

Supplementary Information - Revolutionizing ORR Catalyst Design through Computational Methodologies and Materials Informatics

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Table 1: Total energies and adsorption free energies of oxygen reduction reaction intermediate species on different transition metal nitride (TMN) surfaces selected for this work.

TMN	$E_{(*)}$ (eV)	$E_{\text{-OOH}}$ (eV)	$\Delta G_{\text{-OOH}}$	$E_{\text{-O}}$ (eV)	$\Delta G_{\text{-O}}$	$E_{\text{-OH}}$ (eV)	$\Delta G_{\text{-OH}}$
Co ₂ N (110)	-171.80	-186.08	4.02	-176.91	2.36	-182.00	0.65
Co ₃ N (110)	-225.35	-239.18	4.47	-229.76	3.05	-234.77	1.43
CoN (100)	-239.19	-253.32	4.16	-245.43	1.21	-248.91	1.12
ReN ₂ (110)	-439.40	-455.89	1.81	-445.11	1.74	-448.37	1.87
ReN ₂ (100)	-222.95	-237.76	3.49	-228.25	2.16	-232.20	1.59
ReN ₂ (110)	-219.68	-231.90	6.08	-223.07	4.07	-227.47	3.06
Ta ₄ N ₅ (100)	-376.79	-393.39	1.70	-382.63	1.62	-386.09	1.54
Ta ₄ N ₅ (110)	-379.51	-396.42	1.39	-383.72	3.25	-387.13	3.22
Ni ₃ N (110)	-189.05	-205.28	2.07	-195.35	1.16	-198.80	1.09
Fe ₃ N (110)	-256.51	-274.53	0.28	-263.42	0.55	-267.05	0.31
Cr ₃ N ₂ (110)	-331.71	-349.50	0.51	-336.88	2.28	-339.81	2.73
Cr ₂ N (110)	-330.04	-343.79	4.55	-335.50	2.00	-339.40	1.49
MnN (100)	-282.00	-296.00	4.29	-287.32	2.13	-291.65	1.19
Nb ₄ N ₅ (100)	-344.47	-358.62	4.15	-350.35	1.58	-353.94	1.37

XYZ Coordinates of DFT optimized output files of pristine TMN surfaces and oxygen reduction reaction intermediate species adsorption on different TMN surfaces selected for this work as listed in Table 1 above.

Co₂N (110) - Surface

Co N

```

1.0000000000000000
 4.5225900000000001  0.0000000000000000  0.0000000000000000
 0.0000000000000000  5.1302700000000003  0.0000000000000000
 0.0000000000000000  0.0000000000000000  28.2963999999999984
  
```

Co N

16 8

Selective dynamics

Direct

```

0.1762400000000000  0.6618899999999996  0.01127000000000032  F F F
0.1762400000000000  0.35871999999999982  0.09461000000000030  F F F
0.8237600000000000  0.67851000000000028  0.13284999999999977  F F F
0.8237600000000000  0.98167999999999972  0.04952000000000011  F F F
0.6762400000000000  0.48167999999999972  0.04952000000000011  F F F
0.6762400000000000  0.17851000000000028  0.13284999999999977  F F F
0.3237600000000000  0.16188999999999996  0.01127000000000032  F F F
0.3237600000000000  0.85871999999999982  0.09461000000000030  F F F
0.1948070208851711  0.0720173292094844  0.1805973476788665  T T T
0.1997946110729193  0.7856626985407047  0.2689117382197175  T T T
0.7892100835392438  0.0552498528873082  0.2971126575434176  T T T
0.8031442439296477  0.3609301699001694  0.2152536966525954  T T T
0.6968513176383098  0.8609327461430699  0.2152524925266610  T T T
0.7107564840541433  0.5552139132099218  0.2971120233389039  T T T
0.3051963419992098  0.5720230108330938  0.1805976097640255  T T T
0.3002124745083504  0.2856625079702546  0.2689135666458114  T T T
0.5000000000000000  0.86701999999999966  0.15538999999999970  F F F
0.5000000000000000  0.17020000000000012  0.07206000000000005  F F F
0.0000000000000000  0.67020000000000012  0.07206000000000005  F F F
0.0000000000000000  0.36701999999999966  0.15538999999999970  F F F
0.5341798528656750  0.2748253925649381  0.3206893546539740  T T T
0.4910596352972943  0.5707104424352100  0.2396328222310840  T T T
0.0089368073320335  0.0707129377203531  0.2396322416109238  T T T
0.9658330800500214  0.7748239585806507  0.3206924786254066  T T T
  
```

Co₂N (110) + *OOH

Co N O H

1.0000000000000000

4.5225900000000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 5.1302700000000003 0.0000000000000000
0.0000000000000000 0.0000000000000000 28.2963999999999984

Co N O H

16 8 2 1

Selective dynamics

Direct

0.1762400000000000 0.6618899999999996 0.0112700000000032 F F F
0.1762400000000000 0.3587199999999982 0.0946100000000030 F F F
0.8237600000000000 0.6785100000000028 0.1328499999999977 F F F
0.8237600000000000 0.9816799999999972 0.0495200000000011 F F F
0.6762400000000000 0.4816799999999972 0.0495200000000011 F F F
0.6762400000000000 0.1785100000000028 0.1328499999999977 F F F
0.2695829646028774 0.1539225459224322 0.0175097212968636 T T T
0.3237600000000000 0.8587199999999982 0.0946100000000030 F F F
0.1888138896800081 0.0682025930824495 0.1806792758302969 T T T
0.1962328492895079 0.7596807608810557 0.2700865525191341 T T T
0.7863673543288781 0.0332564268289710 0.2945935454509129 T T T
0.8157775260053596 0.3687130693371350 0.2165423049027483 T T T
0.6943172504207381 0.8653532153745431 0.2144257892512861 T T T
0.6044571222077987 0.5805107360437497 0.3362930109299797 T T T
0.3112267466586867 0.5675065761223574 0.1793704522353816 T T T
0.3391839544220815 0.2778287687448783 0.2659540272060583 T T T
0.5000000000000000 0.8670199999999966 0.1553899999999970 F F F
0.5000000000000000 0.1702000000000012 0.0720600000000005 F F F
0.0000000000000000 0.6702000000000012 0.0720600000000005 F F F
0.0000000000000000 0.3670199999999966 0.1553899999999970 F F F
0.5439273537474505 0.2570802105103279 0.3202614084180309 T T T
0.4932928044750619 0.5719359425199638 0.2372551573788339 T T T
0.0207323088907422 0.0707280315286156 0.2413298621249615 T T T
0.9227568905335921 0.7349432960208375 0.3164484844296857 T T T
0.5965253627684614 0.5485072544949705 0.3992604166780954 T T T
0.5538501686795414 0.8175568377961756 0.4124475408596878 T T T
0.7553157546889244 0.8714526365394648 0.4214181609850406 T T T

Co₂N (110) + *O

Co N O

1.0000000000000000

4.5225900000000001 0.0000000000000000 0.0000000000000000
0.0000000000000000 5.1302700000000003 0.0000000000000000

0.0000000000000000 0.0000000000000000 28.296399999999984

Co N O
16 8 1

Selective dynamics

Direct

0.1762400000000000	0.6618899999999996	0.0112700000000032	F	F	F
0.1762400000000000	0.3587199999999982	0.0946100000000030	F	F	F
0.8237600000000000	0.6785100000000028	0.1328499999999977	F	F	F
0.8237600000000000	0.9816799999999972	0.0495200000000011	F	F	F
0.6762400000000000	0.4816799999999972	0.0495200000000011	F	F	F
0.6762400000000000	0.1785100000000028	0.1328499999999977	F	F	F
0.2691272069956003	0.1540387379490376	0.0175068372628590	T	T	T
0.3237600000000000	0.8587199999999982	0.0946100000000030	F	F	F
0.1916144012649113	0.0709182842167129	0.1810362484549352	T	T	T
0.1711689106841540	0.7534340311061735	0.2606810056002885	T	T	T
0.8338740017257255	0.0413718127260915	0.3002543188114144	T	T	T
0.8048736455377739	0.3660704021665666	0.2148501209635349	T	T	T
0.6846175900517514	0.8668910332955880	0.2160726139973186	T	T	T
0.8425865097651146	0.4626475331020922	0.3471591023694826	T	T	T
0.3120550703201891	0.5680751845931137	0.1786367446037143	T	T	T
0.3361084317768565	0.2775054875513761	0.2676546715304604	T	T	T
0.5000000000000000	0.8670199999999966	0.1553899999999970	F	F	F
0.5000000000000000	0.1702000000000012	0.0720600000000005	F	F	F
0.0000000000000000	0.6702000000000012	0.0720600000000005	F	F	F
0.0000000000000000	0.3670199999999966	0.1553899999999970	F	F	F
0.5791833635951934	0.2806775528377903	0.3168284934987973	T	T	T
0.4886217449141328	0.5676914022749355	0.2377792953022228	T	T	T
0.0056721768270677	0.0736329120684668	0.2409196240011266	T	T	T
0.9545551880139901	0.7180641343041693	0.3131723568451552	T	T	T
0.8778095900217296	0.4696645882043707	0.4034668285952849	T	T	T

