000000			
0.0000000000000000	0.0000000000000000	11.4687304500000007			
Ag	Pd	C	H		
52	2	2	2		
Selective dynamics					
Direct					
0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3333333329999998	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666659999997	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333329999998	0.0000000000000000	F	F	F
0.3333333329999998	0.3333333329999998	0.0000000000000000	F	F	F
0.6666666659999997	0.3333333329999998	0.0000000000000000	F	F	F
0.0000000000000000	0.6666666659999997	0.0000000000000000	F	F	F
0.3333333329999998	0.6666666659999997	0.0000000000000000	F	F	F
0.6666666659999997	0.6666666659999997	0.0000000000000000	F	F	F
0.1111111109999996	0.1111111109999996	0.0711932869999998	F	F	F
0.4444444439999984	0.1111111109999996	0.0711932869999998	F	F	F
0.7777777699999972	0.1111111109999996	0.0711932869999998	F	F	F
0.1111111109999996	0.4444444439999984	0.0711932869999998	F	F	F
0.4444444439999984	0.4444444439999984	0.0711932869999998	F	F	F
0.7777777699999972	0.4444444439999984	0.0711932869999998	F	F	F
0.1111111109999996	0.7777777699999972	0.0711932869999998	F	F	F
0.4444444439999984	0.7777777699999972	0.0711932869999998	F	F	F
0.7777777699999972	0.7777777699999972	0.0711932869999998	F	F	F
0.2235845760631906	0.2190971190790588	0.1427924177773322	T	T	T
0.5570861415874608	0.2190956608974643	0.1428629779586720	T	T	T
0.8905384138120993	0.2190695288299285	0.1427853365339944	T	T	T
0.2238423459244074	0.5522818535914267	0.1427831050602093	T	T	T
0.5571112614856595	0.5522360482764870	0.1427975891625004	T	T	T
0.8904726225728329	0.5523602116187746	0.1428299660763476	T	T	T
0.2234549048891193	0.8861994494181504	0.1427895618117699	T	T	T
0.5569911407787024	0.8859970991772629	0.1427424603680762	T	T	T
0.8902179316891187	0.8859991406150356	0.1427325129779952	T	T	T
0.0012692043395431	-0.0040442075972123	0.2146421466495469	T	T	T
0.3354806832479609	-0.0041190367375419	0.2146590060212870	T	T	T
0.6686271012504710	-0.0044871764298017	0.2147007687972644	T	T	T
0.0020996913099559	0.3287478221256741	0.2147354455584221	T	T	T
0.3353064287492310	0.3284499810050938	0.2145662935164062	T	T	T
0.6690000982854091	0.3286401945284911	0.2145930401544698	T	T	T

0.0013831085447443	0.6626149345429904	0.2143176350520576	T	T	T
0.3350003145944674	0.6625620524251175	0.2141532068946708	T	T	T
0.6686805568941980	0.6624699583808477	0.2143388454566251	T	T	T
0.1132197988380822	0.1059987788884658	0.2862117257038095	T	T	T
0.4472742825519689	0.1071769731885486	0.2869814062753860	T	T	T
0.7778233376672609	0.1071889117100168	0.2869550073737419	T	T	T
0.1134567719189502	0.4411066254839522	0.2863792941319837	T	T	T
0.4463063246895012	0.4397707686300332	0.2860345390295629	T	T	T
0.7779197807733150	0.4409408234260943	0.2863757833456385	T	T	T
0.1136281292499149	0.7717069962913388	0.2859446604690816	T	T	T
0.4470944187685887	0.7715243802723368	0.2859676787490210	T	T	T
0.7800672025955937	0.7722229782797937	0.2863441867710662	T	T	T
0.2230657821777428	0.2176584966382616	0.3576017235248279	T	T	T
0.5580496713125964	0.2162011192446062	0.3597499603748428	T	T	T
0.8915804864335312	0.2175985037606334	0.3576208355395488	T	T	T
0.8910352229554404	0.5503451988973478	0.3577979622986650	T	T	T
0.2251644126218232	0.8819888386340272	0.3575919562156329	T	T	T
0.5579462217375819	0.8818383652752574	0.3576418334143369	T	T	T
0.8924195948447651	0.8818429970381592	0.3576340521787805	T	T	T
0.5573662436797925	0.5518499658167497	0.3570321735789898	T	T	T
0.2232818978189118	0.5516865594256585	0.3570271567458581	T	T	T
0.5107627809377391	0.4616369383590113	0.4089133871810548	T	T	T
0.3598876683618050	0.4616157493493728	0.4089166378230575	T	T	T
0.6025633940870166	0.4372691179510691	0.4334152099527449	T	T	T
0.2922684680291607	0.4373223262419998	0.4333891363448102	T	T	T
Pd2Ag_AgEmb_PBE_bare					
2.92418893300000					
3.0000000000000000	0.0000000000000000	0.0000000000000000			
1.5000000000000000	2.5980762110000000	0.0000000000000000			
0.0000000000000000	0.0000000000000000	11.4687304500000007			
Ag	Pd				
52	2				
Selective dynamics					
Direct					
0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3333333299999988	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666599999976	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333299999988	0.0000000000000000	F	F	F
0.3333333299999988	0.3333333299999988	0.0000000000000000	F	F	F
0.6666666599999976	0.3333333299999988	0.0000000000000000	F	F	F
0.0000000000000000	0.6666666599999976	0.0000000000000000	F	F	F
0.3333333299999988	0.6666666599999976	0.0000000000000000	F	F	F
0.6666666599999976	0.6666666599999976	0.0000000000000000	F	F	F
0.1111111099999996	0.1111111099999996	0.0711932869999998	F	F	F
0.4444444399999984	0.1111111099999996	0.0711932869999998	F	F	F
0.7777777699999972	0.1111111099999996	0.0711932869999998	F	F	F
0.1111111099999996	0.4444444399999984	0.0711932869999998	F	F	F
0.4444444399999984	0.4444444399999984	0.0711932869999998	F	F	F
0.7777777699999972	0.4444444399999984	0.0711932869999998	F	F	F
0.1111111099999996	0.7777777699999972	0.0711932869999998	F	F	F
0.4444444399999984	0.7777777699999972	0.0711932869999998	F	F	F
0.7777777699999972	0.7777777699999972	0.0711932869999998	F	F	F
0.2220715185214291	0.2220222023787101	0.1429636889559450	T	T	T
0.5557322841350102	0.2218687637299740	0.1427998914031736	T	T	T
0.8892396110998562	0.2220222023787101	0.1429636889559450	T	T	T
0.2220943919089028	0.5554595556361813	0.1426710605076077	T	T	T
0.5557793844549112	0.5554595556361813	0.1426710605076077	T	T	T
0.8890578308225520	0.5552176693548879	0.1427462368219440	T	T	T

0.2219880468697827	0.8893572382604299	0.1428226184491410	T	T	T
0.5554391727804956	0.8891970547457757	0.1428688539033614	T	T	T
0.8886971034737200	0.8891970547457757	0.1428688539033614	T	T	T
-0.0000030507302814	0.0000589626160546	0.2150271151374121	T	T	T
0.3332774211142254	0.0000589626160546	0.2150271151374121	T	T	T
0.6663960270395958	0.0005412779208035	0.2149376737908283	T	T	T
0.0000198194316532	0.3332936941366924	0.2150318739650472	T	T	T
0.3335652194457320	0.3331805404297666	0.2144973988106773	T	T	T
0.6665875721244965	0.3331805404297666	0.2144973988106773	T	T	T
-0.0004153746606721	0.6667421805726067	0.2143398915630177	T	T	T
0.3331864474154990	0.6669604371689971	0.2140902527510720	T	T	T
0.6670065260880605	0.6667421805726067	0.2143398915630177	T	T	T
0.1111793954050734	0.1109745421898519	0.2873167868808049	T	T	T
0.4444952761687649	0.1114578491357456	0.2870067681487897	T	T	T
0.7773802066954847	0.1114578491357456	0.2870067681487897	T	T	T
0.1111489113552817	0.4446499228592679	0.2863510881220198	T	T	T
0.4443025487622012	0.4447282344755931	0.2858810546750312	T	T	T
0.7775344977854453	0.4446499228592679	0.2863510881220198	T	T	T
0.1111132079111325	0.7777600454643309	0.2861332335820124	T	T	T
0.4444600786245319	0.7777600454643309	0.2861332335820124	T	T	T
0.7777453697821429	0.7778425914357050	0.2863805396649379	T	T	T
0.2222090990140576	0.2246125727375951	0.3585455748867253	T	T	T
0.5528112207755500	0.2277108904488952	0.3581865813901717	T	T	T
0.8865116602483427	0.2246125727375951	0.3585455748867253	T	T	T
0.8888373121433712	0.5556587067132494	0.3578814733613156	T	T	T
0.2250153702373517	0.8833025915252921	0.3581520054473896	T	T	T
0.5554230266315763	0.8863459225194705	0.3579580062191212	T	T	T
0.8915643818489445	0.8863459225194705	0.3579580062191212	T	T	T
0.5549346153028500	0.5553354072536778	0.3537570785889469	T	T	T
0.2230633094434675	0.5553354072536778	0.3537570785889469	T	T	T

Pd2Ag\_PdEmb\_0.11ML\_PBE

2.80166844800000

2.9999999999999996	0.0000000000000000	0.0000000000000000
1.4999999999999998	2.5980762110000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	11.4687304500000007

Pd Ag C H  
53 1 2 2

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3333333299999988	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666599999976	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333299999988	0.0000000000000000	F	F	F
0.3333333299999988	0.3333333299999988	0.0000000000000000	F	F	F
0.6666666599999976	0.3333333299999988	0.0000000000000000	F	F	F
0.0000000000000000	0.6666666599999976	0.0000000000000000	F	F	F
0.3333333299999988	0.6666666599999976	0.0000000000000000	F	F	F
0.6666666599999976	0.6666666599999976	0.0000000000000000	F	F	F
0.1111111109999996	0.1111111109999996	0.0711932869999998	F	F	F
0.4444444399999984	0.1111111109999996	0.0711932869999998	F	F	F
0.7777777699999972	0.1111111109999996	0.0711932869999998	F	F	F
0.1111111109999996	0.4444444399999984	0.0711932869999998	F	F	F
0.4444444399999984	0.4444444399999984	0.0711932869999998	F	F	F
0.7777777699999972	0.4444444399999984	0.0711932869999998	F	F	F
0.1111111109999996	0.7777777699999972	0.0711932869999998	F	F	F
0.4444444399999984	0.7777777699999972	0.0711932869999998	F	F	F
0.7777777699999972	0.7777777699999972	0.0711932869999998	F	F	F
0.2234592239848631	0.2234096082384323	0.1417127970249820	T	T	T

0.5566194363069853	0.2235771243339323	0.1421104889447009	T	T	T
0.8895906669861705	0.2236985408597774	0.1417359994738066	T	T	T
0.2237342405108749	0.5564621867013397	0.1420973329820232	T	T	T
0.5568954060574821	0.5567843515266818	0.1421794691403513	T	T	T
0.8899735673810959	0.5572565913174855	0.1419461059101805	T	T	T
0.2237567563263220	0.8895163610601301	0.1417383778781734	T	T	T
0.5573552354392880	0.8898888159194300	0.1419509352643619	T	T	T
0.8898542800775463	0.8898431483126820	0.1419141298494189	T	T	T
0.0029804800832443	0.0028480527575143	0.2121783089853690	T	T	T
0.3366401595352430	0.0022963299775366	0.2122904950779671	T	T	T
0.6696946629218871	0.0032327610192367	0.2130014096586988	T	T	T
0.0025357179446208	0.3363659129323205	0.2122541312911401	T	T	T
0.3363440226001120	0.3361163920011497	0.2130357022469896	T	T	T
0.6695139474163235	0.3365727519084825	0.2132104103719570	T	T	T
0.0034212153083343	0.6694952035073345	0.2129882482107771	T	T	T
0.3367462368495714	0.6694795039878864	0.2132092569533650	T	T	T
0.6695686964406566	0.6693970223643683	0.2131190283330231	T	T	T
0.1157303456252763	0.1154644877976996	0.2824992268922306	T	T	T
0.4494207385478717	0.1161139104922556	0.2837364256974939	T	T	T
0.7813818164058083	0.1156580998397852	0.2837070975540530	T	T	T
0.1162595111330317	0.4492776087849005	0.2837367927736544	T	T	T
0.4496661083809387	0.4494999365008135	0.2845730534933892	T	T	T
0.7808580478940580	0.4499298488895875	0.2843278778596299	T	T	T
0.1158682527807971	0.7811917200779236	0.2837265275860274	T	T	T
0.4501749317958602	0.7805529669548138	0.2843527935947116	T	T	T
0.7822054820025836	0.7819745866208502	0.2831294776899207	T	T	T
0.2255617375906911	0.2252916699048351	0.3543220894553142	T	T	T
0.5608710614832220	0.2237813822228662	0.3571762487648424	T	T	T
0.8973979168008348	0.2235153362189425	0.3539617506348738	T	T	T
0.2239110409045823	0.5606690224846204	0.3571871374099592	T	T	T
0.8947661003407121	0.5606134454323046	0.3541312392136940	T	T	T
0.2238251480575658	0.8970393872648837	0.3539661931155680	T	T	T
0.5610301168066464	0.8944679582596176	0.3541644321718532	T	T	T
0.8935703840743950	0.8933591807358185	0.3541621449791533	T	T	T
0.5626079683154660	0.5624817601977307	0.3621348541260294	T	T	T
0.3511802899114866	0.5094164040403156	0.4122283138560704	T	T	T
0.5095313797226892	0.3510723250652895	0.4122302291778350	T	T	T
0.2791154736916929	0.6054701484303188	0.4377046235590621	T	T	T
0.6055791402292497	0.2789919236415291	0.4377094371465147	T	T	T
Pd2Ag_PdEmb_PBE_bare					
2.80166844800000					
2.9999999999999996	0.0000000000000000	0.0000000000000000			
1.4999999999999998	2.5980762110000000	0.0000000000000000			
0.0000000000000000	0.0000000000000000	11.4687304500000007			
Pd Ag					
53 1					
Selective dynamics					
Direct					
0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3333333299999988	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666599999976	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333299999988	0.0000000000000000	F	F	F
0.3333333299999988	0.3333333299999988	0.0000000000000000	F	F	F
0.6666666599999976	0.3333333299999988	0.0000000000000000	F	F	F
0.0000000000000000	0.6666666599999976	0.0000000000000000	F	F	F
0.3333333299999988	0.6666666599999976	0.0000000000000000	F	F	F
0.6666666599999976	0.6666666599999976	0.0000000000000000	F	F	F
0.1111111109999996	0.1111111109999996	0.0711932869999998	F	F	F

0.4444444439999984	0.1111111109999996	0.0711932869999998	F	F	F
0.7777777769999972	0.1111111109999996	0.0711932869999998	F	F	F
0.1111111109999996	0.4444444439999984	0.0711932869999998	F	F	F
0.4444444439999984	0.4444444439999984	0.0711932869999998	F	F	F
0.7777777769999972	0.4444444439999984	0.0711932869999998	F	F	F
0.1111111109999996	0.7777777769999972	0.0711932869999998	F	F	F
0.4444444439999984	0.7777777769999972	0.0711932869999998	F	F	F
0.7777777769999972	0.7777777769999972	0.0711932869999998	F	F	F
0.2222222219999992	0.2222222219999992	0.1415678970537615	T	T	T
0.5556448267333380	0.2223424777679055	0.1419494885626348	T	T	T
0.8886793604987502	0.2223424777679055	0.1419494885626348	T	T	T
0.2223424777679055	0.5556448267333380	0.1419494885626348	T	T	T
0.555555549999980	0.555555549999980	0.1422178187698170	T	T	T
0.8886793604987502	0.5556448267333380	0.1419494885626348	T	T	T
0.2223424777679055	0.8886793604987502	0.1419494885626348	T	T	T
0.5556448267333380	0.8886793604987502	0.1419494885626348	T	T	T
0.8888888879999968	0.8888888879999968	0.1418133890025269	T	T	T
-0.0000838617579316	-0.0000838617579316	0.2125812604029929	T	T	T
0.3334536954696432	-0.0002407249392889	0.2125534465075107	T	T	T
0.6668343895158609	-0.0000838617579316	0.2125812604029929	T	T	T
-0.0002407249392889	0.3334536954696432	0.2125534465075107	T	T	T
0.3334536954696432	0.3334536954696432	0.2125534465075107	T	T	T
0.6663914128875130	0.3338838392249679	0.2131979716882060	T	T	T
-0.0000838617579316	0.6668343895158609	0.2125812604029929	T	T	T
0.3338838392249679	0.6663914128875130	0.2131979716882060	T	T	T
0.6663914128875130	0.6663914128875130	0.2131979716882060	T	T	T
0.1111768889004361	0.1111768889004361	0.2829682707283350	T	T	T
0.4443128881991252	0.1111768889004361	0.2829682707283350	T	T	T
0.7777952439255575	0.1110761771488790	0.2831637635464267	T	T	T
0.1111768889004361	0.4443128881991252	0.2829682707283350	T	T	T
0.4450602037953572	0.4450602037953572	0.2844273258571163	T	T	T
0.7765462574092795	0.4450602037953572	0.2844273258571163	T	T	T
0.1110761771488790	0.7777952439255575	0.2831637635464267	T	T	T
0.4450602037953572	0.7765462574092795	0.2844273258571163	T	T	T
0.7777952439255575	0.7777952439255575	0.2831637635464267	T	T	T
0.2222222219999992	0.2222222219999992	0.3543729714757117	T	T	T
0.5557361107965342	0.2203307071675972	0.3544486536342897	T	T	T
0.8905998470358631	0.2203307071675972	0.3544486536342897	T	T	T
0.2203307071675972	0.5557361107965342	0.3544486536342897	T	T	T
0.8905998470358631	0.5557361107965342	0.3544486536342897	T	T	T
0.2203307071675972	0.8905998470358631	0.3544486536342897	T	T	T
0.5557361107965342	0.8905998470358631	0.3544486536342897	T	T	T
0.8888888879999968	0.8888888879999968	0.3541014568466057	T	T	T
0.555555549999980	0.555555549999980	0.3607089301499666	T	T	T

Pd3\_AgEmb\_0.11ML\_PBE  
2.92418893300000  
3.0000000000000000 0.0000000000000000 0.0000000000000000  
1.5000000000000000 2.5980762110000000 0.0000000000000000  
0.0000000000000000 0.0000000000000000 11.4687304500000007

Ag	Pd	C	H	
51	3	2	2	

Selective dynamics  
Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.333333329999988	0.0000000000000000	0.0000000000000000	F	F	F
0.666666659999976	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.333333329999988	0.0000000000000000	F	F	F
0.333333329999988	0.333333329999988	0.0000000000000000	F	F	F

0.6666666659999976	0.3333333329999988	0.0000000000000000	F	F	F
0.0000000000000000	0.6666666659999976	0.0000000000000000	F	F	F
0.3333333329999988	0.6666666659999976	0.0000000000000000	F	F	F
0.6666666659999976	0.6666666659999976	0.0000000000000000	F	F	F
0.1111111109999996	0.1111111109999996	0.0711932869999998	F	F	F
0.4444444439999984	0.1111111109999996	0.0711932869999998	F	F	F
0.7777777769999972	0.1111111109999996	0.0711932869999998	F	F	F
0.1111111109999996	0.4444444439999984	0.0711932869999998	F	F	F
0.4444444439999984	0.4444444439999984	0.0711932869999998	F	F	F
0.7777777769999972	0.4444444439999984	0.0711932869999998	F	F	F
0.1111111109999996	0.7777777769999972	0.0711932869999998	F	F	F
0.4444444439999984	0.7777777769999972	0.0711932869999998	F	F	F
0.7777777769999972	0.7777777769999972	0.0711932869999998	F	F	F
0.2218514271472709	0.2224711697852497	0.1428115947250076	T	T	T
0.5556805095318090	0.2219516064659907	0.1427872235242388	T	T	T
0.8889119423483319	0.2225139086722701	0.1428110798207624	T	T	T
0.2222618160071996	0.5557104112368856	0.1428131210711744	T	T	T
0.5553653322677464	0.5556749155852018	0.1428240690654962	T	T	T
0.8890469080688016	0.5552025774434044	0.1428529147737385	T	T	T
0.2222196983894414	0.8887744603637964	0.1427780843861702	T	T	T
0.5553121554329888	0.8890073481389313	0.1426760158203771	T	T	T
0.8888950971993435	0.8890191666890015	0.1426771632595775	T	T	T
-0.0004272327502079	0.0005578752455485	0.2144922402897390	T	T	T
0.3329493167279115	0.0004929971597980	0.2144942805858583	T	T	T
0.6669791742526732	0.9991534504625811	0.2142386173816584	T	T	T
-0.0000822040608088	0.3333788520469612	0.2150110786269727	T	T	T
0.3332786905902184	0.3330739125229295	0.2144544692528586	T	T	T
0.6667077946207974	0.3330973816878119	0.2145130537655020	T	T	T
0.9994527761940020	0.6669953284118093	0.2143884269602160	T	T	T
0.3333733260658707	0.6665209964410816	0.2145732206514945	T	T	T
0.6666634545546277	0.6669922899233087	0.2144372292755411	T	T	T
0.1105354843420387	0.1113625146758583	0.2863263088674474	T	T	T
0.4464387646846769	0.1104700197577665	0.2863203804262258	T	T	T
0.7754464573630099	0.1105871271683535	0.2863645589706375	T	T	T
0.1115852210282656	0.4457953386536332	0.2864775082317004	T	T	T
0.4445683871067584	0.4432138197398901	0.2865484117343195	T	T	T
0.7752236709831709	0.4458246538555251	0.2865549412039747	T	T	T
0.1111287055412051	0.7769823414096055	0.2860126226270885	T	T	T
0.4443927464313569	0.7768491353919998	0.2860764009904909	T	T	T
0.7778622021932181	0.7767460192720382	0.2864770428222218	T	T	T
0.2229249690333373	0.2210492083176894	0.3571761621028584	T	T	T
0.8883913653173743	0.2212154647076907	0.3572322962439021	T	T	T
0.8887628236729093	0.5547450384911107	0.3576558758536358	T	T	T
0.2231596576070896	0.8861574705561022	0.3575797539011412	T	T	T
0.5558938615509302	0.8866068488706954	0.3572963492804704	T	T	T
0.8896559427236213	0.8869848217211209	0.3573114760958183	T	T	T
0.5535423148661922	0.5560700315240011	0.3570259859318053	T	T	T
0.2219056245290518	0.5563906501673147	0.3569274815429255	T	T	T
0.5571461515478962	0.2180002916237362	0.3571730535258115	T	T	T
0.5371978153277035	0.4094995335402872	0.4025506837956412	T	T	T
0.3836700366110914	0.4089178453129156	0.4024636295011061	T	T	T
0.6253973623275308	0.3871617368575004	0.4277217135861829	T	T	T
0.3178833921224657	0.3858263754159438	0.4275249660335846	T	T	T
Pd3_AgEmb_PBE_bare					
2.92418893300000					
3.0000000000000000	0.0000000000000000	0.0000000000000000			
1.5000000000000000	2.5980762110000000	0.0000000000000000			
0.0000000000000000	0.0000000000000000	11.4687304500000007			

Ag Pd  
 51 3  
 Selective dynamics  
 Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3333333329999988	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666659999976	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333329999988	0.0000000000000000	F	F	F
0.3333333329999988	0.3333333329999988	0.0000000000000000	F	F	F
0.6666666659999976	0.3333333329999988	0.0000000000000000	F	F	F
0.0000000000000000	0.6666666659999976	0.0000000000000000	F	F	F
0.3333333329999988	0.6666666659999976	0.0000000000000000	F	F	F
0.6666666659999976	0.6666666659999976	0.0000000000000000	F	F	F
0.1111111109999996	0.1111111109999996	0.0711932869999998	F	F	F
0.4444444439999984	0.1111111109999996	0.0711932869999998	F	F	F
0.7777777769999972	0.1111111109999996	0.0711932869999998	F	F	F
0.1111111109999996	0.4444444439999984	0.0711932869999998	F	F	F
0.4444444439999984	0.4444444439999984	0.0711932869999998	F	F	F
0.7777777769999972	0.4444444439999984	0.0711932869999998	F	F	F
0.1111111109999996	0.7777777769999972	0.0711932869999998	F	F	F
0.4444444439999984	0.7777777769999972	0.0711932869999998	F	F	F
0.7777777769999972	0.7777777769999972	0.0711932869999998	F	F	F
0.2219694924547805	0.2219694924547805	0.1428787744182712	T	T	T
0.5557577462230502	0.2218178395538942	0.1425252778026051	T	T	T
0.8893943470904342	0.2219694924547805	0.1428787744182712	T	T	T
0.2218178395538942	0.5557577462230502	0.1425252778026051	T	T	T
0.5557577462230502	0.5557577462230502	0.1425252778026051	T	T	T
0.8890277030676720	0.5552779248646469	0.1427911033879370	T	T	T
0.2219694924547805	0.8893943470904342	0.1428787744182712	T	T	T
0.5552779248646469	0.8890277030676720	0.1427911033879370	T	T	T
0.8890277030676720	0.8890277030676720	0.1427911033879370	T	T	T
0.0000428380720427	0.0000428380720427	0.2150352090786281	T	T	T
0.3332476568559135	0.0000428380720427	0.2150352090786281	T	T	T
0.6667853289398529	-0.0002373258797111	0.2143599179359731	T	T	T
0.0000428380720427	0.3332476568559135	0.2150352090786281	T	T	T
0.3333186457335678	0.3333186457335678	0.2140223809847200	T	T	T
0.6666960405328595	0.3333186457335678	0.2140223809847200	T	T	T
-0.0002373258797111	0.6667853289398529	0.2143599179359731	T	T	T
0.3333186457335678	0.6666960405328595	0.2140223809847200	T	T	T
0.6667853289398529	0.6667853289398529	0.2143599179359731	T	T	T
0.1111111109999996	0.1111111109999996	0.2875298320936091	T	T	T
0.4446999971085417	0.1112245878003666	0.2862589769693832	T	T	T
0.7774087470910866	0.1112245878003666	0.2862589769693832	T	T	T
0.1112245878003666	0.4446999971085417	0.2862589769693832	T	T	T
0.4444444439999984	0.4444444439999984	0.2853397787198268	T	T	T
0.7774087470910865	0.4446999971085417	0.2862589769693832	T	T	T
0.1112245878003666	0.7774087470910865	0.2862589769693832	T	T	T
0.4446999971085417	0.7774087470910865	0.2862589769693832	T	T	T
0.7777777769999972	0.7777777769999972	0.2862390762007777	T	T	T
0.2249131619959415	0.2249131619959415	0.3582116843775850	T	T	T
0.8835070080081122	0.2249131619959415	0.3582116843775850	T	T	T
0.8889087941766017	0.5555157426467882	0.3575835105345600	T	T	T
0.2249131619959415	0.8835070080081122	0.3582116843775850	T	T	T
0.5555157426467882	0.8889087941766017	0.3575835105345600	T	T	T
0.8889087941766017	0.8889087941766017	0.3575835105345600	T	T	T
0.5537694838318431	0.5537694838318431	0.3535533701359381	T	T	T
0.2257943643363091	0.5537694838318431	0.3535533701359381	T	T	T
0.5537694838318431	0.2257943643363091	0.3535533701359381	T	T	T

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Pd3_PdEmb_PBE_bare
2.80166844800000
2.9999999999999996 0.0000000000000000 0.0000000000000000
1.4999999999999998 2.5980762110000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 11.4687304500000007

```