Co₂N (110) + *OH

Co N O H

1.0000000000000000		
4.5225900000000001	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.1302700000000003	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.296399999999984

Co N O H
16 8 1 1

Selective dynamics

Direct

0.1762400000000000	0.6618899999999996	0.0112700000000032	F	F	F
--------------------	--------------------	--------------------	---	---	---

0.1762400000000000	0.3587199999999982	0.0946100000000030	F	F	F
0.8237600000000000	0.6785100000000028	0.1328499999999977	F	F	F
0.8237600000000000	0.9816799999999972	0.0495200000000011	F	F	F
0.6762400000000000	0.4816799999999972	0.0495200000000011	F	F	F
0.6762400000000000	0.1785100000000028	0.1328499999999977	F	F	F
0.2690786621477744	0.1539705884966786	0.0175059985565231	T	T	T
0.3237600000000000	0.8587199999999982	0.0946100000000030	F	F	F
0.1927028056263800	0.0713341608502116	0.1812107816814758	T	T	T
0.1731272615008890	0.7565129993722631	0.2614513591549037	T	T	T
0.8174749053393500	0.0389613386423462	0.2983314388231190	T	T	T
0.8044622795803525	0.3641033922906107	0.2152483530193064	T	T	T
0.6872490642524587	0.8628624267811856	0.2157807087684065	T	T	T
0.8563774812636976	0.4594250787457706	0.3463857754662923	T	T	T
0.3114614138257957	0.5683443869475806	0.1786787145864654	T	T	T
0.3400196141017572	0.2790967831308947	0.2687312024606514	T	T	T
0.5000000000000000	0.8670199999999966	0.1553899999999970	F	F	F
0.5000000000000000	0.1702000000000012	0.0720600000000005	F	F	F
0.0000000000000000	0.6702000000000012	0.0720600000000005	F	F	F
0.0000000000000000	0.3670199999999966	0.1553899999999970	F	F	F
0.5784338191331537	0.2850983945062173	0.3182260644464443	T	T	T
0.4871111648236391	0.5663870876698061	0.2376910726092473	T	T	T
0.0088947475245986	0.0742412882940832	0.2407382395471199	T	T	T
0.9421854544427747	0.7179353188462197	0.3123680851479533	T	T	T
0.9830734508533580	0.4094762929991440	0.4045660494031574	T	T	T
0.1837292337455971	0.3469975138141968	0.4102664702112061	T	T	T

Co₃N (110) - Surface

Co N

1.0000000000000000		
4.3237399999999999	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.8388600000000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.1545999999999985

Co N

24 8

Selective dynamics

Direct

0.0000000000000000	0.6628499999999988	0.0416700000000034	F	F	F
0.0000000000000000	0.1628499999999988	0.1250000000000000	F	F	F
0.0000000000000000	0.3371500000000012	0.0416700000000034	F	F	F
0.0000000000000000	0.8371500000000012	0.1250000000000000	F	F	F
0.5000000000000000	0.8371500000000012	0.0126199999999983	F	F	F
0.5000000000000000	0.3371500000000012	0.0959500000000020	F	F	F

0.0000000000000000	0.5000000000000000	0.1230899999999977	F	F	F
0.0000000000000000	0.0000000000000000	0.0397600000000011	F	F	F
0.5000000000000000	0.1628499999999988	0.0126199999999983	F	F	F
0.5000000000000000	0.6628499999999988	0.0959500000000020	F	F	F
0.5000000000000000	0.5000000000000000	0.0145300000000006	F	F	F
0.5000000000000000	0.0000000000000000	0.0978599999999972	F	F	F
0.9936075328320877	0.6619494646645058	0.2074857613077082	T	T	T
0.9828557829534553	0.1627822731834923	0.2889812355561187	T	T	T
0.0063924671679123	0.3380505353354945	0.2074857613077082	T	T	T
0.0171442170465447	0.8372177268165076	0.2889812355561187	T	T	T
0.5006031903773847	0.8368758104890105	0.1794659363353883	T	T	T
0.5050754647799763	0.3403777501021108	0.2654835860954005	T	T	T
0.0000000000000000	0.5000000000000000	0.2888398609682909	T	T	T
0.0000000000000000	-0.0000000000000000	0.2077794853202022	T	T	T
0.4993968096226157	0.1631241895109896	0.1794659363353883	T	T	T
0.4949245352200233	0.6596222498978893	0.2654835860954005	T	T	T
0.5000000000000000	0.5000000000000000	0.1818496849102124	T	T	T
0.5000000000000000	-0.0000000000000000	0.2626914226711384	T	T	T
0.7500000000000000	0.3333299999999966	0.1521400000000028	F	F	F
0.7500000000000000	0.8333299999999966	0.0688099999999991	F	F	F
0.2500000000000000	0.6666700000000034	0.1521400000000028	F	F	F
0.2500000000000000	0.1666700000000034	0.0688099999999991	F	F	F
0.7763643243541954	0.3337559255335522	0.3136467737155938	T	T	T
0.7437342300979194	0.8278101621713015	0.2377152662223739	T	T	T
0.2236356756458045	0.6662440744664478	0.3136467737155938	T	T	T
0.2562657699020808	0.1721898378286983	0.2377152662223739	T	T	T

Co₃N (110) + *OOH

Co N O H

1.0000000000000000		
4.3237399999999999	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.8388600000000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.1545999999999985

Co N O H

24 8 2 1

Selective dynamics

Direct

0.0000000000000000	0.6628499999999988	0.0416700000000034	F	F	F
0.0000000000000000	0.1628499999999988	0.1250000000000000	F	F	F
0.0000000000000000	0.3371500000000012	0.0416700000000034	F	F	F
0.0000000000000000	0.8371500000000012	0.1250000000000000	F	F	F
0.5000000000000000	0.8371500000000012	0.0126199999999983	F	F	F

0.5000000000000000	0.337150000000012	0.095950000000020	F	F	F
0.0000000000000000	0.5000000000000000	0.123089999999977	F	F	F
0.0000000000000000	0.0000000000000000	0.039760000000011	F	F	F
0.5000000000000000	0.162849999999988	0.012619999999983	F	F	F
0.5000000000000000	0.662849999999988	0.095950000000020	F	F	F
0.5000000000000000	0.5000000000000000	0.014530000000006	F	F	F
0.5000000000000000	0.0000000000000000	0.097859999999972	F	F	F
0.0041064525326446	0.6618806893089991	0.2084247665899627	T	T	T
0.9713411792638783	0.1655265610215740	0.2877516718342570	T	T	T
-0.0001003393034808	0.3383106098964976	0.2079020055559008	T	T	T
0.0191398303967603	0.8420147256452080	0.2888805093840336	T	T	T
0.5005005854685100	0.8362421579040961	0.1799432229541702	T	T	T
0.4920658711101087	0.3470994821348793	0.2666084611862661	T	T	T
0.0696060154237560	0.4900062164383002	0.3206936427490947	T	T	T
0.0003613176117724	-0.0003705647861821	0.2071242162813640	T	T	T
0.5005835223408478	0.1635515675653163	0.1801696520524667	T	T	T
0.4971087945522252	0.6598562808104538	0.2677078320121470	T	T	T
0.4999406621927327	0.4999408643701120	0.1817529953693292	T	T	T
0.4994433084930576	0.9988142198336027	0.2609833449877084	T	T	T
0.7500000000000000	0.333329999999966	0.152140000000028	F	F	F
0.7500000000000000	0.833329999999966	0.068809999999991	F	F	F
0.2500000000000000	0.666670000000034	0.152140000000028	F	F	F
0.2500000000000000	0.166670000000034	0.068809999999991	F	F	F
0.7676315130464895	0.3337573196528060	0.3122950664032790	T	T	T
0.7461183950554203	0.8211900460132038	0.2381123160354423	T	T	T
0.2509863903869509	0.6943527429419252	0.3172013761892656	T	T	T
0.2536156790018090	0.1756699788726422	0.2379452443466225	T	T	T
0.1115885011397237	0.4378929694765651	0.3855563656640782	T	T	T
0.3310017599977055	0.5341904256189994	0.4135570609052193	T	T	T
0.5243578724292779	0.4696487868673533	0.4086348769257362	T	T	T