```

Pd
54

```

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3333333329999988	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666659999976	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333329999988	0.0000000000000000	F	F	F
0.3333333329999988	0.3333333329999988	0.0000000000000000	F	F	F
0.6666666659999976	0.3333333329999988	0.0000000000000000	F	F	F
0.0000000000000000	0.6666666659999976	0.0000000000000000	F	F	F
0.3333333329999988	0.6666666659999976	0.0000000000000000	F	F	F
0.6666666659999976	0.6666666659999976	0.0000000000000000	F	F	F
0.1111111109999996	0.1111111109999996	0.0711932869999998	F	F	F
0.4444444439999984	0.1111111109999996	0.0711932869999998	F	F	F
0.7777777769999972	0.1111111109999996	0.0711932869999998	F	F	F
0.1111111109999996	0.4444444439999984	0.0711932869999998	F	F	F
0.4444444439999984	0.4444444439999984	0.0711932869999998	F	F	F
0.7777777769999972	0.4444444439999984	0.0711932869999998	F	F	F
0.1111111109999996	0.7777777769999972	0.0711932869999998	F	F	F
0.4444444439999984	0.7777777769999972	0.0711932869999998	F	F	F
0.7777777769999972	0.7777777769999972	0.0711932869999998	F	F	F
0.2222222219999992	0.2222222219999992	0.1418432811439177	T	T	T
0.5555555549999980	0.2222222219999992	0.1418432811439177	T	T	T
0.8888888879999968	0.2222222219999992	0.1418432811439177	T	T	T
0.2222222219999992	0.5555555549999980	0.1418432811439177	T	T	T
0.5555555549999980	0.5555555549999980	0.1418432811439177	T	T	T
0.8888888879999968	0.5555555549999980	0.1418432811439177	T	T	T
0.2222222219999992	0.8888888879999968	0.1418432811439177	T	T	T
0.5555555549999980	0.8888888879999968	0.1418432811439177	T	T	T
0.8888888879999968	0.8888888879999968	0.1418432811439177	T	T	T
-0.0000000000000000	-0.0000000000000000	0.2126047287731679	T	T	T
0.3333333329999988	0.0000000000000000	0.2126047287731679	T	T	T
0.6666666659999976	-0.0000000000000000	0.2126047287731679	T	T	T
-0.0000000000000000	0.3333333329999988	0.2126047287731679	T	T	T
0.3333333329999988	0.3333333329999988	0.2126047287731679	T	T	T
0.6666666659999976	0.3333333329999988	0.2126047287731679	T	T	T
-0.0000000000000000	0.6666666659999976	0.2126047287731679	T	T	T
0.3333333329999988	0.6666666659999976	0.2126047287731679	T	T	T
0.6666666659999976	0.6666666659999976	0.2126047287731679	T	T	T
0.1111111109999996	0.1111111109999996	0.2831538900484000	T	T	T
0.4444444439999984	0.1111111109999996	0.2831538900484000	T	T	T
0.7777777769999972	0.1111111109999996	0.2831538900484000	T	T	T
0.1111111109999996	0.4444444439999984	0.2831538900484000	T	T	T
0.4444444439999984	0.4444444439999984	0.2831538900484000	T	T	T
0.7777777769999972	0.4444444439999984	0.2831538900484000	T	T	T
0.1111111109999996	0.7777777769999972	0.2831538900484000	T	T	T
0.4444444439999984	0.7777777769999972	0.2831538900484000	T	T	T
0.7777777769999972	0.7777777769999972	0.2831538900484000	T	T	T
0.2222222219999992	0.2222222219999992	0.3543985364233493	T	T	T
0.5555555549999980	0.2222222219999992	0.3543985364233493	T	T	T
0.8888888879999968	0.2222222219999992	0.3543985364233493	T	T	T
0.2222222219999992	0.5555555549999980	0.3543985364233493	T	T	T



0.555555549999980	0.555555549999980	0.3543985364233493	T	T	T
0.888888879999968	0.555555549999980	0.3543985364233493	T	T	T
0.222222219999992	0.888888879999968	0.3543985364233493	T	T	T
0.555555549999980	0.888888879999968	0.3543985364233493	T	T	T
0.888888879999968	0.888888879999968	0.3543985364233493	T	T	T
Pd3_PdEmb_Pd3_0.11ML_PBE					
2.80166844800000					
2.999999999999996	0.000000000000000	0.000000000000000			
1.499999999999998	2.598076211000000	0.000000000000000			
0.000000000000000	0.000000000000000	11.468730450000007			
Pd	C	H			
54	2	2			
Selective dynamics					
Direct					
0.000000000000000	0.000000000000000	0.000000000000000	F	F	F
0.333333329999988	0.000000000000000	0.000000000000000	F	F	F
0.666666659999976	0.000000000000000	0.000000000000000	F	F	F
0.000000000000000	0.333333329999988	0.000000000000000	F	F	F
0.333333329999988	0.333333329999988	0.000000000000000	F	F	F
0.666666659999976	0.333333329999988	0.000000000000000	F	F	F
0.000000000000000	0.666666659999976	0.000000000000000	F	F	F
0.333333329999988	0.666666659999976	0.000000000000000	F	F	F
0.666666659999976	0.666666659999976	0.000000000000000	F	F	F
0.111111109999996	0.111111109999996	0.071193286999998	F	F	F
0.444444439999984	0.111111109999996	0.071193286999998	F	F	F
0.777777769999972	0.111111109999996	0.071193286999998	F	F	F
0.111111109999996	0.444444439999984	0.071193286999998	F	F	F
0.444444439999984	0.444444439999984	0.071193286999998	F	F	F
0.777777769999972	0.444444439999984	0.071193286999998	F	F	F
0.111111109999996	0.777777769999972	0.071193286999998	F	F	F
0.444444439999984	0.777777769999972	0.071193286999998	F	F	F
0.777777769999972	0.777777769999972	0.071193286999998	F	F	F
0.2196955626906044	0.2242733322847193	0.1417016497639351	T	T	T
0.5530575329837478	0.2238652169012775	0.1420934718041806	T	T	T
0.8861678664155527	0.2243054874174288	0.1417208206475286	T	T	T
0.2196050638726435	0.5574420926795518	0.1420987010324554	T	T	T
0.5529900236462253	0.5574321541215075	0.1420934668427724	T	T	T
0.8861971317768935	0.5578142110410335	0.1419965190973948	T	T	T
0.2199260167125835	0.8902578729096888	0.1417276489952593	T	T	T
0.5536267330643393	0.8903493604201570	0.1419657384052963	T	T	T
0.8860850576576612	0.8904684436661833	0.1419576109180172	T	T	T
0.9944722079295110	0.0037018225210048	0.2121816887374884	T	T	T
0.3284464299353275	0.0036905963739791	0.2121447350726786	T	T	T
0.6617822887241437	0.0031963029564777	0.2131634285852764	T	T	T
-0.0053601702298397	0.3368589414206884	0.2124369446550070	T	T	T
0.3282519021491896	0.3363568230107792	0.2129179176694632	T	T	T
0.6615796561964410	0.3363616631981789	0.2129493117531045	T	T	T
-0.0048456816358849	0.6699614781278544	0.2131001823688373	T	T	T
0.3278818526699254	0.6705774622847476	0.2130791987538029	T	T	T
0.6613035732473775	0.6698987920107007	0.2130985439843438	T	T	T
0.1060756824164069	0.1132263477007071	0.2827223181394078	T	T	T
0.4404477802121622	0.1128424395184272	0.2840086587002046	T	T	T
0.7720884706070028	0.1130034426566179	0.2841278498315107	T	T	T
0.1057678884601966	0.4472637752912743	0.2836933861285197	T	T	T
0.4390301832810046	0.4466772557562477	0.2837083205785026	T	T	T
0.7716756974155013	0.4474542313344401	0.2837406890903555	T	T	T
0.1052910818483318	0.7802193902097314	0.2839993526102654	T	T	T
0.4393773586683583	0.7802198571022939	0.2839582440215945	T	T	T

0.7726549361038899	0.7800590136055118	0.2835093404349889	T	T	T
0.2154253102404106	0.2217685982228845	0.3542690569023880	T	T	T
0.5540603239377359	0.2173180326513493	0.3571256392621859	T	T	T
0.8885271026785345	0.2218407980326328	0.3543458140941756	T	T	T
0.2151664330422152	0.5590879631484400	0.3568733198212879	T	T	T
0.5507817731188751	0.5588311738069376	0.3569108687972856	T	T	T
0.8834988329142461	0.5581976880549878	0.3546864506678900	T	T	T
0.2167130656504608	0.8922756242181992	0.3545809042066618	T	T	T
0.5511929443100566	0.8883844306818399	0.3549118814801761	T	T	T
0.8854729809013601	0.8886096460556041	0.3550211102339796	T	T	T
0.5397552279922602	0.4084106363185789	0.4041949771098000	T	T	T
0.3764823527450708	0.4083491107201980	0.4041258845616776	T	T	T
0.6349255166221788	0.3777123741876027	0.4302413009152111	T	T	T
0.3118393558894495	0.3774020628391124	0.4300956814191628	T	T	T
PdAg2_AgEmb_0.11ML_PBE					
2.92418893300000					
3.0000000000000000	0.0000000000000000	0.0000000000000000			
1.5000000000000000	2.5980762110000000	0.0000000000000000			
0.0000000000000000	0.0000000000000000	11.4687304500000007			
Ag	Pd	C	H		
53	1	2	2		
Selective dynamics					
Direct					
0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3333333329999998	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666659999976	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333329999998	0.0000000000000000	F	F	F
0.3333333329999998	0.3333333329999998	0.0000000000000000	F	F	F
0.6666666659999976	0.3333333329999998	0.0000000000000000	F	F	F
0.0000000000000000	0.6666666659999976	0.0000000000000000	F	F	F
0.3333333329999998	0.6666666659999976	0.0000000000000000	F	F	F
0.6666666659999976	0.6666666659999976	0.0000000000000000	F	F	F
0.1111111109999996	0.1111111109999996	0.0711932869999998	F	F	F
0.4444444439999984	0.1111111109999996	0.0711932869999998	F	F	F
0.7777777769999972	0.1111111109999996	0.0711932869999998	F	F	F
0.1111111109999996	0.4444444439999984	0.0711932869999998	F	F	F
0.4444444439999984	0.4444444439999984	0.0711932869999998	F	F	F
0.7777777769999972	0.4444444439999984	0.0711932869999998	F	F	F
0.1111111109999996	0.7777777769999972	0.0711932869999998	F	F	F
0.4444444439999984	0.7777777769999972	0.0711932869999998	F	F	F
0.7777777769999972	0.7777777769999972	0.0711932869999998	F	F	F
0.2211292157013794	0.2221725008210281	0.1431990164684683	T	T	T
0.5540756891125710	0.2221975517007543	0.1428238314262318	T	T	T
0.8879825349286480	0.2221025334200457	0.1427960340426139	T	T	T
0.2209296374635329	0.5553459033222932	0.1428155241913960	T	T	T
0.5543491740897780	0.5554844580557362	0.1426903990746191	T	T	T
0.8879914993426972	0.5551644911776356	0.1427590480479300	T	T	T
0.2207967638377850	0.8891788504357561	0.1428359701376566	T	T	T
0.5539809885307597	0.8891023183329924	0.1428214709817486	T	T	T
0.8875369065059431	0.8888634544333549	0.1428046985601695	T	T	T
-0.0022023849545036	-0.0003838645668092	0.2144573903213895	T	T	T
0.3320421680605180	0.9980830407913666	0.2150806712198453	T	T	T
0.6641221273219603	-0.0002355295395015	0.2145263192832716	T	T	T
0.9969260779488265	0.3333824918601692	0.2149127713676350	T	T	T
0.3320443600589165	0.3336414852096940	0.2150738578329849	T	T	T
0.6643386213914980	0.3333000080790571	0.2144606691108732	T	T	T
-0.0021086031870433	0.6660855147860435	0.2144427732658890	T	T	T
0.3316019491445013	0.6659963407446619	0.2144414522747506	T	T	T

0.6643239255312464	0.6659948512074156	0.2144403690227810	T	T	T
0.1083787639910748	0.1102329945702057	0.2859503923600373	T	T	T
0.4416595318247176	0.1106174308589462	0.2861488039657419	T	T	T
0.7746292198917022	0.1110574010872973	0.2859021625800364	T	T	T
0.1083595396749128	0.4439648103297916	0.2860207275720746	T	T	T
0.4443214965893953	0.4459686032213953	0.2876661743184672	T	T	T
0.7708523871271855	0.4460160567349640	0.2874253790576489	T	T	T
0.1094123213431120	0.7764586169829810	0.2858272435301846	T	T	T
0.4441660366626926	0.7725069212746917	0.2876216168963709	T	T	T
0.7746675073337239	0.7770550416134672	0.2858910523736189	T	T	T
0.2186027223567985	0.2218947878589534	0.3578232732960056	T	T	T
0.5526874411644261	0.2201573433017722	0.3576475524311147	T	T	T
0.8855769584758403	0.2211522043363543	0.3572427633675611	T	T	T
0.2177388982739318	0.5557386084734923	0.3574106089237666	T	T	T
0.8854929444858596	0.5556699135007324	0.3573812254986434	T	T	T
0.2178466789467288	0.8888301353860134	0.3573196229049589	T	T	T
0.5524026510983914	0.8893647105651067	0.3575773808829109	T	T	T
0.8855215752582682	0.8883256530895949	0.3576604099779476	T	T	T
0.5514095465849702	0.5552617084667409	0.3629808816231702	T	T	T
0.4703086178585019	0.5982200351894706	0.4247881442983604	T	T	T
0.6353554752531129	0.5061794029236664	0.4247318477707221	T	T	T
0.3429474113159912	0.6687719693528914	0.4388405311207270	T	T	T
0.7629379236788462	0.4345105859242078	0.4386489057087271	T	T	T
PdAg2_AgEmb_PBE_bare					
2.92418893300000					
3.0000000000000000	0.0000000000000000	0.0000000000000000			
1.5000000000000000	2.5980762110000000	0.0000000000000000			
0.0000000000000000	0.0000000000000000	11.4687304500000007			
Ag	Pd				
53	1				
Selective dynamics					
Direct					
0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3333333299999988	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666599999976	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333299999988	0.0000000000000000	F	F	F
0.3333333299999988	0.3333333299999988	0.0000000000000000	F	F	F
0.6666666599999976	0.3333333299999988	0.0000000000000000	F	F	F
0.0000000000000000	0.6666666599999976	0.0000000000000000	F	F	F
0.3333333299999988	0.6666666599999976	0.0000000000000000	F	F	F
0.6666666599999976	0.6666666599999976	0.0000000000000000	F	F	F
0.1111111099999996	0.1111111099999996	0.0711932869999998	F	F	F
0.4444444399999984	0.1111111099999996	0.0711932869999998	F	F	F
0.7777777699999972	0.1111111099999996	0.0711932869999998	F	F	F
0.1111111099999996	0.4444444399999984	0.0711932869999998	F	F	F
0.4444444399999984	0.4444444399999984	0.0711932869999998	F	F	F
0.7777777699999972	0.4444444399999984	0.0711932869999998	F	F	F
0.1111111099999996	0.7777777699999972	0.0711932869999998	F	F	F
0.4444444399999984	0.7777777699999972	0.0711932869999998	F	F	F
0.7777777699999972	0.7777777699999972	0.0711932869999998	F	F	F
0.2222222199999992	0.2222222199999992	0.1428815610372541	T	T	T
0.5554747791975229	0.2220274407585888	0.1427923481067185	T	T	T
0.8891644450438826	0.2220274407585888	0.1427923481067185	T	T	T
0.2220274407585888	0.5554747791975229	0.1427923481067185	T	T	T
0.5555555499999980	0.5555555499999980	0.1426886647606909	T	T	T
0.8891644450438826	0.5554747791975229	0.1427923481067185	T	T	T
0.2220274407585888	0.8891644450438826	0.1427923481067185	T	T	T
0.5554747791975229	0.8891644450438826	0.1427923481067185	T	T	T

0.8888888879999968	0.8888888879999968	0.1428605727388942	T	T	T
0.0000007235126703	0.0000007235126703	0.2145689774494132	T	T	T
0.3333882211554186	-0.0001097763108395	0.2146556540635279	T	T	T
0.6666652189746568	0.0000007235126703	0.2145689774494132	T	T	T
-0.0001097763108395	0.3333882211554186	0.2146556540635279	T	T	T
0.3333882211554186	0.3333882211554186	0.2146556540635279	T	T	T
0.6668065756729511	0.3330535136540916	0.2142474670894634	T	T	T
0.0000007235126703	0.6666652189746568	0.2145689774494132	T	T	T
0.3330535136540916	0.6668065756729511	0.2142474670894634	T	T	T
0.6668065756729511	0.6668065756729511	0.2142474670894634	T	T	T
0.1110867241226075	0.1110867241226075	0.2863806262786215	T	T	T
0.4444932177547824	0.1110867241226075	0.2863806262786215	T	T	T
0.7777564840644110	0.1111536968711723	0.2861323790297829	T	T	T
0.1110867241226075	0.4444932177547824	0.2863806262786215	T	T	T
0.4445203949718187	0.4445203949718187	0.2859320607154920	T	T	T
0.7776258750563565	0.4445203949718187	0.2859320607154920	T	T	T
0.1111536968711723	0.7777564840644110	0.2861323790297829	T	T	T
0.4445203949718187	0.7776258750563565	0.2859320607154920	T	T	T
0.7777564840644110	0.7777564840644110	0.2861323790297829	T	T	T
0.222222219999992	0.222222219999992	0.3582288188497139	T	T	T
0.5554914782872484	0.2246184576660263	0.3578691840964184	T	T	T
0.8865567290467194	0.2246184576660263	0.3578691840964184	T	T	T
0.2246184576660263	0.5554914782872484	0.3578691840964184	T	T	T
0.8865567290467194	0.5554914782872484	0.3578691840964184	T	T	T
0.2246184576660263	0.8865567290467194	0.3578691840964184	T	T	T
0.5554914782872484	0.8865567290467194	0.3578691840964184	T	T	T
0.8888888879999968	0.8888888879999968	0.3576469210336692	T	T	T
0.5555555499999980	0.5555555499999980	0.3536901148585790	T	T	T

PdAg2\_PdEmb\_0.11ML\_PBE  
2.80166844800000  
2.999999999999996 0.0000000000000000 0.0000000000000000  
1.499999999999998 2.5980762110000000 0.0000000000000000  
0.0000000000000000 0.0000000000000000 11.4687304500000007

Pd	Ag	C	H	
52	2	2	2	2

Selective dynamics  
Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3333333299999988	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666599999976	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333299999988	0.0000000000000000	F	F	F
0.3333333299999988	0.3333333299999988	0.0000000000000000	F	F	F
0.6666666599999976	0.3333333299999988	0.0000000000000000	F	F	F
0.0000000000000000	0.6666666599999976	0.0000000000000000	F	F	F
0.3333333299999988	0.6666666599999976	0.0000000000000000	F	F	F
0.6666666599999976	0.6666666599999976	0.0000000000000000	F	F	F
0.1111111099999996	0.1111111099999996	0.0711932869999998	F	F	F
0.4444444399999984	0.1111111099999996	0.0711932869999998	F	F	F
0.7777777699999972	0.1111111099999996	0.0711932869999998	F	F	F
0.1111111099999996	0.4444444399999984	0.0711932869999998	F	F	F
0.4444444399999984	0.4444444399999984	0.0711932869999998	F	F	F
0.7777777699999972	0.4444444399999984	0.0711932869999998	F	F	F
0.1111111099999996	0.7777777699999972	0.0711932869999998	F	F	F
0.4444444399999984	0.7777777699999972	0.0711932869999998	F	F	F
0.7777777699999972	0.7777777699999972	0.0711932869999998	F	F	F
0.2220498482301292	0.2226247747628276	0.1416195855934308	T	T	T
0.5553286442063243	0.2225436907220475	0.1420769681187315	T	T	T
0.8883123202717357	0.2227246275527618	0.1416971911544162	T	T	T

0.2221643876025629	0.5556685751763516	0.1421531705486676	T	T	T
0.5554200177815825	0.5555828758986077	0.1421789282133367	T	T	T
0.8884401662876015	0.5561126452948487	0.1419866314239462	T	T	T
0.2222906734740889	0.8885299723960735	0.1417761609076837	T	T	T
0.5556707255305451	0.8888007240765698	0.1419031785024542	T	T	T
0.8885538093380666	0.8889052584387945	0.1418864090496344	T	T	T
-0.0008045374047891	0.0006350509337467	0.2123272413734439	T	T	T
0.3324421344561040	0.0005196235401875	0.2123032574672030	T	T	T
0.6657227091516251	0.0011345319727702	0.2127335958988724	T	T	T
-0.0009903103449623	0.3346394245456619	0.2125041352946570	T	T	T
0.3321485186216709	0.3344910712006908	0.2129897944865257	T	T	T
0.6659080818825568	0.3345372556130256	0.2131808730659751	T	T	T
-0.0001947876337645	0.6674541910480144	0.2129991347159908	T	T	T
0.3324197117265996	0.6676613455881513	0.2134422135907711	T	T	T
0.6654579768437840	0.6672994931634489	0.2130582420116539	T	T	T
0.1088649475236938	0.1135707539021585	0.2824789625897344	T	T	T
0.4427467612863959	0.1140321820548726	0.2833115196160290	T	T	T
0.7742527479808456	0.1146043700939406	0.2836274913558416	T	T	T
0.1099982147975521	0.4480280592028903	0.2842658600857098	T	T	T
0.4422631831850806	0.4465439444924427	0.2846912547695181	T	T	T
0.7734184240482080	0.4480901408326297	0.2844384730257123	T	T	T
0.1104349929889217	0.7779512025097931	0.2843338827774511	T	T	T
0.4436510071173656	0.7775971058044198	0.2843597807574928	T	T	T
0.7758508361477375	0.7804944522346430	0.2828376989767257	T	T	T
0.2184793105827399	0.2231739048065057	0.3540331889986508	T	T	T
0.5562922827395931	0.2183896224581394	0.3575378327426937	T	T	T
0.8908682645215716	0.2229305830314756	0.3541780778843723	T	T	T
0.8849015859499162	0.5621723391622581	0.3537896611822257	T	T	T
0.2169676558908667	0.8988813051440239	0.3541112688999066	T	T	T
0.5538048754099382	0.8932039072215122	0.3537700094465597	T	T	T
0.8846714347020569	0.8935385651164429	0.3538335622807737	T	T	T
0.5538388559155473	0.5600657150528341	0.3619291027905395	T	T	T
0.2154708689297263	0.5632201033618403	0.3620590251203109	T	T	T
0.4270215332645062	0.4928424029244809	0.4154550367907791	T	T	T
0.4889036884372631	0.3148369310655840	0.4153287864969188	T	T	T
0.3826181058711047	0.5937657893351661	0.4405281244311295	T	T	T
0.5110132616498568	0.2162850914869271	0.4400487181445733	T	T	T

PdAg2\_PdEmb\_PBE\_bare

2.80166844800000

2.9999999999999996 0.0000000000000000 0.0000000000000000

1.4999999999999998 2.5980762110000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 11.4687304500000007

Pd Ag

52 2

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3333333299999988	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666599999976	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333299999988	0.0000000000000000	F	F	F
0.3333333299999988	0.3333333299999988	0.0000000000000000	F	F	F
0.6666666599999976	0.3333333299999988	0.0000000000000000	F	F	F
0.0000000000000000	0.6666666599999976	0.0000000000000000	F	F	F
0.3333333299999988	0.6666666599999976	0.0000000000000000	F	F	F
0.6666666599999976	0.6666666599999976	0.0000000000000000	F	F	F
0.1111111109999996	0.1111111109999996	0.0711932869999998	F	F	F
0.4444444399999984	0.1111111109999996	0.0711932869999998	F	F	F
0.7777777699999972	0.1111111109999996	0.0711932869999998	F	F	F

0.1111111109999996	0.4444444439999984	0.0711932869999998	F	F	F
0.4444444439999984	0.4444444439999984	0.0711932869999998	F	F	F
0.7777777769999972	0.4444444439999984	0.0711932869999998	F	F	F
0.1111111109999996	0.7777777769999972	0.0711932869999998	F	F	F
0.4444444439999984	0.7777777769999972	0.0711932869999998	F	F	F
0.7777777769999972	0.7777777769999972	0.0711932869999998	F	F	F
0.2223033847228169	0.2221847378677912	0.1416110899425994	T	T	T
0.5555394181460387	0.2222544957079181	0.1419729105384211	T	T	T
0.8888452094093872	0.2221847378677912	0.1416110899425994	T	T	T
0.2223909544565134	0.5556320469000612	0.1422322483529098	T	T	T
0.5553103306434205	0.5556320469000612	0.1422322483529098	T	T	T
0.8888157797954435	0.5557017714091049	0.1419281922631252	T	T	T
0.2225086908405663	0.8883159503188622	0.1420074115217905	T	T	T
0.5556391298474882	0.8886151335233896	0.1418482418775051	T	T	T
0.8890790676291142	0.8886151335233896	0.1418482418775051	T	T	T
0.0003029663330837	-0.0009173210117822	0.2124879634101085	T	T	T
0.3339476876786973	-0.0009173210117822	0.2124879634101085	T	T	T
0.6670450439549251	-0.0007567559098553	0.2125185130917021	T	T	T
0.0000599699381709	0.3332133931236571	0.2123569050366201	T	T	T
0.3333447772779461	0.3336455436947055	0.2128916738062219	T	T	T
0.6663430110273433	0.3336455436947055	0.2128916738062219	T	T	T
0.0006104149493328	0.6663521438535223	0.2130552983844980	T	T	T
0.3335419121043366	0.6662495077913219	0.2139376381773307	T	T	T
0.6663707731971398	0.6663521438535223	0.2130552983844980	T	T	T
0.1112418819169731	0.1108495691660526	0.2827125677152162	T	T	T
0.4444811280462120	0.1109855720088690	0.2828734452681591	T	T	T
0.7778666319449142	0.1109855720088690	0.2828734452681591	T	T	T
0.1122061027438402	0.4443376214373930	0.2838680873811089	T	T	T
0.4444532768638478	0.4444267782722996	0.2852897824647355	T	T	T
0.7767896078187621	0.4443376214373930	0.2838680873811089	T	T	T
0.1120627961350116	0.7759428647301543	0.2845495967851451	T	T	T
0.4453276711348293	0.7759428647301543	0.2845495967851451	T	T	T
0.7779450117047159	0.7774433075905595	0.2831416903317530	T	T	T
0.2221671494407723	0.2206574147682224	0.3542239714576102	T	T	T
0.5571187612066528	0.2190958095866900	0.3543360517674339	T	T	T
0.8905087677910002	0.2206574147682224	0.3542239714576102	T	T	T
0.8883585870397602	0.5566161569204714	0.3542191897857189	T	T	T
0.2196785194344769	0.8939762931310413	0.3546752244449545	T	T	T
0.5555849856636539	0.8914465056306912	0.3541363509025802	T	T	T
0.8863018397056459	0.8914465056306912	0.3541363509025802	T	T	T
0.5563632742611564	0.5563010559941077	0.3605464186752415	T	T	T
0.2206690017447311	0.5563010559941077	0.3605464186752415	T	T	T
sqrt3_0.33ML_PBE					
2.80166844800000					
1.4999999999999998	0.8660254038000000	0.0000000000000000			
-1.4999999999999998	0.8660254038000000	0.0000000000000000			
0.0000000000000000	0.0000000000000000	7.3484692279999999			
Pd C H					
15 2 2					
Selective dynamics					
Direct					
0.0040559071272305	0.0161648846875829	0.4452409026362578	T	T	T
0.3396781944686784	0.0119601506063686	0.3340795054738740	T	T	T
0.3344095461759400	0.3377555948544291	0.2214054901888091	T	T	T
0.0000000000000000	0.0000000000000000	0.1111111111000014	F	F	F
0.3333333329999988	0.0000000000000000	0.0000000000000000	F	F	F
0.6758459760312969	0.3452402989105300	0.4453134642431716	T	T	T
0.3432302766456852	0.6841593937466851	0.4467628173334410	T	T	T

0.6716166313037892	0.6797346473074223	0.3340220567960840	T	T	T
0.0074566457188997	0.3475995579145362	0.3312370701905549	T	T	T
0.6662380629717992	0.0043438358914431	0.2221305478404213	T	T	T
-0.0000633675811414	0.6723199949232928	0.2214272612428392	T	T	T
0.6666666670000012	0.3333333329999988	0.1111111111000014	F	F	F
0.3333333329999988	0.6666666670000012	0.1111111111000014	F	F	F
0.6666666670000012	0.6666666670000012	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333329999988	0.0000000000000000	F	F	F
0.1401708849361257	0.3179572610038495	0.5213876680615470	T	T	T
-0.0221290764064117	0.4802757493818972	0.5214454633491115	T	T	T
0.2621478414411100	0.2788489260291341	0.5620331723604514	T	T	T
0.9390142419768018	0.6019628553494500	0.5621759767003561	T	T	T

sqrt3\_PBE\_bare

2.80166844800000					
1.4999999999999998	0.8660254038000000	0.0000000000000000			
-1.4999999999999998	0.8660254038000000	0.0000000000000000			
0.0000000000000000	0.0000000000000000	7.3484692279999999			

Pd  
15

Selective dynamics

Direct

-0.0000000000000000	-0.0000000000000000	0.4419627266061198	T	T	T
0.3333333329999988	-0.0000000000000000	0.3309646693832750	T	T	T
0.3333333329999988	0.3333333329999988	0.2209218209098337	T	T	T
0.0000000000000000	0.0000000000000000	0.1111111111000014	F	F	F
0.3333333329999988	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666670000012	0.3333333329999988	0.4419627266061198	T	T	T
0.3333333329999988	0.6666666670000012	0.4419627266061198	T	T	T
0.6666666670000012	0.6666666670000012	0.3309646693832750	T	T	T
-0.0000000000000000	0.3333333329999988	0.3309646693832750	T	T	T
0.6666666670000012	0.0000000000000000	0.2209218209098337	T	T	T
-0.0000000000000000	0.6666666670000012	0.2209218209098337	T	T	T
0.6666666670000012	0.3333333329999988	0.1111111111000014	F	F	F
0.3333333329999988	0.6666666670000012	0.1111111111000014	F	F	F
0.6666666670000012	0.6666666670000012	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333329999988	0.0000000000000000	F	F	F

### PBE-dDsC Geometries

2x2\_0.25ML\_dDsC

2.77984000000000					
2.0000000000000000	0.0000000000000000	0.0000000000000000			
1.0000000000000000	1.7320508079999999	0.0000000000000000			
0.0000000000000000	0.0000000000000000	9.3825138849999998			

Pd C H  
24 2 2

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666670000012	0.6666666670000012	0.0870232210000026	F	F	F
0.3322047309530523	0.3322047309530096	0.1730309311715425	T	T	T
0.9982033779621535	0.9982033779620256	0.2601994809474664	T	T	T
0.6668174168092138	0.6668174168091285	0.3449122675187432	T	T	T
0.8377121832963011	0.8377121832962159	0.4351556316551313	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.1666666670000012	0.1666666670000012	0.0870232210000026	F	F	F

0.6666666670000012	0.16666666670000012	0.0870232210000026	F	F	F
0.16666666670000012	0.66666666670000012	0.0870232210000026	F	F	F
0.8322047314758161	0.3316144420263043	0.1729859412103791	T	T	T
0.3316144420263611	0.8322047314757450	0.1729859412103791	T	T	T
0.8320494727150539	0.8320494727149687	0.1731003265681015	T	T	T
0.4982375050054258	0.9982719550360674	0.2589121803020498	T	T	T
0.9982719550361597	0.4982375050053547	0.2589121803020498	T	T	T
0.4980664681285556	0.4980664681285130	0.2592805836767127	T	T	T
0.1666621405104583	0.1666621405104370	0.3456085945347301	T	T	T
0.1657873793149751	0.6677848953432430	0.3466270150863899	T	T	T
0.6677848953433070	0.1657873793149325	0.3466270150863899	T	T	T
0.3338356645736758	0.3338356645736332	0.4314918763620842	T	T	T
0.8330119611190567	0.3335127064068197	0.4337107905440562	T	T	T
0.3335127064068766	0.8330119611189857	0.4337107905440562	T	T	T
0.8175382333964568	0.5701275603421091	0.4925805349453533	T	T	T
0.5701275603422086	0.8175382333963573	0.4925805349453533	T	T	T
0.9598669901225062	0.4737464889246381	0.5249090866925705	T	T	T
0.4737464889247162	0.9598669901223996	0.5249090866925705	T	T	T
2x2_0.5ML_dDsc					
2.77984000000000					
2.0000000000000000	0.0000000000000000	0.0000000000000000			
1.0000000000000000	1.7320508079999999	0.0000000000000000			
0.0000000000000000	0.0000000000000000	9.3825138849999998			
Pd	C	H			
24	4	4			
Selective dynamics					
Direct					
0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666670000012	0.66666666670000012	0.0870232210000026	F	F	F
0.3306383255939910	0.3340355131313824	0.1733289298395065	T	T	T
0.9966515128849962	0.0014233744580026	0.2593962810245523	T	T	T
0.6623863109531484	0.6735650974441145	0.3468373883592928	T	T	T
0.8389095036054717	0.8294366321016521	0.4390589110618510	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.16666666670000012	0.16666666670000012	0.0870232210000026	F	F	F
0.66666666670000012	0.16666666670000012	0.0870232210000026	F	F	F
0.16666666670000012	0.66666666670000012	0.0870232210000026	F	F	F
0.8306380556249999	0.3340366837625269	0.1732797913570680	T	T	T
0.3306378885390189	0.8340285879912436	0.1730839612035585	T	T	T
0.8306399170544930	0.8340366848084767	0.1730548599757107	T	T	T
0.4966505643861172	0.0014220549857404	0.2593479118857119	T	T	T
0.9966253911259165	0.5014942555046066	0.2597022079322094	T	T	T
0.4966247774564041	0.5014204666669531	0.2600170074172505	T	T	T
0.1648903161469898	0.1706351328452389	0.3461010808814042	T	T	T
0.1621188210697105	0.6736421653022714	0.3471697154482067	T	T	T
0.6652758982726059	0.1677597456497155	0.3463837149140028	T	T	T
0.3386760124080497	0.3246077781431340	0.4334125939370250	T	T	T
0.8287229651083509	0.3294414827195688	0.4323204631683282	T	T	T
0.3287256821531505	0.8403343406220130	0.4362770303039862	T	T	T
0.7777454263667396	0.5380660510852235	0.4962006977755029	T	T	T
0.5781308579514883	0.8132133826266665	0.4958273568761243	T	T	T
0.2890752019304761	0.50931711137505080	0.4998205257485791	T	T	T
0.1109175960082799	0.7878668576439011	0.4974839477133727	T	T	T
0.9095332873322360	0.4253650095195462	0.5290495843197501	T	T	T
0.5001112507178705	0.9521751570832120	0.5289103758630561	T	T	T
0.4073903128074261	0.3874943988374878	0.5332345807614616	T	T	T



0.0338100663327062	0.9326811422764203	0.5297992334049333	T	T	T
2x2_dDsC_bare					
2.779840000000000					
2.0000000000000000	0.0000000000000000	0.0000000000000000			
1.0000000000000000	1.7320508079999999	0.0000000000000000			
0.0000000000000000	0.0000000000000000	9.3825138849999998			

Pd  
24

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666670000012	0.6666666670000012	0.0870232210000026	F	F	F
0.3333172372281896	0.3333172372281405	0.1729985602609900	T	T	T
0.9990530243831043	0.9990530243829693	0.2589744566418394	T	T	T
0.6658306510337600	0.6658306510336606	0.3450519431502795	T	T	T
0.8335346079824094	0.8335346079823241	0.4318881474106241	T	T	T
0.5000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.5000000000000000	0.5000000000000000	0.0000000000000000	F	F	F
0.1666666670000012	0.1666666670000012	0.0870232210000026	F	F	F
0.6666666670000012	0.1666666670000012	0.0870232210000026	F	F	F
0.1666666670000012	0.6666666670000012	0.0870232210000026	F	F	F
0.8327345501857021	0.3332531435327324	0.1729676421043221	T	T	T
0.3332531435327892	0.8327345501856310	0.1729676421043221	T	T	T
0.8326711698713379	0.8326711698712516	0.1729397070287041	T	T	T
0.4997126107827425	0.9990460998050034	0.2589760703509728	T	T	T
0.9990460998051013	0.4997126107826573	0.2589760703509728	T	T	T
0.4997184086239843	0.4997184086239346	0.2589766939639518	T	T	T
0.1662434244091116	0.1662434244090902	0.3448913966723076	T	T	T
0.1665499303349806	0.6655217231921232	0.3449719449098781	T	T	T
0.6655217231921801	0.1665499303349308	0.3449719449098781	T	T	T
0.3323537696376507	0.3323537696376080	0.4319787664002098	T	T	T
0.8335383311306489	0.3323233471613345	0.4319366762585643	T	T	T
0.3323233471613984	0.8335383311305921	0.4319366762585643	T	T	T

3x3\_0.11ML\_dDsC

2.779840000000000					
2.9999999999999996	0.0000000000000000	0.0000000000000000			
1.4999999999999998	2.5980762110000000	0.0000000000000000			
0.0000000000000000	0.0000000000000000	11.4687304500000007			

Pd C H  
54 2 2

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3333333299999988	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666659999976	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333299999988	0.0000000000000000	F	F	F
0.3333333299999988	0.3333333299999988	0.0000000000000000	F	F	F
0.6666666659999976	0.3333333299999988	0.0000000000000000	F	F	F
0.0000000000000000	0.6666666659999976	0.0000000000000000	F	F	F
0.3333333299999988	0.6666666659999976	0.0000000000000000	F	F	F
0.6666666659999976	0.6666666659999976	0.0000000000000000	F	F	F
0.1111111109999996	0.1111111109999996	0.0711932869999998	F	F	F
0.4444444439999984	0.1111111109999996	0.0711932869999998	F	F	F
0.7777777699999972	0.1111111109999996	0.0711932869999998	F	F	F
0.1111111109999996	0.4444444439999984	0.0711932869999998	F	F	F
0.4444444439999984	0.4444444439999984	0.0711932869999998	F	F	F
0.7777777699999972	0.4444444439999984	0.0711932869999998	F	F	F

0.1111111109999996	0.7777777769999972	0.0711932869999998	F	F	F
0.4444444439999984	0.7777777769999972	0.0711932869999998	F	F	F
0.7777777769999972	0.7777777769999972	0.0711932869999998	F	F	F
0.2212213198157148	0.2234676357717996	0.1411878168732619	T	T	T
0.5548669509137438	0.2227513543591999	0.1416345254402141	T	T	T
0.8878019165525047	0.2234807913654737	0.1411852128467322	T	T	T
0.2213593163774979	0.5563664776307838	0.1416503055784822	T	T	T
0.5547203497154685	0.5563801630307300	0.1416439740939650	T	T	T
0.8877781746171642	0.5569700022167469	0.1415820055911673	T	T	T
0.2216221494357619	0.8892219917671734	0.1411711181255404	T	T	T
0.5552626196357362	0.8893945471292105	0.1415115711560448	T	T	T
0.8878588232560155	0.8893982385106499	0.1415170510196333	T	T	T
0.9979474672410021	0.0018369592229745	0.2112320495974189	T	T	T
0.3316647161150187	0.0017400665099894	0.2112252760518955	T	T	T
0.6652620224730512	0.0009739228859041	0.2123113897187351	T	T	T
0.9982655991646038	0.3348510485985341	0.2116156567733020	T	T	T
0.3318647107279293	0.3342730107510269	0.2120038759536756	T	T	T
0.6652712007178697	0.3343237452090594	0.2120074738712044	T	T	T
0.9986721056927539	0.6679732547566414	0.2122703018612797	T	T	T
0.3313711698760842	0.6686393078350775	0.2121668906225927	T	T	T
0.6647193925440418	0.6679756790237027	0.2122666626333518	T	T	T
0.1094735569057789	0.1114520486765445	0.2815251170504989	T	T	T
0.4437140964043161	0.1106595292498811	0.2827055087239772	T	T	T
0.7759224233191381	0.1107511815247566	0.2827025790296335	T	T	T
0.1095247791456757	0.4453511597120447	0.2824859998311059	T	T	T
0.4428273333899497	0.4445182686470168	0.2823501978092156	T	T	T
0.7753853566743091	0.4454433509750015	0.2825037231157973	T	T	T
0.1090536128296974	0.7782866092940458	0.2826905409973327	T	T	T
0.4430123998246989	0.7782526161670013	0.2827025976655727	T	T	T
0.7762732559849230	0.7777973130383390	0.2823668484364950	T	T	T
0.2182196904193767	0.2207469135778191	0.3529256435157322	T	T	T
0.5572980732940757	0.2153156202442402	0.3550333285959797	T	T	T
0.8907731436075439	0.2209159216727354	0.3529301021822904	T	T	T
0.2178544764951285	0.5579084009424096	0.3550650164299762	T	T	T
0.5534402853811268	0.5577638689120330	0.3550993941671289	T	T	T
0.8864255648357992	0.5567305663537992	0.3533772364699579	T	T	T
0.2193092050725109	0.8910381964929507	0.3531053454952144	T	T	T
0.5540585149848741	0.8869989244040720	0.3535578974658963	T	T	T
0.8886691814547196	0.8872469201318735	0.3535129453826185	T	T	T
0.5439639552057927	0.4053337510868855	0.4022259179783064	T	T	T
0.3791535392552358	0.4048444662918084	0.4021773814047446	T	T	T
0.6395348614531440	0.3737130877018518	0.4285636990474484	T	T	T
0.3152361549835430	0.3725223719896509	0.4284173379744754	T	T	T
3x3 0.44ML_dDsc					
2.77984000000000					
2.9999999999999996	0.0000000000000000	0.0000000000000000			
1.4999999999999998	2.5980762110000000	0.0000000000000000			
0.0000000000000000	0.0000000000000000	11.4687304500000007			
Pd C H					
54 8 8					
Selective dynamics					
Direct					
0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3333333299999988	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666659999976	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333299999988	0.0000000000000000	F	F	F
0.3333333299999988	0.3333333299999988	0.0000000000000000	F	F	F
0.6666666659999976	0.3333333299999988	0.0000000000000000	F	F	F

0.0000000000000000	0.6666666659999976	0.0000000000000000	F	F	F
0.3333333329999988	0.6666666659999976	0.0000000000000000	F	F	F
0.6666666659999976	0.6666666659999976	0.0000000000000000	F	F	F
0.1111111109999996	0.1111111109999996	0.0711932869999998	F	F	F