Co₃N (110) + *O

Co N O

1.0000000000000000		
4.323739999999999	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.8388600000000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.154599999999985

Co N O

24 8 1

Selective dynamics

Direct

0.0000000000000000	0.662849999999988	0.041670000000034	F	F	F
--------------------	-------------------	-------------------	---	---	---

0.0000000000000000	0.1628499999999988	0.1250000000000000	F	F	F
0.0000000000000000	0.3371500000000012	0.0416700000000034	F	F	F
0.0000000000000000	0.8371500000000012	0.1250000000000000	F	F	F
0.5000000000000000	0.8371500000000012	0.0126199999999983	F	F	F
0.5000000000000000	0.3371500000000012	0.0959500000000020	F	F	F
0.0000000000000000	0.5000000000000000	0.1230899999999977	F	F	F
0.0000000000000000	0.0000000000000000	0.0397600000000011	F	F	F
0.5000000000000000	0.1628499999999988	0.0126199999999983	F	F	F
0.5000000000000000	0.6628499999999988	0.0959500000000020	F	F	F
0.5000000000000000	0.5000000000000000	0.0145300000000006	F	F	F
0.5000000000000000	0.0000000000000000	0.0978599999999972	F	F	F
-0.0049281764886683	0.6633614784427622	0.2073611125681853	T	T	T
0.9783098478369922	0.1670216892808400	0.2880449177120347	T	T	T
0.0036360529010814	0.3370640089150721	0.2075099647857422	T	T	T
0.0179725636015947	0.8402531905448365	0.2898379867325946	T	T	T
0.4994639038349971	0.8370440072997237	0.1802041123387148	T	T	T
0.5046385853972147	0.3494423869446392	0.2666155926628017	T	T	T
0.1102589559846695	0.4751011148174115	0.3301146950656307	T	T	T
0.0017977204229517	0.9998223661479484	0.2078259772189765	T	T	T
0.5022308409485114	0.1630079052545742	0.1802575930439833	T	T	T
0.4744930337503517	0.6608886054050495	0.2646575000355704	T	T	T
0.4977998000164066	0.4990873714379206	0.1815746916880811	T	T	T
0.5029993287853991	0.0006654789551114	0.2610848345985590	T	T	T
0.7500000000000000	0.3333299999999966	0.1521400000000028	F	F	F
0.7500000000000000	0.8333299999999966	0.0688099999999991	F	F	F
0.2500000000000000	0.6666700000000034	0.1521400000000028	F	F	F
0.2500000000000000	0.1666700000000034	0.0688099999999991	F	F	F
0.7940130481810878	0.3473250501793680	0.3103262103154499	T	T	T
0.7452630908111305	0.8203849615459704	0.2391077073832215	T	T	T
0.2450928418505798	0.6847303530193297	0.3168880242438643	T	T	T
0.2600754759361155	0.1791955369961440	0.2386137106358317	T	T	T
0.2250981892152037	0.4165724911586171	0.3843559114675782	T	T	T

Co₃N (110) + *OH

Co N O H

1.0000000000000000		
4.3237399999999999	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.8388600000000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.1545999999999985

Co N O H

24 8 1 1

Selective dynamics

Direct

0.0000000000000000	0.6628499999999988	0.0416700000000034	F	F	F
0.0000000000000000	0.1628499999999988	0.1250000000000000	F	F	F
0.0000000000000000	0.3371500000000012	0.0416700000000034	F	F	F
0.0000000000000000	0.8371500000000012	0.1250000000000000	F	F	F
0.5000000000000000	0.8371500000000012	0.0126199999999983	F	F	F
0.5000000000000000	0.3371500000000012	0.0959500000000020	F	F	F
0.0000000000000000	0.5000000000000000	0.1230899999999977	F	F	F
0.0000000000000000	0.0000000000000000	0.0397600000000011	F	F	F
0.5000000000000000	0.1628499999999988	0.0126199999999983	F	F	F
0.5000000000000000	0.6628499999999988	0.0959500000000020	F	F	F
0.5000000000000000	0.5000000000000000	0.0145300000000006	F	F	F
0.5000000000000000	0.0000000000000000	0.0978599999999972	F	F	F
0.0060296340381266	0.6616548952128396	0.2085777087044553	T	T	T
0.9747538746926234	0.1650185167971606	0.2877406951987044	T	T	T
0.0017494693535141	0.3381766465898211	0.2077770166391426	T	T	T
0.0225494722009788	0.8417462665354901	0.2890085268462448	T	T	T
0.5019590794922805	0.8360982205424929	0.1800182978686634	T	T	T
0.4965141307104508	0.3482482052055826	0.2659386067088917	T	T	T
0.0683296021612380	0.4920085673464699	0.3206778723923240	T	T	T
0.0028862823671580	-0.0001830421516005	0.2071088671432206	T	T	T
0.5020687070901938	0.1632115832986949	0.1801399255121933	T	T	T
0.5000501276019449	0.6605733301662217	0.2675919015537727	T	T	T
0.5013919809900910	0.5004110846803718	0.1815583789039427	T	T	T
0.5025121786446957	0.9993150141911271	0.2609944293090752	T	T	T
0.7500000000000000	0.3333299999999966	0.1521400000000028	F	F	F
0.7500000000000000	0.8333299999999966	0.0688099999999991	F	F	F
0.2500000000000000	0.6666700000000034	0.1521400000000028	F	F	F
0.2500000000000000	0.1666700000000034	0.0688099999999991	F	F	F
0.7715787912184254	0.3348984635912193	0.3113998089363015	T	T	T
0.7493104671932463	0.8217243234611961	0.2381884053910515	T	T	T
0.2572912972645012	0.6950012374286532	0.3175125542203761	T	T	T
0.2567968550156581	0.1764028612146708	0.2380878745861623	T	T	T
0.1447765496727720	0.4428346224003512	0.3842768822693506	T	T	T
0.3067261963863205	0.5183035926910595	0.3968674202820815	T	T	T

CoN (100) - Surface

Co N

1.0000000000000000		
5.9912599999999996	0.0000000000000000	0.0000000000000000
2.9956300000000002	5.1885833606775549	0.0000000000000000
0.0000000000000000	0.0000000000000000	29.3510999999999989