0.4444444439999984	0.1111111109999996	0.0711932869999998	F	F	F
0.7777777769999972	0.1111111109999996	0.0711932869999998	F	F	F
0.1111111109999996	0.4444444439999984	0.0711932869999998	F	F	F
0.4444444439999984	0.4444444439999984	0.0711932869999998	F	F	F
0.7777777769999972	0.4444444439999984	0.0711932869999998	F	F	F
0.1111111109999996	0.7777777769999972	0.0711932869999998	F	F	F
0.4444444439999984	0.7777777769999972	0.0711932869999998	F	F	F
0.7777777769999972	0.7777777769999972	0.0711932869999998	F	F	F
0.2221502605400056	0.2227122988138753	0.1415192880066986	T	T	T
0.5559668529718474	0.2226165303773347	0.1413781535156588	T	T	T
0.8891164083295579	0.2228149975603149	0.1416414619409987	T	T	T
0.2227437008197060	0.5560779288562943	0.1415347802037047	T	T	T
0.5558134200308147	0.5567293985864779	0.1415957068061679	T	T	T
0.8889475481333430	0.5560921749889586	0.1417138837067584	T	T	T
0.2224837076580370	0.8888021899869430	0.1414540845008261	T	T	T
0.5563854540102512	0.8885347525336955	0.1413389855399465	T	T	T
0.8893873761741677	0.8889231192842015	0.1415774832660826	T	T	T
0.0012194416639705	0.0007544582014763	0.2121941203119296	T	T	T
0.3336854721363191	0.9991020506974587	0.2114374888711776	T	T	T
0.6684494301147105	0.0005067512967210	0.2118128459127232	T	T	T
0.0004710617017685	0.3335836736601893	0.2125068821251039	T	T	T
0.3330426708395864	0.3350604133797889	0.2117560308058329	T	T	T
0.6663488038549404	0.3345561121456123	0.2121193419185748	T	T	T
0.0010595101587330	0.6679872389379866	0.2124968262114946	T	T	T
0.3332562108815031	0.6674789531535654	0.2125960274601522	T	T	T
0.6673088111632001	0.6671266029403169	0.2126724678516068	T	T	T
0.1149203142367866	0.1115333539634492	0.2841637956675036	T	T	T
0.4424117279259929	0.1118549476871623	0.2806514756594013	T	T	T
0.7818503863521907	0.1116137682645370	0.2823877960817413	T	T	T
0.1092241191108349	0.4475714873589878	0.2831284507827316	T	T	T
0.4405651499361344	0.4511665425353381	0.2834824635355114	T	T	T
0.7755211434508493	0.4469154298816832	0.2837855059377177	T	T	T
0.1116638056345893	0.7812032834199054	0.2841426944274298	T	T	T
0.4450099731368769	0.7754263027496902	0.2835342361457147	T	T	T
0.7768271349115284	0.7783820188202341	0.2833769307225710	T	T	T
0.2218886403861410	0.2327248488207181	0.3567182092387948	T	T	T
0.5553556294243275	0.2190940650290883	0.3487296861541387	T	T	T
0.8904399229431650	0.2191210914254778	0.3533317958226518	T	T	T
0.1945949499156376	0.5752504365699745	0.3576086008381396	T	T	T
0.5461957165591884	0.5296212092933247	0.3781121214442779	T	T	T
0.8662041845654986	0.5658757610862052	0.3577277896707796	T	T	T
0.2269903466471259	0.8861449640048247	0.3566029335837339	T	T	T
0.5490649940598593	0.8937222388053508	0.3529066638038367	T	T	T
0.8727331331857080	0.9092699943013323	0.3540562119374067	T	T	T
0.4037785951560791	0.9154283410758630	0.4044949945634618	T	T	T
0.3872909733179276	0.7636001978843222	0.4119078536171340	T	T	T
0.9262383825165046	0.3783654423245955	0.4038374235443088	T	T	T
0.7802566081740213	0.3513152405196015	0.4103302735735151	T	T	T
0.4706152647685816	0.3258792414694651	0.4054371270100193	T	T	T
0.2870364927318802	0.3769801038009646	0.4028183108486075	T	T	T
0.0200091257935740	0.7402621313063626	0.4040910878225196	T	T	T
0.8564778712851000	0.7400692347416460	0.4035663836052071	T	T	T
0.3779196555209763	0.0241418350250644	0.4272650513869707	T	T	T
0.3290139956087898	0.7389912220352827	0.4403854415904456	T	T	T

0.0307165306143641	0.3481072046854063	0.4278748660164970	T	T	T
0.7641321059234218	0.2810035245137370	0.4375761021510496	T	T	T
0.5552249904098676	0.2637622459631658	0.4334446593827275	T	T	T
0.2019436142887727	0.4029707920889747	0.4310058889003784	T	T	T
0.0792786114332391	0.7782025179476190	0.4301525714446394	T	T	T
0.7564861631452611	0.7795792730508652	0.4291131412047537	T	T	T
3x3_dDsC_bare					
2.77984000000000					
2.9999999999999996	0.0000000000000000	0.0000000000000000			
1.4999999999999998	2.5980762110000000	0.0000000000000000			
0.0000000000000000	0.0000000000000000	11.4687304500000007			
Pd					
54					
Selective dynamics					
Direct					
0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3333333299999988	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666599999976	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333299999988	0.0000000000000000	F	F	F
0.3333333299999988	0.3333333299999988	0.0000000000000000	F	F	F
0.6666666599999976	0.3333333299999988	0.0000000000000000	F	F	F
0.0000000000000000	0.6666666599999976	0.0000000000000000	F	F	F
0.3333333299999988	0.6666666599999976	0.0000000000000000	F	F	F
0.6666666599999976	0.6666666599999976	0.0000000000000000	F	F	F
0.1111111099999996	0.1111111099999996	0.0711932869999998	F	F	F
0.4444444399999984	0.1111111099999996	0.0711932869999998	F	F	F
0.7777777699999972	0.1111111099999996	0.0711932869999998	F	F	F
0.1111111099999996	0.4444444399999984	0.0711932869999998	F	F	F
0.4444444399999984	0.4444444399999984	0.0711932869999998	F	F	F
0.7777777699999972	0.4444444399999984	0.0711932869999998	F	F	F
0.1111111099999996	0.7777777699999972	0.0711932869999998	F	F	F
0.4444444399999984	0.7777777699999972	0.0711932869999998	F	F	F
0.7777777699999972	0.7777777699999972	0.0711932869999998	F	F	F
0.2222222199999992	0.2222222199999992	0.1414754156019031	T	T	T
0.5555555499999980	0.2222222199999992	0.1414754156019031	T	T	T
0.8888888799999968	0.2222222199999992	0.1414754156019031	T	T	T
0.2222222199999992	0.5555555499999980	0.1414754156019031	T	T	T
0.5555555499999980	0.5555555499999980	0.1414754156019031	T	T	T
0.8888888799999968	0.5555555499999980	0.1414754156019031	T	T	T
0.2222222199999992	0.8888888799999968	0.1414754156019031	T	T	T
0.5555555499999980	0.8888888799999968	0.1414754156019031	T	T	T
0.8888888799999968	0.8888888799999968	0.1414754156019031	T	T	T
-0.0000000000000000	0.0000000000000000	0.2118457911057095	T	T	T
0.3333333299999988	0.0000000000000000	0.2118457911057095	T	T	T
0.6666666599999976	0.0000000000000000	0.2118457911057095	T	T	T
-0.0000000000000000	0.3333333299999988	0.2118457911057095	T	T	T
0.3333333299999988	0.3333333299999988	0.2118457911057095	T	T	T
0.6666666599999976	0.3333333299999988	0.2118457911057095	T	T	T
-0.0000000000000000	0.6666666599999976	0.2118457911057095	T	T	T
0.3333333299999988	0.6666666599999976	0.2118457911057095	T	T	T
0.6666666599999976	0.6666666599999976	0.2118457911057095	T	T	T
0.1111111099999996	0.1111111099999996	0.2820181556321751	T	T	T
0.4444444399999984	0.1111111099999996	0.2820181556321751	T	T	T
0.7777777699999972	0.1111111099999996	0.2820181556321751	T	T	T
0.1111111099999996	0.4444444399999984	0.2820181556321751	T	T	T
0.4444444399999984	0.4444444399999984	0.2820181556321751	T	T	T
0.7777777699999972	0.4444444399999984	0.2820181556321751	T	T	T
0.1111111099999996	0.7777777699999972	0.2820181556321751	T	T	T

0.4444444439999984	0.7777777769999972	0.2820181556321751	T	T	T
0.7777777769999972	0.7777777769999972	0.2820181556321751	T	T	T
0.2222222219999992	0.2222222219999992	0.3530829600817724	T	T	T
0.5555555549999980	0.2222222219999992	0.3530829600817724	T	T	T
0.8888888879999968	0.2222222219999992	0.3530829600817724	T	T	T
0.2222222219999992	0.5555555549999980	0.3530829600817724	T	T	T
0.5555555549999980	0.5555555549999980	0.3530829600817724	T	T	T
0.8888888879999968	0.5555555549999980	0.3530829600817724	T	T	T
0.2222222219999992	0.8888888879999968	0.3530829600817724	T	T	T
0.5555555549999980	0.8888888879999968	0.3530829600817724	T	T	T
0.8888888879999968	0.8888888879999968	0.3530829600817724	T	T	T
Ag3_AgEmb_0.11ML_dDsC					
2.92008000000000					
3.0000000000000000	0.0000000000000000	0.0000000000000000			
1.5000000000000000	2.5980762110000000	0.0000000000000000			
0.0000000000000000	0.0000000000000000	11.4687304500000007			
Ag	C	H			
54	2	2			
Selective dynamics					
Direct					
0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3333333329999988	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666659999976	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333329999988	0.0000000000000000	F	F	F
0.3333333329999988	0.3333333329999988	0.0000000000000000	F	F	F
0.6666666659999976	0.3333333329999988	0.0000000000000000	F	F	F
0.0000000000000000	0.6666666659999976	0.0000000000000000	F	F	F
0.3333333329999988	0.6666666659999976	0.0000000000000000	F	F	F
0.6666666659999976	0.6666666659999976	0.0000000000000000	F	F	F
0.1111111109999996	0.1111111109999996	0.0711932869999998	F	F	F
0.4444444439999984	0.1111111109999996	0.0711932869999998	F	F	F
0.7777777769999972	0.1111111109999996	0.0711932869999998	F	F	F
0.1111111109999996	0.4444444439999984	0.0711932869999998	F	F	F
0.4444444439999984	0.4444444439999984	0.0711932869999998	F	F	F
0.7777777769999972	0.4444444439999984	0.0711932869999998	F	F	F
0.1111111109999996	0.7777777769999972	0.0711932869999998	F	F	F
0.4444444439999984	0.7777777769999972	0.0711932869999998	F	F	F
0.7777777769999972	0.7777777769999972	0.0711932869999998	F	F	F
0.2221637786515773	0.2222523845778955	0.1413414858812404	T	T	T
0.5555693851883430	0.2221597176563157	0.1411424022097218	T	T	T
0.8888649642968989	0.2221581375656256	0.1411359513339728	T	T	T
0.222248170544565	0.5555777209271242	0.1411663541259229	T	T	T
0.5555673967057505	0.5555377083340787	0.1411116457353747	T	T	T
0.8888256893803970	0.5555515917648953	0.1411420205445497	T	T	T
0.2222178924119028	0.8888456424679543	0.1411619675954128	T	T	T
0.5555886905478729	0.8888735135187975	0.1411403226179463	T	T	T
0.8888101935013882	0.8888733434080098	0.1411898979311513	T	T	T
-0.0001994787714904	0.0000068995775304	0.2112582853061101	T	T	T
0.3337730976295226	0.9991454913153780	0.2114065314426870	T	T	T
0.6663288750152951	0.0000549889948524	0.2113187142744115	T	T	T
-0.0009337454718123	0.3337014105547940	0.2113747385605860	T	T	T
0.3337260750801451	0.3336275243407942	0.2113872279632820	T	T	T
0.6663290872522249	0.3337151508961008	0.2113869043681438	T	T	T
-0.0001772303588333	0.6666058051989534	0.2112582741403893	T	T	T
0.3336188165070150	0.6664260462735566	0.2113952136774898	T	T	T
0.6663306189478099	0.6664223346584236	0.2113955788748419	T	T	T
0.1109848568803874	0.1112560623599806	0.2808122681617244	T	T	T
0.4438803155798116	0.1111960016751041	0.2811188770293945	T	T	T

0.7775103243845329	0.1109796628589391	0.2811813642369124	T	T	T
0.1108153433063464	0.4439758661388702	0.2808678524125697	T	T	T
0.4449191654619158	0.4449564970099741	0.2818860447752842	T	T	T
0.7757028092882867	0.4452530876974278	0.2818732449543835	T	T	T
0.1107106634307504	0.7777562099735715	0.2810626447723800	T	T	T
0.4449906066310607	0.7762218521264912	0.2819088288105042	T	T	T
0.7774809478813550	0.7778073975482503	0.2811886892354418	T	T	T
0.2214307057509677	0.2221317584978685	0.3515693953566876	T	T	T
0.8897683032571065	0.2206428959521337	0.3511082205354650	T	T	T
0.8894245798087582	0.5555257947539041	0.3512196772796921	T	T	T
0.2201061906400113	0.8902512447353927	0.3510301119438686	T	T	T
0.5553330160476716	0.8897721135333178	0.3514277550374328	T	T	T
0.8885975283798209	0.8886412165876886	0.3517837226851208	T	T	T
0.5549405571646193	0.5553237523993642	0.3535570178344721	T	T	T
0.2198041958375808	0.5556502520464388	0.3510245432733864	T	T	T
0.5553547799584969	0.2205358365312064	0.3513536430086620	T	T	T
0.4653922995421644	0.5954980408625831	0.4369845670589928	T	T	T
0.6251346957924602	0.5090527192158754	0.4372994016721156	T	T	T
0.3243005830956437	0.6716420505633306	0.4377344480896074	T	T	T
0.7660930993157482	0.4327157705573246	0.4386901443827830	T	T	T
Ag3_AgEmb_dDsC_bare					
2.92008000000000					
3.0000000000000000	0.0000000000000000	0.0000000000000000			
1.5000000000000000	2.5980762110000000	0.0000000000000000			
0.0000000000000000	0.0000000000000000	11.4687304500000007			
Ag					
54					
Selective dynamics					
Direct					
0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3333333299999988	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666599999976	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333299999988	0.0000000000000000	F	F	F
0.3333333299999988	0.3333333299999988	0.0000000000000000	F	F	F
0.6666666599999976	0.3333333299999988	0.0000000000000000	F	F	F
0.0000000000000000	0.6666666599999976	0.0000000000000000	F	F	F
0.3333333299999988	0.6666666599999976	0.0000000000000000	F	F	F
0.6666666599999976	0.6666666599999976	0.0000000000000000	F	F	F
0.1111111109999996	0.1111111109999996	0.0711932869999998	F	F	F
0.4444444399999984	0.1111111109999996	0.0711932869999998	F	F	F
0.7777777699999972	0.1111111109999996	0.0711932869999998	F	F	F
0.1111111109999996	0.4444444399999984	0.0711932869999998	F	F	F
0.4444444399999984	0.4444444399999984	0.0711932869999998	F	F	F
0.7777777699999972	0.4444444399999984	0.0711932869999998	F	F	F
0.1111111109999996	0.7777777699999972	0.0711932869999998	F	F	F
0.4444444399999984	0.7777777699999972	0.0711932869999998	F	F	F
0.7777777699999972	0.7777777699999972	0.0711932869999998	F	F	F
0.2222222199999992	0.2222222199999992	0.1411301544382417	T	T	T
0.5555555499999980	0.2222222199999992	0.1411301544382417	T	T	T
0.8888888799999968	0.2222222199999992	0.1411301544382417	T	T	T
0.2222222199999992	0.5555555499999980	0.1411301544382417	T	T	T
0.5555555499999980	0.5555555499999980	0.1411301544382417	T	T	T
0.8888888799999968	0.5555555499999980	0.1411301544382417	T	T	T
0.2222222199999992	0.8888888799999968	0.1411301544382417	T	T	T
0.5555555499999980	0.8888888799999968	0.1411301544382417	T	T	T
0.8888888799999968	0.8888888799999968	0.1411301544382417	T	T	T
-0.0000000000000000	0.0000000000000000	0.2112088768668099	T	T	T
0.3333333299999988	0.0000000000000000	0.2112088768668099	T	T	T

0.6666666659999976	0.0000000000000000	0.2112088768668099	T	T	T
-0.0000000000000000	0.3333333329999988	0.2112088768668099	T	T	T
0.3333333329999988	0.3333333329999988	0.2112088768668099	T	T	T
0.6666666659999976	0.3333333329999988	0.2112088768668099	T	T	T
-0.0000000000000000	0.6666666659999976	0.2112088768668099	T	T	T
0.3333333329999988	0.6666666659999976	0.2112088768668099	T	T	T
0.6666666659999976	0.6666666659999976	0.2112088768668099	T	T	T
0.1111111109999996	0.1111111109999996	0.2811234587646212	T	T	T
0.4444444439999984	0.1111111109999996	0.2811234587646212	T	T	T
0.7777777769999972	0.1111111109999996	0.2811234587646212	T	T	T
0.1111111109999996	0.4444444439999984	0.2811234587646212	T	T	T
0.4444444439999984	0.4444444439999984	0.2811234587646212	T	T	T
0.7777777769999972	0.4444444439999984	0.2811234587646212	T	T	T
0.1111111109999996	0.7777777769999972	0.2811234587646212	T	T	T
0.4444444439999984	0.7777777769999972	0.2811234587646212	T	T	T
0.7777777769999972	0.7777777769999972	0.2811234587646212	T	T	T
0.2222222219999992	0.2222222219999992	0.3513698862819497	T	T	T
0.8888888879999968	0.2222222219999992	0.3513698862819497	T	T	T
0.8888888879999968	0.555555549999980	0.3513698862819497	T	T	T
0.2222222219999992	0.8888888879999968	0.3513698862819497	T	T	T
0.555555549999980	0.8888888879999968	0.3513698862819497	T	T	T
0.8888888879999968	0.8888888879999968	0.3513698862819497	T	T	T
0.555555549999980	0.555555549999980	0.3513698862819497	T	T	T
0.2222222219999992	0.555555549999980	0.3513698862819497	T	T	T
0.555555549999980	0.2222222219999992	0.3513698862819497	T	T	T
Ag3_PdEmb_0.11ML_dDsC					
2.77984000000000					
2.9999999999999996	0.0000000000000000	0.0000000000000000			
1.4999999999999998	2.5980762110000000	0.0000000000000000			
0.0000000000000000	0.0000000000000000	11.4687304500000007			
Pd	Ag	C	H		
51	3	2	2		
Selective dynamics					
Direct					
0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3333333329999988	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666659999976	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333329999988	0.0000000000000000	F	F	F
0.3333333329999988	0.3333333329999988	0.0000000000000000	F	F	F
0.6666666659999976	0.3333333329999988	0.0000000000000000	F	F	F
0.0000000000000000	0.6666666659999976	0.0000000000000000	F	F	F
0.3333333329999988	0.6666666659999976	0.0000000000000000	F	F	F
0.6666666659999976	0.6666666659999976	0.0000000000000000	F	F	F
0.1111111109999996	0.1111111109999996	0.0711932869999998	F	F	F
0.4444444439999984	0.1111111109999996	0.0711932869999998	F	F	F
0.7777777769999972	0.1111111109999996	0.0711932869999998	F	F	F
0.1111111109999996	0.4444444439999984	0.0711932869999998	F	F	F
0.4444444439999984	0.4444444439999984	0.0711932869999998	F	F	F
0.7777777769999972	0.4444444439999984	0.0711932869999998	F	F	F
0.1111111109999996	0.7777777769999972	0.0711932869999998	F	F	F
0.4444444439999984	0.7777777769999972	0.0711932869999998	F	F	F
0.7777777769999972	0.7777777769999972	0.0711932869999998	F	F	F
0.2222424438541515	0.2222606124775988	0.1411759811583981	T	T	T
0.5550778754724611	0.2223933115065234	0.1417195402169037	T	T	T
0.8882628633280383	0.2223952816268145	0.1411510586453562	T	T	T
0.2223434157690506	0.5551479340495751	0.1417154325235412	T	T	T
0.5553088435347912	0.5553320166014973	0.1417113947207803	T	T	T
0.8886168211798969	0.5554455827957961	0.1414073094668804	T	T	T

0.2223609931752972	0.8882930539508364	0.1411419986116684	T	T	T
0.5554719422883860	0.8886149045110312	0.1414047311053739	T	T	T
0.8885904344553177	0.8885919009133738	0.1413403468814084	T	T	T
0.9992656902258297	0.9993037727990726	0.2111644336000285	T	T	T
0.3335151866543241	0.9991080982817929	0.2113884728048475	T	T	T
0.6661855055730382	-0.0002590820463121	0.2118862622282849	T	T	T
0.9990178821415756	0.3335424707076718	0.2113754722510382	T	T	T
0.3331401501245163	0.3331871851721006	0.2125271302670699	T	T	T
0.6656493097956889	0.3332381761791859	0.2123997080751509	T	T	T
-0.0003489141741662	0.6662054627689991	0.2119105024880006	T	T	T
0.3331356837195343	0.6657189388614958	0.2124035483146684	T	T	T
0.6661129439073656	0.6660955566428536	0.2120262985243027	T	T	T
0.1106830125443258	0.1105562915728300	0.2806863401734637	T	T	T
0.4441115982047933	0.1111266811789795	0.2824732259790076	T	T	T
0.7758808157467736	0.1110500352849875	0.2823844271446411	T	T	T
0.1111844239471244	0.4440092190489389	0.2824372583915797	T	T	T
0.4442749011275413	0.4442330185086781	0.2846502383329993	T	T	T
0.7750834361102632	0.4445550196239900	0.2827320310677518	T	T	T
0.1110321078503258	0.7759739928821181	0.2823807041929774	T	T	T
0.4446121968483362	0.7750722601381080	0.2827148285570150	T	T	T
0.7769421041291438	0.7771095035292012	0.2815875815391133	T	T	T
0.2186121197651745	0.2187463143425675	0.3527431638700401	T	T	T
0.8934460651236203	0.2176584921095154	0.3522436908273966	T	T	T
0.8879658329841601	0.5559096438077745	0.3522870617585358	T	T	T
0.2180204382577944	0.8931733305156510	0.3522727180487057	T	T	T
0.5559256594237989	0.8878819653341549	0.3523078926587582	T	T	T
0.8875647575905172	0.8872603929632020	0.3523895198038698	T	T	T
0.5556437910946360	0.5553809664581308	0.3595929098714500	T	T	T
0.2177747372032784	0.5557669423942003	0.3577878262446400	T	T	T
0.5560440110833242	0.2176122928428469	0.3578908385358697	T	T	T
0.4907179541044236	0.6319117790322859	0.4410266303058251	T	T	T
0.6553411762509238	0.5188803975095406	0.4396674333180314	T	T	T
0.3462269442212020	0.7318979463675894	0.4438853287141025	T	T	T
0.8006908204711998	0.4195622751832631	0.4401966456769704	T	T	T

Ag3\_PdEmb\_dDsC\_bare

2.77984000000000		
2.9999999999999996	0.0000000000000000	0.0000000000000000
1.4999999999999998	2.5980762110000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	11.4687304500000007

Pd Ag  
51 3

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3333333299999988	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666659999976	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333299999988	0.0000000000000000	F	F	F
0.3333333299999988	0.3333333299999988	0.0000000000000000	F	F	F
0.6666666659999976	0.3333333299999988	0.0000000000000000	F	F	F
0.0000000000000000	0.6666666659999976	0.0000000000000000	F	F	F
0.3333333299999988	0.6666666659999976	0.0000000000000000	F	F	F
0.6666666659999976	0.6666666659999976	0.0000000000000000	F	F	F
0.1111111109999996	0.1111111109999996	0.0711932869999998	F	F	F
0.4444444439999984	0.1111111109999996	0.0711932869999998	F	F	F
0.7777777699999972	0.1111111109999996	0.0711932869999998	F	F	F
0.1111111109999996	0.4444444439999984	0.0711932869999998	F	F	F
0.4444444439999984	0.4444444439999984	0.0711932869999998	F	F	F
0.7777777699999972	0.4444444439999984	0.0711932869999998	F	F	F



0.1111111109999996	0.7777777769999972	0.0711932869999998	F	F	F
0.4444444439999984	0.7777777769999972	0.0711932869999998	F	F	F
0.7777777769999972	0.7777777769999972	0.0711932869999998	F	F	F
0.2224143047360159	0.2224143047360159	0.1411713098550842	T	T	T
0.5554991709204702	0.2223349901590619	0.1417488383484254	T	T	T
0.8885047225279633	0.2224143047360159	0.1411713098550842	T	T	T
0.2223349901590619	0.5554991709204702	0.1417488383484254	T	T	T
0.5554991709204702	0.5554991709204702	0.1417488383484254	T	T	T
0.8887716745746580	0.5557899818506685	0.1414463067871999	T	T	T
0.2224143047360159	0.8885047225279633	0.1411713098550842	T	T	T
0.5557899818506685	0.8887716745746580	0.1414463067871999	T	T	T
0.8887716745746580	0.8887716745746580	0.1414463067871999	T	T	T
0.9997669824923007	0.9997669824923007	0.2113621427671495	T	T	T
0.3337993680153973	0.9997669824923007	0.2113621427671495	T	T	T
0.6665904531148377	0.0001524257703269	0.2120986854519434	T	T	T
0.9997669824923007	0.3337993680153973	0.2113621427671495	T	T	T
0.3335430223154200	0.3335430223154200	0.2123984570076932	T	T	T
0.6662472873691480	0.3335430223154200	0.2123984570076932	T	T	T
0.0001524257703269	0.6665904531148377	0.2120986854519434	T	T	T
0.3335430223154200	0.6662472873691480	0.2123984570076932	T	T	T
0.6665904531148377	0.6665904531148377	0.2120986854519434	T	T	T
0.1111111109999996	0.1111111109999996	0.2809024188247198	T	T	T
0.4448736236350798	0.1118934599598955	0.2826047812822958	T	T	T
0.7765662484050199	0.1118934599598955	0.2826047812822958	T	T	T
0.1118934599598955	0.4448736236350798	0.2826047812822958	T	T	T
0.4444444439999984	0.4444444439999984	0.2843875036775103	T	T	T
0.7765662484050199	0.4448736236350798	0.2826047812822958	T	T	T
0.1118934599598955	0.7765662484050199	0.2826047812822958	T	T	T
0.4448736236350798	0.7765662484050199	0.2826047812822958	T	T	T
0.7777777769999972	0.7777777769999972	0.2818294679609097	T	T	T
0.2198742029625314	0.2198742029625314	0.3526273388086887	T	T	T
0.8935849260749394	0.2198742029625314	0.3526273388086887	T	T	T
0.8883282116991313	0.5566769076017219	0.3525724027196333	T	T	T
0.2198742029625314	0.8935849260749394	0.3526273388086887	T	T	T
0.5566769076017219	0.8883282116991313	0.3525724027196333	T	T	T
0.8883282116991313	0.8883282116991313	0.3525724027196333	T	T	T
0.5568512561041841	0.5568512561041841	0.3583310514978852	T	T	T
0.2196308197916267	0.5568512561041841	0.3583310514978852	T	T	T
0.5568512561041841	0.2196308197916267	0.3583310514978852	T	T	T

C2H2\_dDsC

1.0000000000000000					
25.0000000000000000	0.0000000000000000	0.0000000000000000			
0.0000000000000000	26.0000000000000000	0.0000000000000000			
0.0000000000000000	0.0000000000000000	27.0000000000000000			

C H

2 2

Selective dynamics

Direct

0.4938336571491644	0.4550479236339607	0.5000000000000000	T	T	T
0.5060449448823353	0.4999861066230900	0.5000000000000000	T	T	T
0.4830295586575902	0.4151918319255086	0.5000000000000000	T	T	T
0.5170918393109100	0.5397741378174373	0.5000000000000000	T	T	T

Pd2Ag\_AgEmb\_0.11ML\_dDsC

2.92418893300000					
3.0000000000000000	0.0000000000000000	0.0000000000000000			
1.5000000000000000	2.5980762110000000	0.0000000000000000			
0.0000000000000000	0.0000000000000000	11.4687304500000007			

Ag Pd C H

52 2 2 2  
 Selective dynamics  
 Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3333333329999988	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666659999976	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333329999988	0.0000000000000000	F	F	F
0.3333333329999988	0.3333333329999988	0.0000000000000000	F	F	F
0.6666666659999976	0.3333333329999988	0.0000000000000000	F	F	F
0.0000000000000000	0.6666666659999976	0.0000000000000000	F	F	F
0.3333333329999988	0.6666666659999976	0.0000000000000000	F	F	F
0.6666666659999976	0.6666666659999976	0.0000000000000000	F	F	F
0.1111111109999996	0.1111111109999996	0.0711932869999998	F	F	F
0.4444444439999984	0.1111111109999996	0.0711932869999998	F	F	F
0.7777777769999972	0.1111111109999996	0.0711932869999998	F	F	F
0.1111111109999996	0.4444444439999984	0.0711932869999998	F	F	F
0.4444444439999984	0.4444444439999984	0.0711932869999998	F	F	F
0.7777777769999972	0.4444444439999984	0.0711932869999998	F	F	F
0.1111111109999996	0.7777777769999972	0.0711932869999998	F	F	F
0.4444444439999984	0.7777777769999972	0.0711932869999998	F	F	F
0.7777777769999972	0.7777777769999972	0.0711932869999998	F	F	F
0.2223028225003869	0.2215849414160322	0.1408735870976803	T	T	T
0.5558672427903950	0.2214811566553620	0.1410198107318439	T	T	T
0.8893306112021456	0.2215819765737976	0.1408762564459922	T	T	T
0.2226048269443096	0.5546133056362014	0.1409624935038057	T	T	T
0.5559748655100816	0.5546019542085615	0.1409669023497058	T	T	T
0.8892306571168360	0.5547149015795704	0.1410331443950376	T	T	T
0.2223418164741299	0.8885021082151101	0.1409441177620956	T	T	T
0.5557477361807934	0.8884535931534173	0.1408969196572579	T	T	T
0.8890213331574865	0.8884519933227180	0.1408890327779156	T	T	T
-0.0001829562325841	0.9994320745139667	0.2109583643800814	T	T	T
0.3338342144109799	0.9994291884889184	0.2109612656416746	T	T	T
0.6672582129675358	0.9984971416731820	0.2110014336306519	T	T	T
0.0006125685175176	0.3318616754613551	0.2111105724169847	T	T	T
0.3338639867549723	0.3313752686659590	0.2109321833460592	T	T	T
0.6678247972772935	0.3313418320836117	0.2109324609698540	T	T	T
-0.0000829963734434	0.6658193021677401	0.2107517422231921	T	T	T
0.3336860345895219	0.6655913878782697	0.2105159435251253	T	T	T
0.6672508298751559	0.6657812737573205	0.2107522454852026	T	T	T
0.1117410604573097	0.1093343551539910	0.2808500955221876	T	T	T
0.4459779156033792	0.1103270733866814	0.2813425746698197	T	T	T
0.7764574604997081	0.1102611865907725	0.2813469764126587	T	T	T
0.1118541126717264	0.4442836555328759	0.2808260138586787	T	T	T
0.4450121921764044	0.4428453257016348	0.2805043678820709	T	T	T
0.7766606968134724	0.4442641206006965	0.2808342095269094	T	T	T
0.1121882029612996	0.7751334456647995	0.2803444971548091	T	T	T
0.4453474710657144	0.7751162979198102	0.2803493155950618	T	T	T
0.7786409014855146	0.7753828709605859	0.2809349274686717	T	T	T
0.2214409339186992	0.2211954872245662	0.3505408400669954	T	T	T
0.5567666557542765	0.2189152768085158	0.3523139343752111	T	T	T
0.8899397350775559	0.2211341028914525	0.3505318266006144	T	T	T
0.8895370031406037	0.5536639147143859	0.3508128511818795	T	T	T
0.2237945839596719	0.8848938711384992	0.3505245467234183	T	T	T
0.5563062936703814	0.8849504569412813	0.3504754156205486	T	T	T
0.8912278761630659	0.8849736998378532	0.3504919271361208	T	T	T
0.5561554530905503	0.5554936856984848	0.3497783427709578	T	T	T
0.2210421436122653	0.5555111961965967	0.3497598704182566	T	T	T
0.5129140804278211	0.4580899871464738	0.4004095356996780	T	T	T

0.3615047650553087	0.4580917104506356	0.4004192632034146	T	T	T
0.6041199825729167	0.4324149000678105	0.4251256939131213	T	T	T
0.2959266528874706	0.4324376505166032	0.4251325558062219	T	T	T
Pd2Ag_AgEmb_dDsC_bare					
2.92418893300000					
3.0000000000000000	0.0000000000000000	0.0000000000000000			
1.5000000000000000	2.5980762110000000	0.0000000000000000			
0.0000000000000000	0.0000000000000000	11.4687304500000007			
Ag	Pd				
52	2				
Selective dynamics					
Direct					
0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3333333329999988	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666659999976	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333329999988	0.0000000000000000	F	F	F
0.3333333329999988	0.3333333329999988	0.0000000000000000	F	F	F
0.6666666659999976	0.3333333329999988	0.0000000000000000	F	F	F
0.0000000000000000	0.6666666659999976	0.0000000000000000	F	F	F
0.3333333329999988	0.6666666659999976	0.0000000000000000	F	F	F
0.6666666659999976	0.6666666659999976	0.0000000000000000	F	F	F
0.1111111109999996	0.1111111109999996	0.0711932869999998	F	F	F
0.4444444439999984	0.1111111109999996	0.0711932869999998	F	F	F
0.7777777769999972	0.1111111109999996	0.0711932869999998	F	F	F
0.1111111109999996	0.4444444439999984	0.0711932869999998	F	F	F
0.4444444439999984	0.4444444439999984	0.0711932869999998	F	F	F
0.7777777769999972	0.4444444439999984	0.0711932869999998	F	F	F
0.1111111109999996	0.7777777769999972	0.0711932869999998	F	F	F
0.4444444439999984	0.7777777769999972	0.0711932869999998	F	F	F
0.7777777769999972	0.7777777769999972	0.0711932869999998	F	F	F
0.2221877025897244	0.2220384066006531	0.1411457197527022	T	T	T
0.5557478984550778	0.2218375350898399	0.1409559449743041	T	T	T
0.8891072228096181	0.2220384066006531	0.1411457197527022	T	T	T
0.2220717811665639	0.5554975974246075	0.1408536823312159	T	T	T
0.5557639534088235	0.5554975974246075	0.1408536823312159	T	T	T
0.8889868821941470	0.5553595666116969	0.1409071397668795	T	T	T
0.2219556111737291	0.8894221096525369	0.1409399350802155	T	T	T
0.5555422559875790	0.8891003795018017	0.1410475358211222	T	T	T
0.8886906955106114	0.8891003795018017	0.1410475358211222	T	T	T
0.0000768289825010	-0.0000146305046939	0.2112261053876456	T	T	T
0.3332711345221918	-0.0000146305046939	0.2112261053876456	T	T	T
0.6666011685018048	0.0001309949963851	0.2111676580649985	T	T	T
-0.0000191355025093	0.3333716040050244	0.2112958361512429	T	T	T
0.3336037588391247	0.3331001328291164	0.2109423877818710	T	T	T
0.6666294403317538	0.3331001328291164	0.2109423877818710	T	T	T
-0.0002866087424238	0.6665750482456196	0.2108311384740328	T	T	T
0.3332054134874469	0.6669225050251014	0.2104571844766930	T	T	T
0.6670448924967993	0.6665750482456196	0.2108311384740328	T	T	T
0.1112622710956959	0.1108087908086069	0.2816355618073494	T	T	T
0.4446916796619965	0.1112236714917274	0.2813516540091233	T	T	T
0.7774179808462712	0.1112236714917274	0.2813516540091233	T	T	T
0.1111724385541509	0.4446847563892696	0.2809803797919014	T	T	T
0.4442949380907723	0.4447434558184504	0.2804578051379843	T	T	T
0.7774761370565746	0.4446847563892696	0.2809803797919014	T	T	T
0.1113424032099989	0.7775095677026899	0.2807113542158308	T	T	T
0.4444813610873066	0.7775095677026899	0.2807113542158308	T	T	T
0.7778338308283024	0.7776656693433939	0.2810540145000391	T	T	T
0.2222141772151784	0.2248050008743049	0.3512292944910594	T	T	T

0.5526882372238799	0.2279568575522417	0.3510037768593210	T	T	T
0.8863141539105189	0.2248050008743049	0.3512292944910594	T	T	T
0.8888290608068021	0.5556752093863951	0.3509512287869423	T	T	T
0.2251600055770387	0.8830133208459177	0.3509866954513280	T	T	T
0.5553673039756498	0.8862980967184280	0.3508479951188772	T	T	T
0.8916679303059065	0.8862980967184280	0.3508479951188772	T	T	T
0.5546420008397580	0.5552877539739629	0.3472896090263102	T	T	T
0.2234035771862741	0.5552877539739629	0.3472896090263102	T	T	T
Pd2Ag_PdEmb_0.11ML_dDsC					
2.77984000000000					
2.9999999999999996	0.0000000000000000	0.0000000000000000			
1.4999999999999998	2.5980762110000000	0.0000000000000000			
0.0000000000000000	0.0000000000000000	11.4687304500000007			
Pd	Ag	C	H		
53	1	2	2		
Selective dynamics					
Direct					
0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3333333329999988	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666659999976	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333329999988	0.0000000000000000	F	F	F
0.3333333329999988	0.3333333329999988	0.0000000000000000	F	F	F
0.6666666659999976	0.3333333329999988	0.0000000000000000	F	F	F
0.0000000000000000	0.6666666659999976	0.0000000000000000	F	F	F
0.3333333329999988	0.6666666659999976	0.0000000000000000	F	F	F
0.6666666659999976	0.6666666659999976	0.0000000000000000	F	F	F
0.1111111109999996	0.1111111109999996	0.0711932869999998	F	F	F
0.4444444439999984	0.1111111109999996	0.0711932869999998	F	F	F
0.7777777769999972	0.1111111109999996	0.0711932869999998	F	F	F
0.1111111109999996	0.4444444439999984	0.0711932869999998	F	F	F
0.4444444439999984	0.4444444439999984	0.0711932869999998	F	F	F
0.7777777769999972	0.4444444439999984	0.0711932869999998	F	F	F
0.1111111109999996	0.7777777769999972	0.0711932869999998	F	F	F
0.4444444439999984	0.7777777769999972	0.0711932869999998	F	F	F
0.7777777769999972	0.7777777769999972	0.0711932869999998	F	F	F
0.2225759830728256	0.2225431012962619	0.1411832754291490	T	T	T
0.5556883982010602	0.2227121352546881	0.1416407681226265	T	T	T
0.8886340869683104	0.2228206685976244	0.1412035198974285	T	T	T
0.2227180135591443	0.5556733156349396	0.1416401755040138	T	T	T
0.5559848289829999	0.5559540018616763	0.1417038610374638	T	T	T
0.8889563168325723	0.5563048841537471	0.1415109003261365	T	T	T
0.2228676850223044	0.8886176500210977	0.1412010627729807	T	T	T
0.5563660810730622	0.8889198003777632	0.1415142956727014	T	T	T
0.8889579446079907	0.8889645064132077	0.1414272068371352	T	T	T
0.0010656585691731	0.0009931157692870	0.2112188570719039	T	T	T
0.3344934109329926	0.0002623171447407	0.2113936798901823	T	T	T
0.6677311395700741	0.0012225378892711	0.2120569482507666	T	T	T
0.0003008078992797	0.3344145438466657	0.2113939424203861	T	T	T
0.3341731461152373	0.3341555106215227	0.2120906977759590	T	T	T
0.6675276854277632	0.3346596928824667	0.2122783411848573	T	T	T
0.0012634713568801	0.6676820474681200	0.2120504984101642	T	T	T
0.3346881615870360	0.6674875944370904	0.2122718844695715	T	T	T
0.6675639335036341	0.6674849057974630	0.2122828682693458	T	T	T
0.1134624170762996	0.1134062968581859	0.2813005384042802	T	T	T
0.4470017561763037	0.1134690049201253	0.2823075376963943	T	T	T
0.7792941817193593	0.1133633509639484	0.2823058037736588	T	T	T
0.1134898350735449	0.4469503647547544	0.2823084346453029	T	T	T
0.4469688904697566	0.4469673062603786	0.2831881103804147	T	T	T

0.7781122918000911	0.4476634549130186	0.2830916651353193	T	T	T
0.1134094731490825	0.7792390565488575	0.2823017871157086	T	T	T
0.4477268913296072	0.7780444105777147	0.2830837089677952	T	T	T
0.7799364913078896	0.7799079643844242	0.2818797751970416	T	T	T
0.2237198565652372	0.2236934163876097	0.3528368541250314	T	T	T
0.5590729295025604	0.2212594539582998	0.3550024092629927	T	T	T
0.8953497944604309	0.2217700335484308	0.3525743957105049	T	T	T
0.2212645072536957	0.5590774918113568	0.3550125271659560	T	T	T
0.8926632729479934	0.5589049719339642	0.3527051983613535	T	T	T
0.2217962891701591	0.8953101925017385	0.3525645322848700	T	T	T
0.5589014450286443	0.8926602463282990	0.3526988782998597	T	T	T
0.8914969197937063	0.8915053297582448	0.3527164712701244	T	T	T
0.5608878000051887	0.5608436424195750	0.3602864054369859	T	T	T
0.3520943559423056	0.5122844465726254	0.4095375784770598	T	T	T
0.5122541899231075	0.3521006883741611	0.4095428208309959	T	T	T
0.2813738259639764	0.6089097090915717	0.4353364361788364	T	T	T
0.6088954386735267	0.2813133137255140	0.4353314753371543	T	T	T
Pd2Ag_PdEmb_dDsC_bare					
2.77984000000000					
2.9999999999999996	0.0000000000000000	0.0000000000000000			
1.4999999999999998	2.5980762110000000	0.0000000000000000			
0.0000000000000000	0.0000000000000000	11.4687304500000007			
Pd Ag					
53 1					
Selective dynamics					
Direct					
0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3333333299999988	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666599999976	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333299999988	0.0000000000000000	F	F	F
0.3333333299999988	0.3333333299999988	0.0000000000000000	F	F	F
0.6666666599999976	0.3333333299999988	0.0000000000000000	F	F	F
0.0000000000000000	0.6666666599999976	0.0000000000000000	F	F	F
0.3333333299999988	0.6666666599999976	0.0000000000000000	F	F	F
0.6666666599999976	0.6666666599999976	0.0000000000000000	F	F	F
0.1111111099999996	0.1111111099999996	0.0711932869999998	F	F	F
0.4444444399999984	0.1111111099999996	0.0711932869999998	F	F	F
0.7777777699999972	0.1111111099999996	0.0711932869999998	F	F	F