Co N

16 16

Selective dynamics

Direct

0.0625000000000000	0.3750000000000000	0.0312500000000000	F	F	F
0.2291700000000034	0.0416600000000003	0.1145799999999966	F	F	F
0.3958329488885254	0.2083324705890763	0.1978594754853196	T	T	T
0.0625012131539842	0.3749986758322464	0.2835984559653617	T	T	T
0.0625000000000000	0.8750000000000000	0.0312500000000000	F	F	F
0.2291700000000034	0.5416600000000003	0.1145799999999966	F	F	F
0.3958317514457508	0.7083369012203634	0.1978599888729220	T	T	T
0.0624996284094849	0.8750015698170077	0.2835988906923768	T	T	T
0.5625000000000000	0.3750000000000000	0.0312500000000000	F	F	F
0.7291700000000034	0.0416600000000003	0.1145799999999966	F	F	F
0.8958329488885255	0.2083324705890763	0.1978594754853196	T	T	T
0.5625012131539843	0.3749986758322464	0.2835984559653617	T	T	T
0.5625000000000000	0.8750000000000000	0.0312500000000000	F	F	F
0.7291700000000034	0.5416600000000003	0.1145799999999966	F	F	F
0.8958317514457508	0.7083369012203634	0.1978599888729220	T	T	T
0.5624996284094850	0.8750015698170077	0.2835988906923768	T	T	T
0.2291700000000034	0.0416600000000003	0.0520799999999966	F	F	F
0.3958299999999966	0.2083299999999966	0.1354200000000034	F	F	F
0.0624965575386414	0.3750055620693777	0.2206018743607968	T	T	T
0.2291632806983572	0.0416733793417275	0.3015466230879810	T	T	T
0.2291700000000034	0.5416600000000003	0.0520799999999966	F	F	F
0.3958299999999966	0.7083399999999997	0.1354200000000034	F	F	F
0.0625015180656473	0.8749969356330251	0.2206025450767849	T	T	T
0.2291706388403280	0.5416589108357960	0.3015482586333095	T	T	T
0.7291700000000034	0.0416600000000003	0.0520799999999966	F	F	F
0.8958299999999966	0.2083299999999966	0.1354200000000034	F	F	F
0.5624965575386413	0.3750055620693777	0.2206018743607968	T	T	T
0.7291632806983500	0.0416733793417275	0.3015466230879810	T	T	T
0.7291700000000034	0.5416600000000003	0.0520799999999966	F	F	F
0.8958300000000037	0.7083399999999997	0.1354200000000034	F	F	F
0.5625015180656473	0.8749969356330251	0.2206025450767849	T	T	T
0.7291706388403210	0.5416589108357960	0.3015482586333095	T	T	T

CoN (100) + *OOH

Co N O H

1.0000000000000000

5.9912599999999996 0.0000000000000000 0.0000000000000000

2.9956300000000002 5.1885833606775549 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.3510999999999989

Co N O H

16 16 2 1

Selective dynamics

Direct

0.0625000000000000	0.3750000000000000	0.0312500000000000	F F F
0.22917000000000034	0.04166000000000003	0.11457999999999966	F F F
0.3922020481237577	0.2068506124773554	0.1969969150815920	T T T
0.0526734121270851	0.3854124418052444	0.2833642790053743	T T T
0.0625000000000000	0.8750000000000000	0.0312500000000000	F F F
0.22917000000000034	0.54166000000000003	0.11457999999999966	F F F
0.4010611496240545	0.7050858031815647	0.1989301299882417	T T T
0.0646526988180354	0.8793798765007438	0.280966685226217	T T T
0.5625000000000000	0.3750000000000000	0.0312500000000000	F F F
0.72917000000000034	0.04166000000000003	0.11457999999999966	F F F
0.8909030299706123	0.2152511245447182	0.1989382851241947	T T T
0.5706690529326330	0.3853397565274926	0.2819762877197093	T T T
0.5625000000000000	0.8750000000000000	0.0312500000000000	F F F
0.72917000000000034	0.54166000000000003	0.11457999999999966	F F F
0.8924747302601548	0.7066548092338786	0.1985231819596416	T T T
0.5704660771547264	0.8676604091659643	0.2832492786577085	T T T
0.22917000000000034	0.04166000000000003	0.05207999999999966	F F F
0.39582999999999966	0.20832999999999966	0.13542000000000034	F F F
0.0638685479962192	0.3745255112679730	0.2206815381941369	T T T
0.2378975750105647	0.0527678198756720	0.2974652044778839	T T T
0.22917000000000034	0.54166000000000003	0.05207999999999966	F F F
0.39582999999999966	0.70833999999999997	0.13542000000000034	F F F
0.0620159319430702	0.8763715466083023	0.2185559625258862	T T T
0.2349114216670903	0.5364972881269239	0.2975749829564310	T T T
0.72917000000000034	0.04166000000000003	0.05207999999999966	F F F
0.89582999999999966	0.20832999999999966	0.13542000000000034	F F F
0.5570498571530558	0.3714652999316601	0.2203033052444281	T T T
0.7216898734146914	0.0496471895901225	0.2975619905954255	T T T
0.72917000000000034	0.54166000000000003	0.05207999999999966	F F F
0.89583000000000037	0.70833999999999997	0.13542000000000034	F F F
0.5599945072014026	0.8785127638197584	0.2206096662505992	T T T
0.7327520883753939	0.5477516362330889	0.3180467335483049	T T T
0.7175291805257119	0.5351890055054059	0.3599417918454416	T T T
0.8659205263272517	0.6927111070794335	0.3908841986412995	T T T
0.8044160698886470	0.6686246522480261	0.4204369018366380	T T T

CoN (100) + *O

Co N O

1.0000000000000000

5.991259999999996 0.000000000000000 0.000000000000000
2.9956300000000002 5.188583360677549 0.000000000000000
0.0000000000000000 0.000000000000000 29.351099999999989

Co N O

16 16 1

Selective dynamics

Direct

0.0625000000000000	0.3750000000000000	0.0312500000000000	F	F	F
0.2291700000000034	0.0416600000000003	0.1145799999999966	F	F	F
0.3980728234810614	0.2096281594345961	0.1975578173990670	T	T	T
0.0637371338312782	0.3779275663946539	0.2827461086690782	T	T	T
0.0625000000000000	0.8750000000000000	0.0312500000000000	F	F	F
0.2291700000000034	0.5416600000000003	0.1145799999999966	F	F	F
0.4023341830765143	0.7073818339632491	0.1985972476033698	T	T	T
0.0659724981265316	0.8769196232745970	0.2817674365790499	T	T	T
0.5625000000000000	0.3750000000000000	0.0312500000000000	F	F	F
0.7291700000000034	0.0416600000000003	0.1145799999999966	F	F	F
0.8958666355246828	0.2138723985813598	0.1985990144134462	T	T	T
0.5672160247809057	0.3780636361008166	0.2827580744130507	T	T	T
0.5625000000000000	0.8750000000000000	0.0312500000000000	F	F	F
0.7291700000000034	0.5416600000000003	0.1145799999999966	F	F	F
0.8959461953412007	0.7073749977027735	0.1985901401787441	T	T	T
0.5669981193879033	0.8746754522816194	0.2827475070289751	T	T	T
0.2291700000000034	0.0416600000000003	0.0520799999999966	F	F	F
0.3958299999999966	0.2083299999999966	0.1354200000000034	F	F	F
0.0667322472362013	0.3753487500932968	0.2202357001755790	T	T	T
0.2353641574111821	0.0463333980344138	0.2998220917003594	T	T	T
0.2291700000000034	0.5416600000000003	0.0520799999999966	F	F	F
0.3958299999999966	0.7083399999999997	0.1354200000000034	F	F	F
0.0649080189567582	0.8763467574222941	0.2190807834756231	T	T	T
0.2354419519728984	0.5379733100574170	0.2997335088974835	T	T	T
0.7291700000000034	0.0416600000000003	0.0520799999999966	F	F	F
0.8958299999999966	0.2083299999999966	0.1354200000000034	F	F	F
0.5639551424670671	0.3753645864931030	0.2202729425238914	T	T	T
0.7269859691082422	0.0463946773597235	0.2997704513162534	T	T	T
0.7291700000000034	0.5416600000000003	0.0520799999999966	F	F	F
0.8958300000000037	0.7083399999999997	0.1354200000000034	F	F	F
0.5639338442714683	0.8781923169456860	0.2202419969589720	T	T	T
0.7329701667414493	0.5438288723371369	0.3139958482755006	T	T	T
0.7332292151962155	0.5441063411818248	0.3557987948639795	T	T	T

CoN (100) + *OH

Co N O H

1.0000000000000000

5.9912599999999996 0.0000000000000000 0.0000000000000000

2.9956300000000002 5.1885833606775549 0.0000000000000000

0.0000000000000000 0.0000000000000000 29.3510999999999989

Co N O H

16 16 1 1

Selective dynamics

Direct

0.0625000000000000 0.3750000000000000 0.0312500000000000 F F F

0.2291700000000034 0.0416600000000003 0.1145799999999966 F F F

0.3979436939672130 0.2084989700975169 0.1993267721583549 T T T

0.0916836035274513 0.3599111422015733 0.2818598276194994 T T T

0.0625000000000000 0.8750000000000000 0.0312500000000000 F F F

0.2291700000000034 0.5416600000000003 0.1145799999999966 F F F

0.4010539648463100 0.7050305046614180 0.1978597803252826 T T T

0.0639918373974718 0.8738220489235085 0.2831736832558495 T T T

0.5625000000000000 0.3750000000000000 0.0312500000000000 F F F

0.7291700000000034 0.0416600000000003 0.1145799999999966 F F F

0.8933830540750569 0.2124166711411653 0.1978370319824089 T T T

0.5501398529066308 0.3612206800022209 0.2829433906680472 T T T

0.5625000000000000 0.8750000000000000 0.0312500000000000 F F F

0.7291700000000034 0.5416600000000003 0.1145799999999966 F F F

0.8951158737078870 0.7069480141733829 0.1977486266729846 T T T

0.5502599863056625 0.9010715837659679 0.2820567903250462 T T T

0.2291700000000034 0.0416600000000003 0.0520799999999966 F F F

0.3958299999999966 0.2083299999999966 0.1354200000000034 F F F

0.0620112570012302 0.3754691243302474 0.2198635316110557 T T T

0.2283166216304280 0.0385073187728355 0.3028079256302633 T T T

0.2291700000000034 0.5416600000000003 0.0520799999999966 F F F

0.3958299999999966 0.7083399999999997 0.1354200000000034 F F F

0.0640649611525719 0.8752586866019915 0.2193004398782747 T T T

0.2271587123851823 0.5449239851388706 0.3037202488160471 T T T

0.7291700000000034 0.0416600000000003 0.0520799999999966 F F F

0.8958299999999966 0.2083299999999966 0.1354200000000034 F F F

0.5643305934128334 0.3758731427827077 0.2207309951614599 T T T

0.7347397259644395 0.0380801356774946 0.3034390180545057 T T T

0.7291700000000034 0.5416600000000003 0.0520799999999966 F F F

0.8958300000000037 0.7083399999999997 0.1354200000000034 F F F

0.5644062258332441 0.8728358887719168 0.2200654477817889 T T T

0.7324678688072912 0.5410457149932977 0.3022387999615345 T T T

0.7314326797583974 0.5394933742948230 0.3504810261615095 T T T

0.8342137140984837 0.6189886619043793 0.3596697896099253 T T T

ReN₂ (110) - Surface

Re N

1.0000000000000000
9.5357500000000002 0.0000000000000000 0.0000000000000000
0.0000000000000000 5.0288700000000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 28.1466999999999992

Re N

16 32

Selective dynamics

Direct

0.3913599999999988	0.9949999999999974	0.1482699999999966	F	F	F
0.3913599999999988	0.3148499999999999	0.0649400000000000	F	F	F
0.8913599999999988	0.8402099999999990	0.0067900000000023	F	F	F
0.8913599999999988	0.5203599999999966	0.0901199999999989	F	F	F
0.6086400000000012	0.3402099999999990	0.0067900000000023	F	F	F
0.6086400000000012	0.0203599999999966	0.0901199999999989	F	F	F
0.1086400000000012	0.4949999999999974	0.1482699999999966	F	F	F
0.1086400000000012	0.8148499999999999	0.0649400000000000	F	F	F
0.3779247282523819	0.3429204041731813	0.3124337782787390	T	T	T
0.3987270371120062	0.6341397744196324	0.2348338686166088	T	T	T
0.8913211015547602	0.2021041058317532	0.1709482628095874	T	T	T
0.8873249037943943	0.8256375150099177	0.2635999808885629	T	T	T
0.6097387756446675	0.7020693503432337	0.1704804094026810	T	T	T
0.6105189047697778	0.3284131856404612	0.2638843291537446	T	T	T
0.1129151383355576	0.8397722193997392	0.3143490947790991	T	T	T
0.1023846099238402	0.1310807656134352	0.2357581516331657	T	T	T
0.3263999999999996	0.7173700000000025	0.0529999999999973	F	F	F
0.3263999999999996	0.3975200000000001	0.1363300000000010	F	F	F
0.8263999999999996	0.4376900000000035	0.0187299999999979	F	F	F
0.8263999999999996	0.1178400000000011	0.1020600000000016	F	F	F
0.6736000000000004	0.6178400000000011	0.1020600000000016	F	F	F
0.6736000000000004	0.9376900000000035	0.0187299999999979	F	F	F
0.1736000000000004	0.8975200000000001	0.1363300000000010	F	F	F
0.1736000000000004	0.2173700000000025	0.0529999999999973	F	F	F
0.4049499999999995	0.5897300000000030	0.1598800000000011	F	F	F
0.4049499999999995	0.9095799999999983	0.0765499999999975	F	F	F
0.9049499999999995	0.6057800000000029	0.1618500000000012	F	F	F
0.9049499999999995	0.9256299999999982	0.0785100000000014	F	F	F
0.5950500000000005	0.1057800000000029	0.1618500000000012	F	F	F
0.5950500000000005	0.4256299999999982	0.0785100000000014	F	F	F
0.0982411504415803	0.0884553253913684	0.1616577458285578	T	T	T

0.0950500000000005	0.4095799999999983	0.0765499999999975	F	F	F
0.3279060603023116	0.0360595802054665	0.2211213548387357	T	T	T
0.3682253609601452	0.7475351952743167	0.3048297171580606	T	T	T
0.8284756638969930	0.7999563230831016	0.1859808134668909	T	T	T
0.8244276515364475	0.4418259671219348	0.2662893423838604	T	T	T
0.6771076629694404	0.9372403319655725	0.2663222629246319	T	T	T
0.6726484418514548	0.2993780734733161	0.1854912127561104	T	T	T
0.1500253275113676	0.2394595419276359	0.3046080066178877	T	T	T
0.1725485872832490	0.5346136750084797	0.2214075223292795	T	T	T
0.3456355214513410	0.9347577399017543	0.3340942582821333	T	T	T
0.4051391714807107	0.2275470000749607	0.2452425982214927	T	T	T
0.9295936022553503	0.8727801197512556	0.3324488985396078	T	T	T
0.8983315787223843	0.2404675752901849	0.2462362536690938	T	T	T
0.5706106698457759	0.3580091222517604	0.3305737762421984	T	T	T
0.6038285117700992	0.7384539630612376	0.2456049301433849	T	T	T
0.1663032540459924	0.4457555551080692	0.3329325582536439	T	T	T
0.0949019428241314	0.7239448297688005	0.2461591583788810	T	T	T

ReN₂ (110) + *OOH

Re N O H

1.0000000000000000		
9.5357500000000002	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.0288700000000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.146699999999992

Re N O H

16 32 2 1

Selective dynamics

Direct

0.3913599999999988	0.9949999999999974	0.1482699999999966	F	F	F
0.3913599999999988	0.3148499999999999	0.0649400000000000	F	F	F
0.8913599999999988	0.8402099999999990	0.0067900000000023	F	F	F
0.8913599999999988	0.5203599999999966	0.0901199999999989	F	F	F
0.6086400000000012	0.3402099999999990	0.0067900000000023	F	F	F
0.6086400000000012	0.0203599999999966	0.0901199999999989	F	F	F
0.1086400000000012	0.4949999999999974	0.1482699999999966	F	F	F
0.1086400000000012	0.8148499999999999	0.0649400000000000	F	F	F
0.3903285604949228	0.3109478014692605	0.3122048190298199	T	T	T
0.3948145359231364	0.6316844966220472	0.2349891354582536	T	T	T
0.8908430034772539	0.2024320227984007	0.1711393629642062	T	T	T
0.8913438131199738	0.8407886792350117	0.2634286106655707	T	T	T
0.6087807865005409	0.7024034000082107	0.1707148765004848	T	T	T
0.6109430651867898	0.3351812872447925	0.2634986778156554	T	T	T