0.1111111099999996	0.4444444399999984	0.0711932869999998	F	F	F
0.4444444399999984	0.4444444399999984	0.0711932869999998	F	F	F
0.7777777699999972	0.4444444399999984	0.0711932869999998	F	F	F
0.1111111099999996	0.7777777699999972	0.0711932869999998	F	F	F
0.4444444399999984	0.7777777699999972	0.0711932869999998	F	F	F
0.7777777699999972	0.7777777699999972	0.0711932869999998	F	F	F
0.2222222199999992	0.2222222199999992	0.1411334940853339	T	T	T
0.5556677343633448	0.2223458616794982	0.1415089711651052	T	T	T
0.8886530689571436	0.2223458616794982	0.1415089711651052	T	T	T
0.2223458616794982	0.5556677343633448	0.1415089711651052	T	T	T
0.5555555499999980	0.5555555499999980	0.1417508562004393	T	T	T
0.8886530689571436	0.5556677343633448	0.1415089711651052	T	T	T
0.2223458616794982	0.8886530689571436	0.1415089711651052	T	T	T
0.5556677343633448	0.8886530689571436	0.1415089711651052	T	T	T
0.8888888799999968	0.8888888799999968	0.1413700413877670	T	T	T
0.9999099892270435	0.9999099892270435	0.2117768389557468	T	T	T
0.3334433614421896	0.9997799431156185	0.2117104434209257	T	T	T
0.6668466875459172	0.9999099892270435	0.2117768389557468	T	T	T
0.9997799431156185	0.3334433614421896	0.2117104434209257	T	T	T
0.3334433614421896	0.3334433614421896	0.2117104434209257	T	T	T

0.6664352118040232	0.3337962413919476	0.2123562753519808	T	T	T
0.9999099892270435	0.6668466875459172	0.2117768389557468	T	T	T
0.3337962413919476	0.6664352118040232	0.2123562753519808	T	T	T
0.6664352118040232	0.6664352118040232	0.2123562753519808	T	T	T
0.1111982131826882	0.1111982131826882	0.2817925233107466	T	T	T
0.4442702396346282	0.1111982131826882	0.2817925233107466	T	T	T
0.7778165140521295	0.1110336368957420	0.2819981397330548	T	T	T
0.1111982131826882	0.4442702396346282	0.2817925233107466	T	T	T
0.4450680684071500	0.4450680684071500	0.2831881177147034	T	T	T
0.7765305281856940	0.4450680684071500	0.2831881177147034	T	T	T
0.1110336368957420	0.7778165140521295	0.2819981397330548	T	T	T
0.4450680684071500	0.7765305281856940	0.2831881177147034	T	T	T
0.7778165140521295	0.7778165140521295	0.2819981397330548	T	T	T
0.2222222219999992	0.2222222219999992	0.3530121490111675	T	T	T
0.5557081402820389	0.2204130784596400	0.3530302787322818	T	T	T
0.8905454462583147	0.2204130784596400	0.3530302787322818	T	T	T
0.2204130784596400	0.5557081402820389	0.3530302787322818	T	T	T
0.8905454462583147	0.5557081402820389	0.3530302787322818	T	T	T
0.2204130784596400	0.8905454462583147	0.3530302787322818	T	T	T
0.5557081402820389	0.8905454462583147	0.3530302787322818	T	T	T
0.8888888879999968	0.8888888879999968	0.3527779841553760	T	T	T
0.5555555549999980	0.5555555549999980	0.3592060623491551	T	T	T
Pd3_AgEmb_0.11ML_dDsC					
2.92008000000000					
3.0000000000000000	0.0000000000000000	0.0000000000000000			
1.5000000000000000	2.5980762110000000	0.0000000000000000			
0.0000000000000000	0.0000000000000000	11.4687304500000007			
Ag	Pd	C	H		
51	3	2	2		
Selective dynamics					
Direct					
0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3333333329999988	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666659999976	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333329999988	0.0000000000000000	F	F	F
0.3333333329999988	0.3333333329999988	0.0000000000000000	F	F	F
0.6666666659999976	0.3333333329999988	0.0000000000000000	F	F	F
0.0000000000000000	0.6666666659999976	0.0000000000000000	F	F	F
0.3333333329999988	0.6666666659999976	0.0000000000000000	F	F	F
0.6666666659999976	0.6666666659999976	0.0000000000000000	F	F	F
0.1111111109999996	0.1111111109999996	0.0711932869999998	F	F	F
0.4444444439999984	0.1111111109999996	0.0711932869999998	F	F	F
0.7777777769999972	0.1111111109999996	0.0711932869999998	F	F	F
0.1111111109999996	0.4444444439999984	0.0711932869999998	F	F	F
0.4444444439999984	0.4444444439999984	0.0711932869999998	F	F	F
0.7777777769999972	0.4444444439999984	0.0711932869999998	F	F	F
0.1111111109999996	0.7777777769999972	0.0711932869999998	F	F	F
0.4444444439999984	0.7777777769999972	0.0711932869999998	F	F	F
0.7777777769999972	0.7777777769999972	0.0711932869999998	F	F	F
0.2218182834317473	0.2224917711133591	0.1411140836240742	T	T	T
0.5556575608782542	0.2218118289283708	0.1411019331800875	T	T	T
0.8887841581410815	0.2224963070054360	0.1411161901475312	T	T	T
0.2222436343471804	0.5555972641182515	0.1411837579348638	T	T	T
0.5553566185838373	0.5555780278251188	0.1411800095998642	T	T	T
0.8890612545681479	0.5550987835868552	0.1412291545909685	T	T	T
0.2222478310781967	0.8885957917333580	0.1411455382818164	T	T	T
0.5552260298481447	0.8889154896054794	0.1410980445598956	T	T	T
0.8890037139535368	0.8888655594160840	0.1410949777237523	T	T	T

0.9997866908567613	0.0005470531708084	0.2112558484230306	T	T	T
0.3327290686743425	0.0005484552032175	0.2112568305636918	T	T	T
0.6669197247111590	0.9992067537647110	0.2110219462633165	T	T	T
0.9998947923705068	0.3332187867032148	0.2115870827307050	T	T	T
0.3332865768005210	0.3329564126793982	0.2112271468168268	T	T	T
0.6667406049207781	0.3329489877681454	0.2112312300541379	T	T	T
0.9994593615703632	0.6669810925305091	0.2112093963623050	T	T	T
0.3334205545264586	0.6662560320996587	0.2113330513385437	T	T	T
0.6666624678425002	0.6669309846995962	0.2112059272717696	T	T	T
0.1104495923228106	0.1116803818491423	0.2816754334686495	T	T	T
0.4463633583002714	0.1106974932706647	0.2814135266197768	T	T	T
0.7755971909390762	0.1106749339261597	0.2814213514254863	T	T	T
0.1112523877762223	0.4460896269482161	0.2815403984581278	T	T	T
0.4445959082173979	0.4433954063473904	0.2815324830986415	T	T	T
0.7751543713239317	0.4460932558407040	0.2815718864559562	T	T	T
0.1111367824905335	0.7773704011831313	0.2811618997533286	T	T	T
0.4442236121769159	0.7773390053613307	0.2811626650477068	T	T	T
0.7777304993127652	0.7771514731012111	0.2816374415325860	T	T	T
0.2227507559917595	0.2220832557172899	0.3510112915352460	T	T	T
0.8877167193668261	0.2221224270536387	0.3510201748151214	T	T	T
0.8884570367293713	0.5554069723482323	0.3514130376122847	T	T	T
0.2228919094996062	0.8867541074736074	0.3514835927158990	T	T	T
0.5554332117943078	0.8876054648641852	0.3510864693658368	T	T	T
0.8894798938757073	0.8876391014475162	0.3510798064286100	T	T	T
0.5531071404645982	0.5573125781436875	0.3506524608469450	T	T	T
0.2218247824731605	0.5572539553908159	0.3506230067743253	T	T	T
0.5570122813703499	0.2185645507796941	0.3509132393916480	T	T	T
0.5381301515457889	0.4098158646822135	0.3956865950296728	T	T	T
0.3839369342742764	0.4096570003966382	0.3956532997729416	T	T	T
0.6260663554531222	0.3876933414856735	0.4209447864818802	T	T	T
0.3182075434103765	0.3872979134365718	0.4208878108058666	T	T	T
Pd3_AgEmb_dDsC_bare					
2.920080000000000					
3.0000000000000000	0.0000000000000000	0.0000000000000000			
1.5000000000000000	2.5980762110000000	0.0000000000000000			
0.0000000000000000	0.0000000000000000	11.4687304500000007			
Ag Pd					
51 3					
Selective dynamics					
Direct					
0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3333333299999988	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666599999976	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333299999988	0.0000000000000000	F	F	F
0.3333333299999988	0.3333333299999988	0.0000000000000000	F	F	F
0.6666666599999976	0.3333333299999988	0.0000000000000000	F	F	F
0.0000000000000000	0.6666666599999976	0.0000000000000000	F	F	F
0.3333333299999988	0.6666666599999976	0.0000000000000000	F	F	F
0.6666666599999976	0.6666666599999976	0.0000000000000000	F	F	F
0.1111111109999996	0.1111111109999996	0.0711932869999998	F	F	F
0.4444444399999984	0.1111111109999996	0.0711932869999998	F	F	F
0.7777777699999972	0.1111111109999996	0.0711932869999998	F	F	F
0.1111111109999996	0.4444444399999984	0.0711932869999998	F	F	F
0.4444444399999984	0.4444444399999984	0.0711932869999998	F	F	F
0.7777777699999972	0.4444444399999984	0.0711932869999998	F	F	F
0.1111111109999996	0.7777777699999972	0.0711932869999998	F	F	F
0.4444444399999984	0.7777777699999972	0.0711932869999998	F	F	F
0.7777777699999972	0.7777777699999972	0.0711932869999998	F	F	F

0.2220153085278607	0.2220153085278607	0.1412203607380970	T	T	T
0.5557623886702886	0.2218085546594177	0.1409645851036914	T	T	T
0.8893027149442807	0.2220153085278607	0.1412203607380970	T	T	T
0.2218085546594177	0.5557623886702886	0.1409645851036914	T	T	T
0.5557623886702886	0.5557623886702886	0.1409645851036914	T	T	T
0.8889776325088523	0.5553780659822800	0.1411199437934675	T	T	T
0.2220153085278607	0.8893027149442807	0.1412203607380970	T	T	T
0.5553780659822800	0.8889776325088523	0.1411199437934675	T	T	T
0.8889776325088523	0.8889776325088523	0.1411199437934675	T	T	T
0.0000385037057322	0.0000385037057322	0.2115596061013932	T	T	T
0.3332563255885271	0.0000385037057322	0.2115596061013932	T	T	T
0.6668089543292151	-0.0002845766584347	0.2111685838722685	T	T	T
0.0000385037057322	0.3332563255885271	0.2115596061013932	T	T	T
0.3332893180258216	0.3332893180258216	0.2109207660043339	T	T	T
0.6667546959483591	0.3332893180258216	0.2109207660043339	T	T	T
-0.0002845766584347	0.6668089543292151	0.2111685838722685	T	T	T
0.3332893180258216	0.6667546959483591	0.2109207660043339	T	T	T
0.6668089543292151	0.6668089543292151	0.2111685838722685	T	T	T
0.1111111109999996	0.1111111109999996	0.2823418719368524	T	T	T
0.4448588463671247	0.1111506750403853	0.2814479718064287	T	T	T
0.7773238105924851	0.1111506750403853	0.2814479718064287	T	T	T
0.1111506750403853	0.4448588463671247	0.2814479718064287	T	T	T
0.4444444439999984	0.4444444439999984	0.2805251807626664	T	T	T
0.7773238105924851	0.4448588463671247	0.2814479718064287	T	T	T
0.1111506750403853	0.7773238105924851	0.2814479718064287	T	T	T
0.4448588463671247	0.7773238105924851	0.2814479718064287	T	T	T
0.7777777769999972	0.7777777769999972	0.2815484524847102	T	T	T
0.2249132356529110	0.2249132356529110	0.3517149660145610	T	T	T
0.8835068606941731	0.2249132356529110	0.3517149660145610	T	T	T
0.8889336606428451	0.5554660097143015	0.3514305433793714	T	T	T
0.2249132356529110	0.8835068606941731	0.3517149660145610	T	T	T
0.5554660097143015	0.8889336606428451	0.3514305433793714	T	T	T
0.8889336606428451	0.8889336606428451	0.3514305433793714	T	T	T
0.5535200592989036	0.5535200592989036	0.3478654585465253	T	T	T
0.2262932134021882	0.5535200592989036	0.3478654585465253	T	T	T
0.5535200592989036	0.2262932134021882	0.3478654585465253	T	T	T

Pd3\_PdEmb\_0.11ML\_dDsC

2.77984000000000		
2.9999999999999996	0.0000000000000000	0.0000000000000000
1.4999999999999998	2.5980762110000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	11.4687304500000007

Pd C H  
54 2 2

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3333333299999988	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666659999976	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333299999988	0.0000000000000000	F	F	F
0.3333333299999988	0.3333333299999988	0.0000000000000000	F	F	F
0.6666666659999976	0.3333333299999988	0.0000000000000000	F	F	F
0.0000000000000000	0.6666666659999976	0.0000000000000000	F	F	F
0.3333333299999988	0.6666666659999976	0.0000000000000000	F	F	F
0.6666666659999976	0.6666666659999976	0.0000000000000000	F	F	F
0.1111111109999996	0.1111111109999996	0.0711932869999998	F	F	F
0.4444444439999984	0.1111111109999996	0.0711932869999998	F	F	F
0.7777777769999972	0.1111111109999996	0.0711932869999998	F	F	F
0.1111111109999996	0.4444444439999984	0.0711932869999998	F	F	F



0.4444444439999984	0.4444444439999984	0.0711932869999998	F	F	F
0.7777777769999972	0.4444444439999984	0.0711932869999998	F	F	F
0.1111111109999996	0.7777777769999972	0.0711932869999998	F	F	F
0.4444444439999984	0.7777777769999972	0.0711932869999998	F	F	F
0.7777777769999972	0.7777777769999972	0.0711932869999998	F	F	F
0.2210213181338775	0.2235464727965098	0.1411704052085471	T	T	T
0.5546474887012588	0.2228652500191632	0.1416007704799215	T	T	T
0.8875677978468903	0.2235881300829365	0.1411802602219945	T	T	T
0.2211257761475623	0.5564872220299065	0.1416152659186510	T	T	T
0.5544798638593508	0.5564925319492015	0.1416270981624858	T	T	T
0.8875069991660564	0.5570928934351700	0.1415707451933858	T	T	T
0.2213133136217282	0.8893923039953628	0.1411749947046898	T	T	T
0.5550110908727101	0.8894498632910515	0.1415081485518319	T	T	T
0.8875407148597371	0.8895460003148258	0.1414972883829105	T	T	T
0.9969981717412106	0.0022720677975168	0.2112147924773272	T	T	T
0.3307794917904063	0.0022532169453585	0.2112060072798523	T	T	T
0.6643891252040112	0.0013495213923903	0.2122805321152187	T	T	T
0.9974782401556334	0.3351992760963520	0.2115699280978421	T	T	T
0.3312011342651440	0.3345937633033222	0.2119408639731431	T	T	T
0.6645725637546742	0.3345737335069048	0.2120017788005046	T	T	T
0.9978758194495170	0.6683797988427469	0.2122137261108415	T	T	T
0.3306785973116842	0.6689292050750438	0.2121190489965349	T	T	T
0.6639833254602618	0.6682755125202696	0.2122633704519235	T	T	T
0.1081184559075369	0.1120592469227304	0.2814930615638805	T	T	T
0.4425037726690707	0.1113150039752362	0.2826520773485660	T	T	T
0.7747377123336889	0.1112808578587063	0.2827326363913830	T	T	T
0.1084248206458958	0.4458295031486123	0.2824003956972885	T	T	T
0.4418596131336814	0.4450434651558164	0.2822829136550760	T	T	T
0.7743668174165610	0.4459678807882245	0.2824993648643159	T	T	T
0.1079541400473559	0.7789383549976063	0.2826368329534821	T	T	T
0.4418330514260938	0.7789556939662513	0.2826659383806604	T	T	T
0.7752340245512932	0.7784093562572523	0.2823548748675397	T	T	T
0.2168223067754171	0.2214756555421527	0.3528865722501219	T	T	T
0.5559702185209695	0.2161613721971136	0.3550575181437782	T	T	T
0.8893156633116619	0.2218887063377686	0.3529816299212655	T	T	T
0.2166521900297050	0.5586919092545359	0.3548508090350044	T	T	T
0.5520823957156826	0.5587174255505016	0.3550356510714034	T	T	T
0.8851701105291179	0.5574886280933521	0.3533544272249962	T	T	T
0.2180659302061608	0.8919409444447557	0.3530684646549942	T	T	T
0.5528697384078066	0.8879403575448772	0.3535053401398839	T	T	T
0.8875695936999314	0.8880236206595596	0.3535378266422020	T	T	T
0.5420669489648903	0.4066430396690677	0.4021827857380556	T	T	T
0.3773131143969546	0.4061237687108243	0.4020675869571102	T	T	T
0.6373436717725309	0.3755528251969508	0.4285544533599741	T	T	T
0.3128434125981940	0.3745211783129094	0.4282927793481797	T	T	T
Pd3_PdEmb_dDsC_bare					
2.77984000000000					
2.9999999999999996	0.0000000000000000	0.0000000000000000			
1.4999999999999998	2.5980762110000000	0.0000000000000000			
0.0000000000000000	0.0000000000000000	11.4687304500000007			
Pd					
54					
Selective dynamics					
Direct					
0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3333333299999988	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666599999976	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333299999988	0.0000000000000000	F	F	F

0.333333329999988	0.333333329999988	0.000000000000000	F	F	F
0.666666659999976	0.333333329999988	0.000000000000000	F	F	F
0.000000000000000	0.666666659999976	0.000000000000000	F	F	F
0.333333329999988	0.666666659999976	0.000000000000000	F	F	F
0.666666659999976	0.666666659999976	0.000000000000000	F	F	F
0.111111109999996	0.111111109999996	0.071193286999998	F	F	F
0.444444439999984	0.111111109999996	0.071193286999998	F	F	F
0.777777769999972	0.111111109999996	0.071193286999998	F	F	F
0.111111109999996	0.444444439999984	0.071193286999998	F	F	F
0.444444439999984	0.444444439999984	0.071193286999998	F	F	F
0.777777769999972	0.444444439999984	0.071193286999998	F	F	F
0.111111109999996	0.777777769999972	0.071193286999998	F	F	F
0.444444439999984	0.777777769999972	0.071193286999998	F	F	F
0.777777769999972	0.777777769999972	0.071193286999998	F	F	F
0.222222219999992	0.222222219999992	0.1414754156019031	T	T	T
0.555555549999980	0.222222219999992	0.1414754156019031	T	T	T
0.888888879999968	0.222222219999992	0.1414754156019031	T	T	T
0.222222219999992	0.555555549999980	0.1414754156019031	T	T	T
0.555555549999980	0.555555549999980	0.1414754156019031	T	T	T
0.888888879999968	0.555555549999980	0.1414754156019031	T	T	T
0.222222219999992	0.888888879999968	0.1414754156019031	T	T	T
0.555555549999980	0.888888879999968	0.1414754156019031	T	T	T
0.888888879999968	0.888888879999968	0.1414754156019031	T	T	T
-0.000000000000000	0.000000000000000	0.2118457911057095	T	T	T
0.333333329999988	0.000000000000000	0.2118457911057095	T	T	T
0.666666659999976	0.000000000000000	0.2118457911057095	T	T	T
-0.000000000000000	0.333333329999988	0.2118457911057095	T	T	T
0.333333329999988	0.333333329999988	0.2118457911057095	T	T	T
0.666666659999976	0.333333329999988	0.2118457911057095	T	T	T
-0.000000000000000	0.666666659999976	0.2118457911057095	T	T	T
0.333333329999988	0.666666659999976	0.2118457911057095	T	T	T
0.666666659999976	0.666666659999976	0.2118457911057095	T	T	T
0.111111109999996	0.111111109999996	0.2820181556321751	T	T	T
0.444444439999984	0.111111109999996	0.2820181556321751	T	T	T
0.777777769999972	0.111111109999996	0.2820181556321751	T	T	T
0.111111109999996	0.444444439999984	0.2820181556321751	T	T	T
0.444444439999984	0.444444439999984	0.2820181556321751	T	T	T
0.777777769999972	0.444444439999984	0.2820181556321751	T	T	T
0.111111109999996	0.777777769999972	0.2820181556321751	T	T	T
0.444444439999984	0.777777769999972	0.2820181556321751	T	T	T
0.777777769999972	0.777777769999972	0.2820181556321751	T	T	T
0.222222219999992	0.222222219999992	0.3530829600817724	T	T	T
0.555555549999980	0.222222219999992	0.3530829600817724	T	T	T
0.888888879999968	0.222222219999992	0.3530829600817724	T	T	T
0.222222219999992	0.555555549999980	0.3530829600817724	T	T	T
0.555555549999980	0.555555549999980	0.3530829600817724	T	T	T
0.888888879999968	0.555555549999980	0.3530829600817724	T	T	T
0.222222219999992	0.888888879999968	0.3530829600817724	T	T	T
0.555555549999980	0.888888879999968	0.3530829600817724	T	T	T
0.888888879999968	0.888888879999968	0.3530829600817724	T	T	T

PdAg2\_AgEmb\_0.11ML\_dDsC

2.920080000000000

3.000000000000000	0.000000000000000	0.000000000000000