0.1111235855415995	0.8612895563019891	0.3171574734619435	T	T	T
0.1026469536491857	0.1434549282589114	0.2350193952248412	T	T	T
0.3263999999999996	0.7173700000000025	0.0529999999999973	F	F	F
0.3263999999999996	0.3975200000000001	0.1363300000000010	F	F	F
0.8263999999999996	0.4376900000000035	0.0187299999999979	F	F	F
0.8263999999999996	0.1178400000000011	0.1020600000000016	F	F	F
0.6736000000000004	0.6178400000000011	0.1020600000000016	F	F	F
0.6736000000000004	0.9376900000000035	0.0187299999999979	F	F	F
0.1704039845040551	0.8954045278385815	0.1377176486446166	T	T	T
0.1736000000000004	0.2173700000000025	0.0529999999999973	F	F	F
0.4049499999999995	0.5897300000000030	0.1598800000000011	F	F	F
0.4049499999999995	0.9095799999999983	0.0765499999999975	F	F	F
0.9049499999999995	0.6057800000000029	0.1618500000000012	F	F	F
0.9049499999999995	0.9256299999999982	0.0785100000000014	F	F	F
0.5950500000000005	0.1057800000000029	0.1618500000000012	F	F	F
0.5950500000000005	0.4256299999999982	0.0785100000000014	F	F	F
0.0950500000000005	0.0897300000000030	0.1598800000000011	F	F	F
0.0950500000000005	0.4095799999999983	0.0765499999999975	F	F	F
0.3273357520795273	0.0352950493129279	0.2202648841965419	T	T	T
0.3333256402641221	0.7193206073425040	0.3077682886290009	T	T	T
0.8269441801146434	0.8001066451164348	0.1849038816779430	T	T	T
0.8253096861394634	0.4530162819512702	0.2660827095980162	T	T	T
0.6748243580453228	0.9490464108317945	0.2654332693366884	T	T	T
0.6722846969625675	0.3007627313323754	0.1850824024542718	T	T	T
0.1466534956833016	0.2571150919432635	0.3075823336575997	T	T	T
0.1707426214486936	0.5462948708049118	0.2213893868687128	T	T	T
0.3676450331976943	0.9440889640679768	0.3275245826949759	T	T	T
0.4063158781590854	0.2242987197215069	0.2441525885068418	T	T	T
0.9151386141518962	0.8879701934109208	0.3302456312645307	T	T	T
0.8988798999763673	0.2537399428151647	0.2459734591032181	T	T	T
0.5772945598833720	0.3841335008466599	0.3306240924485728	T	T	T
0.5988826885567563	0.7500586931221269	0.2461667578321682	T	T	T
0.0783769484231125	0.4453893044476875	0.3343805797249272	T	T	T
0.0949290941122478	0.7371516028254701	0.2463965836585489	T	T	T
0.0066132203596357	0.3735187050553186	0.3680404009535181	T	T	T
0.1491686639612201	0.8746528341585040	0.3856526568818970	T	T	T
0.0624927876856809	0.8674287321198229	0.4040792174989957	T	T	T

ReN₂ (110) + *O

Re N O

1.0000000000000000

9.5357500000000002 0.0000000000000000 0.0000000000000000

0.0000000000000000 5.0288700000000004 0.0000000000000000
0.0000000000000000 0.0000000000000000 28.1466999999999992

Re N O
16 32 1

Selective dynamics

Direct

0.39135999999999988	0.99499999999999974	0.14826999999999966	F	F	F
0.39135999999999988	0.31484999999999999	0.06494000000000000	F	F	F
0.89135999999999988	0.84020999999999990	0.00679000000000023	F	F	F
0.89135999999999988	0.52035999999999966	0.09011999999999989	F	F	F
0.60864000000000012	0.34020999999999990	0.00679000000000023	F	F	F
0.60864000000000012	0.02035999999999966	0.09011999999999989	F	F	F
0.10864000000000012	0.49499999999999974	0.14826999999999966	F	F	F
0.10864000000000012	0.81484999999999999	0.06494000000000000	F	F	F
0.3875668476283004	0.3147801450375483	0.3120407499546771	T	T	T
0.3986056686388846	0.6233940064902848	0.2347767618751641	T	T	T
0.8912115829070196	0.2018805164840667	0.1713429899658439	T	T	T
0.8916179138489425	0.8432070198883360	0.2648407461158352	T	T	T
0.6096373802137300	0.7016485888571241	0.1709108243844668	T	T	T
0.6128867888277139	0.3248534851293932	0.2645345407485211	T	T	T
0.1222080014907163	0.8329634288441912	0.3152064018580347	T	T	T
0.1027578933603817	0.1397065960940634	0.2357787107403510	T	T	T
0.32639999999999996	0.71737000000000025	0.05299999999999973	F	F	F
0.32639999999999996	0.39752000000000001	0.13633000000000010	F	F	F
0.82639999999999996	0.43769000000000035	0.01872999999999979	F	F	F
0.82639999999999996	0.11784000000000011	0.10206000000000016	F	F	F
0.67360000000000004	0.61784000000000011	0.10206000000000016	F	F	F
0.67360000000000004	0.93769000000000035	0.01872999999999979	F	F	F
0.1708454540146606	0.8953666740409231	0.1379127265056733	T	T	T
0.17360000000000004	0.21737000000000025	0.05299999999999973	F	F	F
0.40494999999999995	0.58973000000000030	0.15988000000000011	F	F	F
0.40494999999999995	0.90957999999999983	0.07654999999999975	F	F	F
0.90494999999999995	0.60578000000000029	0.16185000000000012	F	F	F
0.90494999999999995	0.92562999999999982	0.07851000000000014	F	F	F
0.59505000000000005	0.10578000000000029	0.16185000000000012	F	F	F
0.59505000000000005	0.42562999999999982	0.07851000000000014	F	F	F
0.09505000000000005	0.08973000000000030	0.15988000000000011	F	F	F
0.09505000000000005	0.40957999999999983	0.07654999999999975	F	F	F
0.3286423071473916	0.0266222700276177	0.2205776761836161	T	T	T
0.3409937822163535	0.7076704156268376	0.3037415677059340	T	T	T
0.8279969007966999	0.8001356023689935	0.1848863015949915	T	T	T
0.8244843615746099	0.4490901394760478	0.2673944180698617	T	T	T
0.6755442683516726	0.9435080625359755	0.2657330790235162	T	T	T
0.6723113854771261	0.2997266178310151	0.1856817171860228	T	T	T

0.1524674285154160	0.2572478643140741	0.3051766506143725	T	T	T
0.1712854507644221	0.5432916999914589	0.2211686855806645	T	T	T
0.3346937161484557	0.9280490256564832	0.3294554027233192	T	T	T
0.4083685739437857	0.2159366057600266	0.2442547680713808	T	T	T
0.9234763453451179	0.8865946463034952	0.3298928670160595	T	T	T
0.8996699625617673	0.2540255775222006	0.2466084893366443	T	T	T
0.5720782182131601	0.3664475093204062	0.3325730510530338	T	T	T
0.6017839782897226	0.7401284540259516	0.2463481403269283	T	T	T
0.0763085258765181	0.4310245727216532	0.3306603643376805	T	T	T
0.0959117453660205	0.7353256528825415	0.2464265477909518	T	T	T
0.1552532527284073	0.5379609136281372	0.3670761185806236	T	T	T

ReN₂ (110) + *OH

Re N O H

1.0000000000000000		
9.5357500000000002	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.0288700000000004	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.146699999999992

Re N O H

16 32 1 1

Selective dynamics

Direct

0.3913599999999988	0.9949999999999974	0.1482699999999966	F	F	F
0.3913599999999988	0.3148499999999999	0.0649400000000000	F	F	F
0.8913599999999988	0.8402099999999990	0.0067900000000023	F	F	F
0.8913599999999988	0.5203599999999966	0.0901199999999989	F	F	F
0.6086400000000012	0.3402099999999990	0.0067900000000023	F	F	F
0.6086400000000012	0.0203599999999966	0.0901199999999989	F	F	F
0.1086400000000012	0.4949999999999974	0.1482699999999966	F	F	F
0.1086400000000012	0.8148499999999999	0.0649400000000000	F	F	F
0.3998593724523081	0.3024170179200893	0.3135499977537446	T	T	T
0.3945465484717516	0.6357322587221581	0.2355217679994939	T	T	T
0.8915840914065665	0.2027319052295911	0.1711565620995013	T	T	T
0.8848290341964422	0.8448996136424669	0.2613135429369841	T	T	T
0.6081192508433021	0.7022487793630687	0.1705137865857996	T	T	T
0.6133318920077218	0.3463501269155332	0.2626367200912976	T	T	T
0.0965903179299204	0.8297365497115152	0.3126368744372765	T	T	T
0.1050990002843991	0.1380756325816220	0.2362816948876258	T	T	T
0.3263999999999996	0.7173700000000025	0.0529999999999973	F	F	F
0.3263999999999996	0.3975200000000001	0.1363300000000010	F	F	F
0.8263999999999996	0.4376900000000035	0.0187299999999979	F	F	F
0.8263999999999996	0.1178400000000011	0.1020600000000016	F	F	F

0.6736000000000004	0.6178400000000011	0.1020600000000016	F	F	F
0.6736000000000004	0.9376900000000035	0.0187299999999979	F	F	F
0.1708212597175985	0.8947612065956013	0.1381144120719104	T	T	T
0.1736000000000004	0.2173700000000025	0.0529999999999973	F	F	F
0.4049499999999995	0.5897300000000030	0.1598800000000011	F	F	F
0.4049499999999995	0.9095799999999983	0.0765499999999975	F	F	F
0.9049499999999995	0.6057800000000029	0.1618500000000012	F	F	F
0.9049499999999995	0.9256299999999982	0.0785100000000014	F	F	F
0.5950500000000005	0.1057800000000029	0.1618500000000012	F	F	F
0.5950500000000005	0.4256299999999982	0.0785100000000014	F	F	F
0.0950500000000005	0.0897300000000030	0.1598800000000011	F	F	F
0.0950500000000005	0.4095799999999983	0.0765499999999975	F	F	F
0.3278477332473942	0.0396345944597940	0.2209378960386864	T	T	T
0.3338170193126044	0.7260690065951002	0.3105638355130287	T	T	T
0.8267217770734366	0.8008517108644656	0.1847289310675148	T	T	T
0.8264740110702135	0.4614899647533086	0.2650957195825042	T	T	T
0.6740701012086442	0.9548297461014138	0.2651560028107110	T	T	T
0.6733056252483387	0.3007593737671977	0.1843127967573527	T	T	T
0.1663801100052421	0.2365007550978396	0.3095241801983189	T	T	T
0.1717673804743339	0.5380896634566470	0.2210935012478036	T	T	T
0.3905688139152199	0.9458460072779377	0.3276636586518197	T	T	T
0.4076665956675380	0.2288512321470743	0.2446619141948182	T	T	T
0.9111472752772307	0.9042765188339035	0.3293122433524762	T	T	T
0.9013737904419350	0.2617114907800460	0.2457556557413520	T	T	T
0.5908015695761082	0.3995376379360047	0.3287802568950389	T	T	T
0.5982797839813502	0.7579373593761908	0.2457170807026245	T	T	T
0.0887920332817544	0.4401475642975928	0.3280908405968783	T	T	T
0.0913808886473277	0.7305376000497454	0.2441499410580525	T	T	T
0.1295550031734876	0.5231553753980417	0.3772423271915735	T	T	T
0.2342563619891198	0.5103022459926139	0.3775587072687872	T	T	T

ReN₂ (100) - Surface

Re N

1.0000000000000000		
3.6890100000000001	0.0000000000000000	0.0000000000000000
0.5760683759820097	5.7184370321437870	0.0000000000000000
0.0000000000000000	0.0000000000000000	31.1944000000000017

Re N

8 16

Selective dynamics

Direct

0.2131200000000035	0.7777299999999983	0.0386299999999977	F	F	F
--------------------	--------------------	--------------------	---	---	---

0.616999999999973	0.233199999999965	0.009509999999988	F	F	F
0.919100000000003	0.796649999999996	0.121969999999975	F	F	F
0.322969999999980	0.252110000000018	0.092849999999985	F	F	F
0.6207282129553875	0.8171167160285093	0.2054171499885287	T	T	T
0.0281657429345899	0.2700029551515175	0.1763376370339614	T	T	T
0.3064345371346194	0.8381566180521710	0.2886277937575879	T	T	T
0.7199580003062069	0.2856907802097500	0.2628452175247672	T	T	T
0.7018750934457765	0.8841296739447463	0.0141329256172098	T	T	T
0.131560000000003	0.142940000000030	0.034649999999992	F	F	F
0.602679999999994	0.484420000000001	0.057659999999985	F	F	F
0.933419999999981	0.545430000000032	0.073819999999978	F	F	F
0.404539999999972	0.886910000000003	0.096829999999971	F	F	F
0.837530000000010	0.161859999999972	0.117980000000029	F	F	F
0.308650000000001	0.503329999999983	0.140999999999982	F	F	F
0.639389999999988	0.564349999999975	0.157150000000015	F	F	F
0.1046825920575910	0.9021376859371317	0.1812413765397526	T	T	T
0.5428810723538408	0.1840639950950401	0.2009682820144004	T	T	T
0.0040496692307065	0.5199875123089758	0.2254317440548591	T	T	T
0.3337295196607157	0.5818940810389419	0.2421030477659352	T	T	T
0.8061651799745798	0.9252445376267977	0.2625798856681270	T	T	T
0.2424643869171555	0.1895698086268543	0.2828082931858699	T	T	T
0.7158884382921356	0.5545132992254156	0.3102451303135826	T	T	T
-0.0150920761160732	0.6558094138219490	0.3207122865742306	T	T	T

ReN₂ (100) + *OOH

Re N O H

1.000000000000000			
3.689010000000001	0.000000000000000	0.000000000000000	
0.5760683759820097	5.7184370321437870	0.000000000000000	
0.000000000000000	0.000000000000000	31.194400000000017	

Re N O H

8 16 2 1

Selective dynamics

Direct

0.213120000000035	0.777729999999983	0.038629999999977	F	F	F
0.616999999999973	0.233199999999965	0.009509999999988	F	F	F
0.919100000000003	0.796649999999996	0.121969999999975	F	F	F
0.322969999999980	0.252110000000018	0.092849999999985	F	F	F
0.6218214963448626	0.8162649496358347	0.2049048998713242	T	T	T
0.0253453523580539	0.2728623479111080	0.1767867952104470	T	T	T
0.3285240077268849	0.8684041915518126	0.2865475731440794	T	T	T
0.7135110136886410	0.2871729892102804	0.2607239831087226	T	T	T

0.6985600000000005	0.8679899999999989	0.0135000000000005	F	F	F
0.1315600000000003	0.1429400000000030	0.0346499999999992	F	F	F
0.6026799999999994	0.4844200000000001	0.0576599999999985	F	F	F
0.9334199999999981	0.5454300000000032	0.0738199999999978	F	F	F
0.4045399999999972	0.8869100000000003	0.0968299999999971	F	F	F
0.8375300000000010	0.1618599999999972	0.1179800000000029	F	F	F
0.3086500000000001	0.5033299999999983	0.1409999999999982	F	F	F
0.6393899999999988	0.5643499999999975	0.1571500000000015	F	F	F
0.1044284481185767	0.9035840835811676	0.1808739773985784	T	T	T
0.5409484302244641	0.1850931699353654	0.2010566987507675	T	T	T
0.0047845064551540	0.5251349129318538	0.2267393686411101	T	T	T
0.3347099995441348	0.5876514095658367	0.2439923024085149	T	T	T
0.8090677514390933	0.9286788332324306	0.2615597163860062	T	T	T
0.2280839490309932	0.2025492363258521	0.2832367289115693	T	T	T
0.7140266154138382	0.6644858622608356	0.3225914548833416	T	T	T
-0.0062391126597465	0.7635180843903023	0.3393543963749508	T	T	T
0.6963814482033783	0.4418298314173206	0.3302819856927169	T	T	T
0.1372230312694901	0.6466254466751992	0.3750994563929075	T	T	T
0.0585211648975094	0.4865518177769930	0.3718620715611442	T	T	T

ReN₂ (100) + *O

Re N O

1.0000000000000000

3.6890100000000001 0.0000000000000000 0.0000000000000000

0.5760683759820097 5.7184370321437870 0.0000000000000000

0.0000000000000000 0.0000000000000000 31.1944000000000017

Re N O

8 16 1

Selective dynamics

Direct

0.2131200000000035	0.7777299999999983	0.0386299999999977	F	F	F
0.6169999999999973	0.2331999999999965	0.0095099999999988	F	F	F
0.9191000000000003	0.7966499999999996	0.1219699999999975	F	F	F
0.3229699999999980	0.2521100000000018	0.0928499999999985	F	F	F
0.6215867100548180	0.8162147471646610	0.2047503797679312	T	T	T
0.0244786468666147	0.2723706515620913	0.1767604632642359	T	T	T
0.3239721140222902	0.8681859747798203	0.2885215610150823	T	T	T
0.7217387740441704	0.2847186591871763	0.2612282167450146	T	T	T
0.6985600000000005	0.8679899999999989	0.0135000000000005	F	F	F
0.1315600000000003	0.1429400000000030	0.0346499999999992	F	F	F
0.6026799999999994	0.4844200000000001	0.0576599999999985	F	F	F
0.9334199999999981	0.5454300000000032	0.0738199999999978	F	F	F