1.500000000000000	2.598076211000000	0.000000000000000
0.000000000000000	0.000000000000000	11.468730450000007

Ag Pd C H

53 1 2 2

Selective dynamics

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3333333329999988	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666659999976	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333329999988	0.0000000000000000	F	F	F
0.3333333329999988	0.3333333329999988	0.0000000000000000	F	F	F
0.6666666659999976	0.3333333329999988	0.0000000000000000	F	F	F
0.0000000000000000	0.6666666659999976	0.0000000000000000	F	F	F
0.3333333329999988	0.6666666659999976	0.0000000000000000	F	F	F
0.6666666659999976	0.6666666659999976	0.0000000000000000	F	F	F
0.1111111109999996	0.1111111109999996	0.0711932869999998	F	F	F
0.4444444439999984	0.1111111109999996	0.0711932869999998	F	F	F
0.7777777769999972	0.1111111109999996	0.0711932869999998	F	F	F
0.1111111109999996	0.4444444439999984	0.0711932869999998	F	F	F
0.4444444439999984	0.4444444439999984	0.0711932869999998	F	F	F
0.7777777769999972	0.4444444439999984	0.0711932869999998	F	F	F
0.1111111109999996	0.7777777769999972	0.0711932869999998	F	F	F
0.4444444439999984	0.7777777769999972	0.0711932869999998	F	F	F
0.7777777769999972	0.7777777769999972	0.0711932869999998	F	F	F
0.2219126068679019	0.2221798804570808	0.1414086629617048	T	T	T
0.5549721975675191	0.2221644816487668	0.1411360773729790	T	T	T
0.8889282765006198	0.2220654180212703	0.1411201648528642	T	T	T
0.2217650492979726	0.5553467733951944	0.1411401832853662	T	T	T
0.5552841320176943	0.5554879058854473	0.1410392052683095	T	T	T
0.8889578193134761	0.5552393555950201	0.1411106570702967	T	T	T
0.2217247246189830	0.8892271673995259	0.1411441266509345	T	T	T
0.5549437501050012	0.8891937425751901	0.1411186213184601	T	T	T
0.8884437721627320	0.8888746175661797	0.1411293007240644	T	T	T
0.9995654941857987	-0.0002171565954007	0.2112028085783147	T	T	T
0.3334020713299941	0.9986463241997604	0.2116145118070501	T	T	T
0.6659214959707911	-0.0000787114596373	0.2112367709033915	T	T	T
0.9985633338255012	0.3335694020737316	0.2115678013086264	T	T	T
0.3334380422941285	0.3336193532377617	0.2116034460883788	T	T	T
0.6661857841972487	0.3331995303468088	0.2110936040410242	T	T	T
0.9995680915525009	0.6663943728478806	0.2112240493962249	T	T	T
0.3329493496601423	0.6664191173072671	0.2110651222599141	T	T	T
0.6661318245443505	0.6664438740478371	0.2110768811963093	T	T	T
0.1097250241020426	0.1106004877162681	0.2810827013512281	T	T	T
0.4429641013255142	0.1107315451300067	0.2812751790583359	T	T	T
0.7758559565014198	0.1112655490640801	0.2809986950844617	T	T	T
0.1098060025812569	0.4441623881478844	0.2811515917294516	T	T	T
0.4452785010062074	0.4461175681433385	0.2821494989337579	T	T	T
0.7724868194084734	0.4458928432557547	0.2820683596236406	T	T	T
0.1106795602031855	0.7768049642712537	0.2809641317949776	T	T	T
0.4453788950458286	0.7729362094390182	0.2821197971680100	T	T	T
0.7758512455582588	0.7771371278111728	0.2810234851036540	T	T	T
0.2197759651442139	0.2218377201539111	0.3515082673710888	T	T	T
0.5538122535065362	0.2204175556980960	0.3511782194805146	T	T	T
0.8868679985021627	0.2209373250837041	0.3508259198860708	T	T	T
0.2190052872602941	0.5556557560530424	0.3509421850550419	T	T	T
0.8868173388058953	0.5554136644182637	0.3509263488958363	T	T	T
0.2190938431491154	0.8888340792352575	0.3508315639261644	T	T	T
0.5535799072136431	0.8894778009981301	0.3511972934414659	T	T	T
0.8867441624193360	0.8882401314294955	0.3512592208714664	T	T	T
0.5525987810129521	0.5554356821087812	0.3549079578062278	T	T	T
0.4716174856869991	0.5980602540625233	0.4161200500839969	T	T	T
0.6374531531150694	0.5076523058929668	0.4160475569215430	T	T	T
0.3453414216794553	0.6667093037732438	0.4308179169113697	T	T	T

0.7640345060199623	0.4382241488843944	0.4305861998427048	T	T	T
PdAg2_AgEmb_dDsC_bare					
2.92008000000000					
3.0000000000000000	0.0000000000000000	0.0000000000000000			
1.5000000000000000	2.5980762110000000	0.0000000000000000			
0.0000000000000000	0.0000000000000000	11.4687304500000007			
Ag	Pd				
53	1				
Selective dynamics					
Direct					
0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3333333329999988	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666659999976	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333329999988	0.0000000000000000	F	F	F
0.3333333329999988	0.3333333329999988	0.0000000000000000	F	F	F
0.6666666659999976	0.3333333329999988	0.0000000000000000	F	F	F
0.0000000000000000	0.6666666659999976	0.0000000000000000	F	F	F
0.3333333329999988	0.6666666659999976	0.0000000000000000	F	F	F
0.6666666659999976	0.6666666659999976	0.0000000000000000	F	F	F
0.1111111109999996	0.1111111109999996	0.0711932869999998	F	F	F
0.4444444439999984	0.1111111109999996	0.0711932869999998	F	F	F
0.7777777769999972	0.1111111109999996	0.0711932869999998	F	F	F
0.1111111109999996	0.4444444439999984	0.0711932869999998	F	F	F
0.4444444439999984	0.4444444439999984	0.0711932869999998	F	F	F
0.7777777769999972	0.4444444439999984	0.0711932869999998	F	F	F
0.1111111109999996	0.7777777769999972	0.0711932869999998	F	F	F
0.4444444439999984	0.7777777769999972	0.0711932869999998	F	F	F
0.7777777769999972	0.7777777769999972	0.0711932869999998	F	F	F
0.2222222219999992	0.2222222219999992	0.1413361824472261	T	T	T
0.5554837202497648	0.2220142224143421	0.1411165885182963	T	T	T
0.8891687223358872	0.2220142224143421	0.1411165885182963	T	T	T
0.2220142224143421	0.5554837202497648	0.1411165885182963	T	T	T
0.555555549999980	0.555555549999980	0.1409974982382214	T	T	T
0.8891687223358872	0.5554837202497648	0.1411165885182963	T	T	T
0.2220142224143421	0.8891687223358872	0.1411165885182963	T	T	T
0.5554837202497648	0.8891687223358872	0.1411165885182963	T	T	T
0.8888888879999968	0.8888888879999968	0.1412177275098495	T	T	T
0.0000682896672614	0.0000682896672614	0.2113093256570993	T	T	T
0.3333921416325594	-0.0001176172651213	0.2113737117588115	T	T	T
0.6665300866654748	0.0000682896672614	0.2113093256570993	T	T	T
-0.0001176172651213	0.3333921416325594	0.2113737117588115	T	T	T
0.3333921416325594	0.3333921416325594	0.2113737117588115	T	T	T
0.6667723034132066	0.3331220581735812	0.2110004462342869	T	T	T
0.0000682896672614	0.6665300866654748	0.2113093256570993	T	T	T
0.3331220581735812	0.6667723034132066	0.2110004462342869	T	T	T
0.6667723034132066	0.6667723034132066	0.2110004462342869	T	T	T
0.1109774156206840	0.1109774156206840	0.2815270253582048	T	T	T
0.4447118347586296	0.1109774156206840	0.2815270253582048	T	T	T
0.7777022131119383	0.1112622387761171	0.2812486914831026	T	T	T
0.1109774156206840	0.4447118347586296	0.2815270253582048	T	T	T
0.4445878918617531	0.4445878918617531	0.2810811241034477	T	T	T
0.7774908812764877	0.4445878918617531	0.2810811241034477	T	T	T
0.1112622387761171	0.7777022131119383	0.2812486914831026	T	T	T
0.4445878918617531	0.7774908812764877	0.2810811241034477	T	T	T
0.7777022131119383	0.7777022131119383	0.2812486914831026	T	T	T
0.2222222219999992	0.2222222219999992	0.3516464842663994	T	T	T
0.5555502570655781	0.2247120015228110	0.3514885387868589	T	T	T
0.8864044064116048	0.2247120015228110	0.3514885387868589	T	T	T

0.2247120015228110	0.5555502570655781	0.3514885387868589	T	T	T
0.8864044064116048	0.5555502570655781	0.3514885387868589	T	T	T
0.2247120015228110	0.8864044064116048	0.3514885387868589	T	T	T
0.5555502570655781	0.8864044064116048	0.3514885387868589	T	T	T
0.8888888879999968	0.8888888879999968	0.3512899911166759	T	T	T
0.5555555549999980	0.5555555549999980	0.3479666217061603	T	T	T
PdAg2_PdEmb_0.11ML_dDsC					
2.77984000000000					
2.999999999999996	0.0000000000000000	0.0000000000000000			
1.499999999999998	2.5980762110000000	0.0000000000000000			
0.0000000000000000	0.0000000000000000	11.4687304500000007			
Pd	Ag	C	H		
52	2	2	2		
Selective dynamics					
Direct					
0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3333333329999988	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666659999976	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333329999988	0.0000000000000000	F	F	F
0.3333333329999988	0.3333333329999988	0.0000000000000000	F	F	F
0.6666666659999976	0.3333333329999988	0.0000000000000000	F	F	F
0.0000000000000000	0.6666666659999976	0.0000000000000000	F	F	F
0.3333333329999988	0.6666666659999976	0.0000000000000000	F	F	F
0.6666666659999976	0.6666666659999976	0.0000000000000000	F	F	F
0.1111111109999996	0.1111111109999996	0.0711932869999998	F	F	F
0.4444444439999984	0.1111111109999996	0.0711932869999998	F	F	F
0.7777777769999972	0.1111111109999996	0.0711932869999998	F	F	F
0.1111111109999996	0.4444444439999984	0.0711932869999998	F	F	F
0.4444444439999984	0.4444444439999984	0.0711932869999998	F	F	F
0.7777777769999972	0.4444444439999984	0.0711932869999998	F	F	F
0.1111111109999996	0.7777777769999972	0.0711932869999998	F	F	F
0.4444444439999984	0.7777777769999972	0.0711932869999998	F	F	F
0.7777777769999972	0.7777777769999972	0.0711932869999998	F	F	F
0.2219749256435887	0.2228226366492747	0.1411432782394762	T	T	T
0.5551455303232304	0.2227954712893063	0.1416222900278766	T	T	T
0.8882662708104760	0.2227653111804581	0.1411893942821188	T	T	T
0.2219265242826355	0.5559178889081489	0.1416798643380437	T	T	T
0.5552934014337915	0.5557815132343150	0.1417005776119249	T	T	T
0.8883093814225822	0.5562940459635036	0.1415790009340895	T	T	T
0.2222765356822371	0.8887020698995761	0.1412345614000899	T	T	T
0.5556306642120177	0.8889391917479894	0.1414398322894639	T	T	T
0.8885107142969860	0.8889625104049386	0.1414607815587492	T	T	T
0.9995180507099585	0.0004987406781078	0.2113888332736199	T	T	T
0.3325640547030909	0.0005450229680493	0.2113607100593048	T	T	T
0.6657242082382739	0.0012142104560525	0.2119017466051049	T	T	T
0.9989487206473249	0.3346752882749882	0.2116313489520159	T	T	T
0.3320206945109330	0.3345018170613760	0.2121172472848677	T	T	T
0.6661944420795428	0.3343378305395626	0.2122590493643589	T	T	T
0.9997861919081806	0.6673403954928827	0.2121824082471037	T	T	T
0.3324520840964073	0.6676852435713277	0.2124045623038209	T	T	T
0.6654920376906395	0.6673155571302253	0.2122282098739801	T	T	T
0.1095852822736845	0.1130205729436497	0.2812641383150434	T	T	T
0.4432428074109852	0.1132609994274525	0.2820473488443776	T	T	T
0.7752783286767062	0.1136052706337242	0.2822886439726633	T	T	T
0.1103791086913271	0.4473028480475852	0.2829728684813668	T	T	T
0.4427415213854757	0.4461240132320194	0.2831854888909724	T	T	T
0.7742437063073989	0.4472766596120364	0.2831282469211498	T	T	T
0.1108254176010916	0.7776248663456738	0.2829233830995863	T	T	T

0.4439451762225474	0.7774047524044199	0.2829558478237807	T	T	T
0.7763126870904622	0.7799196144302528	0.2816588809404447	T	T	T
0.2201896314031881	0.2209059887217675	0.3526470540344842	T	T	T
0.5583503653826563	0.2161649929412522	0.3552874538127581	T	T	T
0.8922090526728800	0.2209099504116080	0.3526927133183168	T	T	T
0.8862602847245294	0.5597367209559833	0.3524443499251850	T	T	T
0.2184255453681515	0.8963608274246740	0.3527174119001524	T	T	T
0.5551942577853631	0.8910743092504255	0.3523945050390834	T	T	T
0.8863418622230126	0.8912856311320911	0.3524246632312573	T	T	T
0.5551968237876904	0.5581286855291138	0.3596240302725955	T	T	T
0.2171332855150465	0.5603731648127902	0.3596305984444129	T	T	T
0.4257699821703209	0.4944842881612268	0.4129565102632484	T	T	T
0.4902214816622982	0.3142472042320355	0.4129352953080923	T	T	T
0.3803189743502279	0.5955954405567881	0.4383513059952475	T	T	T
0.5133977741559230	0.2160350119716157	0.4381731628453328	T	T	T
PdAg2_PdEmb_dDsC_bare					
2.77984000000000					
2.9999999999999996	0.0000000000000000	0.0000000000000000			
1.4999999999999998	2.5980762110000000	0.0000000000000000			
0.0000000000000000	0.0000000000000000	11.4687304500000007			
Pd Ag					
52 2					
Selective dynamics					
Direct					
0.0000000000000000	0.0000000000000000	0.0000000000000000	F	F	F
0.3333333329999998	0.0000000000000000	0.0000000000000000	F	F	F
0.6666666659999976	0.0000000000000000	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333329999998	0.0000000000000000	F	F	F
0.3333333329999998	0.3333333329999998	0.0000000000000000	F	F	F
0.6666666659999976	0.3333333329999998	0.0000000000000000	F	F	F
0.0000000000000000	0.6666666659999976	0.0000000000000000	F	F	F
0.3333333329999998	0.6666666659999976	0.0000000000000000	F	F	F
0.6666666659999976	0.6666666659999976	0.0000000000000000	F	F	F
0.1111111109999996	0.1111111109999996	0.0711932869999998	F	F	F
0.4444444439999984	0.1111111109999996	0.0711932869999998	F	F	F
0.7777777769999972	0.1111111109999996	0.0711932869999998	F	F	F
0.1111111109999996	0.4444444439999984	0.0711932869999998	F	F	F
0.4444444439999984	0.4444444439999984	0.0711932869999998	F	F	F
0.7777777769999972	0.4444444439999984	0.0711932869999998	F	F	F
0.1111111109999996	0.7777777769999972	0.0711932869999998	F	F	F
0.4444444439999984	0.7777777769999972	0.0711932869999998	F	F	F
0.7777777769999972	0.7777777769999972	0.0711932869999998	F	F	F
0.2222984361158780	0.2223422396040156	0.1411242092488233	T	T	T
0.5554582662089020	0.2224167995821912	0.1415061899208940	T	T	T
0.8886926562801015	0.2223422396040156	0.1411242092488233	T	T	T
0.2222970811247266	0.5556717653450296	0.1417089240718826	T	T	T
0.5553644855302391	0.5556717653450296	0.1417089240718826	T	T	T
0.8887157496981394	0.5559018316037132	0.1414946628905327	T	T	T
0.2224579838178471	0.8884173643642937	0.1414878651934932	T	T	T
0.5556254325013196	0.8886895357816312	0.1414060599540098	T	T	T
0.8890183627170336	0.8886895357816312	0.1414060599540098	T	T	T
0.0002701516089526	0.9993437737344991	0.2115174308545240	T	T	T
0.3337194076565400	0.9993437737344991	0.2115174308545240	T	T	T
0.6669087329231383	0.9995158661537256	0.2116551562062629	T	T	T
-0.0000980490120784	0.3335294310241555	0.2114178325157521	T	T	T
0.3331381841565509	0.3336655505725077	0.2120069364031558	T	T	T
0.6665295972709363	0.3336655505725077	0.2120069364031558	T	T	T
0.0003773339734356	0.6665206757282843	0.2121629485825101	T	T	T

0.3337038031187094	0.6659257257625764	0.2126571977052300	T	T	T
0.6664353222982752	0.6665206757282843	0.2121629485825101	T	T	T
0.1112589380574230	0.1108154568851529	0.2812919198717703	T	T	T
0.4445481592113186	0.1106278589195882	0.2815713390740874	T	T	T
0.7781573138690958	0.1106278589195882	0.2815713390740874	T	T	T
0.1120296891950440	0.4443504304969137	0.2826574362899418	T	T	T
0.4445132766565719	0.4443067786868514	0.2837883758196399	T	T	T
0.7769532123080374	0.4443504304969137	0.2826574362899418	T	T	T
0.1122209353538838	0.7758668328742626	0.2830107103754802	T	T	T
0.4452455637718486	0.7758668328742626	0.2830107103754802	T	T	T
0.7780385978013915	0.7772561353972086	0.2818884413851639	T	T	T
0.2224056031139222	0.2201939450349870	0.3526688316758436	T	T	T
0.5573231381234371	0.2186870557531209	0.3526919665840569	T	T	T
0.8907337838510792	0.2201939450349870	0.3526688316758436	T	T	T
0.8886083032057732	0.5561167245884445	0.3528678928379090	T	T	T
0.2198328582207517	0.8936676155584845	0.3529396704576772	T	T	T
0.5557278884894695	0.8909554164492780	0.3525406981663451	T	T	T
0.8866500260612438	0.8909554164492780	0.3525406981663451	T	T	T
0.5563693230851977	0.5560235370700226	0.3586601120531814	T	T	T
0.2209404718447749	0.5560235370700226	0.3586601120531814	T	T	T
sqrt3_0.33ML_dDsC					
2.77984000000000					
1.4999999999999998	0.8660254038000000	0.0000000000000000			
-1.4999999999999998	0.8660254038000000	0.0000000000000000			
0.0000000000000000	0.0000000000000000	7.3484692279999990			
Pd	C	H			
15	2	2			
Selective dynamics					
Direct					
0.0064625252769207	0.0153955440220539	0.4435312049887320	T	T	T
0.3418286849048968	0.0107297558393264	0.3326328636701910	T	T	T
0.3358439324635872	0.3367271174921916	0.2208902745106292	T	T	T
0.0000000000000000	0.0000000000000000	0.1111111111000014	F	F	F
0.3333333329999988	0.0000000000000000	0.0000000000000000	F	F	F
0.6772627064325100	0.3446410363955160	0.4434603508262008	T	T	T
0.3468486571729339	0.6850675783333341	0.4447674942121608	T	T	T
0.6741055558321157	0.6785214528879849	0.3326240527681220	T	T	T
0.0093245743818276	0.3460378508738461	0.3301133830885676	T	T	T
0.6678068796393194	0.0032042212345109	0.2214690451523635	T	T	T
0.0012761925465574	0.6711035410648408	0.2208869024962224	T	T	T
0.6666666670000012	0.3333333329999988	0.1111111111000014	F	F	F
0.3333333329999988	0.6666666670000012	0.1111111111000014	F	F	F
0.6666666670000012	0.6666666670000012	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333329999988	0.0000000000000000	F	F	F
0.1453633044800259	0.3201042555099444	0.5194909348107685	T	T	T
0.9816215221318350	0.4844634101609771	0.5194521657383090	T	T	T
0.2685467346798751	0.2815703300696550	0.5605079833580874	T	T	T
0.9434505153539480	0.6080901364675276	0.5604390991247582	T	T	T
sqrt3_dDsC_bare					
2.77984000000000					
1.4999999999999998	0.8660254038000000	0.0000000000000000			
-1.4999999999999998	0.8660254038000000	0.0000000000000000			
0.0000000000000000	0.0000000000000000	7.3484692279999990			
Pd					
15					
Selective dynamics					
Direct					
0.0049531780968722	0.0103801263402628	0.4406079744991694	T	T	T

0.3377007521171237	0.0088564972017942	0.3299927667547033	T	T	T
0.3357463173122849	0.3384915953375170	0.2205599551972050	T	T	T
0.0000000000000000	0.0000000000000000	0.1111111111000014	F	F	F
0.3333333329999988	0.0000000000000000	0.0000000000000000	F	F	F
0.6715961188391469	0.3437632170590736	0.4406018649194877	T	T	T
0.3382158805067376	0.6769629444927338	0.4406303316617566	T	T	T
0.6709981675890723	0.6755482755850126	0.3299852095478361	T	T	T
0.0042815270117101	0.3421309254079156	0.3300001341183598	T	T	T
0.6691771809358092	0.0052699896950736	0.2205655657574067	T	T	T
0.0024963013092995	0.6718914355576360	0.2205669517104738	T	T	T
0.6666666670000012	0.3333333329999988	0.1111111111000014	F	F	F
0.3333333329999988	0.6666666670000012	0.1111111111000014	F	F	F
0.6666666670000012	0.6666666670000012	0.0000000000000000	F	F	F
0.0000000000000000	0.3333333329999988	0.0000000000000000	F	F	F