0.4045399999999972	0.8869100000000003	0.0968299999999971	F	F	F
0.8375300000000010	0.1618599999999972	0.1179800000000029	F	F	F
0.3086500000000001	0.5033299999999983	0.1409999999999982	F	F	F
0.6393899999999988	0.5643499999999975	0.1571500000000015	F	F	F
0.1033544268241163	0.9026826727463945	0.1810171393954693	T	T	T
0.5387748059280750	0.1847153631261071	0.2009620528668367	T	T	T
0.0101203094098646	0.5232389293819530	0.2272229209432411	T	T	T
0.3438002727016932	0.5850112393405561	0.2440722988613080	T	T	T
0.8130168210504648	0.9297348469087084	0.2602813858364435	T	T	T
0.2304870463902696	0.1997537632381247	0.2832097350919961	T	T	T
0.7180015545713898	0.6690438857302771	0.3218944149859458	T	T	T
0.0138180482885943	0.7455998210668672	0.3316983943944709	T	T	T
0.6968497136807680	0.4386467619547831	0.3248762962172579	T	T	T

ReN₂ (100) + *OH

Re N O H

1.0000000000000000					
3.6890100000000001	0.0000000000000000	0.0000000000000000			
0.5760683759820097	5.7184370321437870	0.0000000000000000			
0.0000000000000000	0.0000000000000000	31.1944000000000017			

Re N O H

8 16 1 1

Selective dynamics

Direct

0.2131200000000035	0.7777299999999983	0.0386299999999977	F	F	F
0.6169999999999973	0.2331999999999965	0.0095099999999988	F	F	F
0.9191000000000003	0.7966499999999996	0.1219699999999975	F	F	F
0.3229699999999980	0.2521100000000018	0.0928499999999985	F	F	F
0.6212123415363787	0.8151246983031359	0.2050620548611697	T	T	T
0.0278621114640001	0.2717963995883196	0.1762056374705980	T	T	T
0.3082421524656795	0.8600259300513524	0.2892175737326454	T	T	T
0.7083798642297430	0.2832790792778055	0.2604837817163280	T	T	T
0.6985600000000005	0.8679899999999989	0.0135000000000005	F	F	F
0.1315600000000003	0.1429400000000030	0.0346499999999992	F	F	F
0.6026799999999994	0.4844200000000001	0.0576599999999985	F	F	F
0.9334199999999981	0.5454300000000032	0.0738199999999978	F	F	F
0.4045399999999972	0.8869100000000003	0.0968299999999971	F	F	F
0.8375300000000010	0.1618599999999972	0.1179800000000029	F	F	F
0.3086500000000001	0.5033299999999983	0.1409999999999982	F	F	F
0.6393899999999988	0.5643499999999975	0.1571500000000015	F	F	F
0.1050131084864591	0.9025238252341781	0.1811611532141001	T	T	T
0.5401543192137392	0.1817717795279482	0.2008904605419021	T	T	T

0.0056752546076472	0.5209743417036046	0.2265917399948451	T	T	T
0.3392568297610872	0.5845718546534405	0.2437488982865271	T	T	T
0.7975004236015557	0.9156887285332136	0.2627314305238121	T	T	T
0.2232696223905765	0.2045839682119229	0.2827214760986003	T	T	T
0.6812322956212593	0.7314443638462236	0.3348148357177989	T	T	T
0.0119693296155256	0.7604613474493688	0.3352910005738013	T	T	T
0.5893396129341151	0.5806434013617434	0.3704460561850645	T	T	T
0.8347867526381302	0.5485156206292771	0.3831459699985652	T	T	T

ReN₂ (110) - Surface

Re N

1.0000000000000000		
5.5853799999999998	0.0000000000000000	0.0000000000000000
1.4576319424392254	5.4095059961960343	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.6293000000000006

Re N

8 16

Selective dynamics

Direct

0.9952600000000018	0.8038200000000018	0.0037700000000029	F	F	F
0.2003500000000003	0.0179600000000022	0.0870999999999995	F	F	F
0.5982199999999978	0.4092899999999986	0.0456100000000035	F	F	F
0.8033100000000033	0.6234299999999990	0.1289400000000001	F	F	F
0.4050002476502463	0.2213888331013139	0.1696897452725484	T	T	T
0.6106361358580811	0.4208062126728720	0.2467419719891142	T	T	T
-0.0150405257809287	0.7946480940932730	0.2102161573765217	T	T	T
0.2100530893711112	0.0208768526407419	0.2815693562420402	T	T	T
0.4185500000000033	0.2233200000000011	0.0858699999999999	F	F	F
0.2134599999999978	0.0091899999999967	0.0025300000000001	F	F	F
0.1101373072023948	0.4995196919580192	0.1640049248954823	T	T	T
0.9019699999999986	0.2868899999999996	0.0791299999999993	F	F	F
0.6874334509060054	0.9228016931723327	0.1640848713142737	T	T	T
0.4946500000000000	0.7062200000000018	0.0808000000000035	F	F	F
0.1814699999999974	0.9903400000000033	0.1567099999999968	F	F	F
0.9763799999999989	0.7762099999999990	0.0733800000000002	F	F	F
0.8225302588897074	0.6327256830623960	0.2495176583065038	T	T	T
0.6303105965372509	0.4413831669653528	0.1735485120189233	T	T	T
0.5973369035126175	0.4361020881419608	0.3710659127120705	T	T	T
0.3113175239306643	0.7051894744186602	0.2514532573110095	T	T	T
0.2417826952873683	0.0506674957391883	0.3451129238035509	T	T	T
0.8932796337768534	0.1211258739968646	0.2514046656483295	T	T	T
0.6046103454061943	0.4259806284255657	0.3292120540079462	T	T	T

0.3866909499162758 0.1994005837923985 0.2443278745297735 T T T
ReN₂ (110) + *OOH

Re N O H

1.0000000000000000

5.5853799999999998 0.0000000000000000 0.0000000000000000

1.4576319424392254 5.4095059961960343 0.0000000000000000

0.0000000000000000 0.0000000000000000 26.6293000000000006

Re N O H

8 16 2 1

Selective dynamics

Direct

0.9952600000000018	0.8038200000000018	0.0037700000000029	F	F	F
0.2003500000000003	0.0179600000000022	0.0870999999999995	F	F	F
0.5982199999999978	0.4092899999999986	0.0456100000000035	F	F	F
0.8033100000000033	0.6234299999999990	0.1289400000000001	F	F	F
0.4109619610170633	0.2204048029238714	0.1714437879066771	T	T	T
0.5980477840261028	0.4476705032722034	0.2472489759174860	T	T	T
-0.0048066097950872	0.8161318582367582	0.2123423485516927	T	T	T
0.1956865001247173	0.0722907157119770	0.2930123285282096	T	T	T
0.4185500000000033	0.2233200000000011	0.0858699999999999	F	F	F
0.2134599999999978	0.0091899999999967	0.0025300000000001	F	F	F
0.1070500000000010	0.5010199999999969	0.1624600000000029	F	F	F
0.9019699999999986	0.2868899999999996	0.0791299999999993	F	F	F
0.6850948854836111	0.9260778110822305	0.1625379414945685	T	T	T
0.4946500000000000	0.7062200000000018	0.0808000000000035	F	F	F
0.1814699999999974	0.9903400000000033	0.1567099999999968	F	F	F
0.9763799999999989	0.7762099999999990	0.0733800000000002	F	F	F
0.8264062185853288	0.6405770511066868	0.2475382804491583	T	T	T
0.6294298631573494	0.4406350016631216	0.1714039044699230	T	T	T
0.3747682388083254	0.7662206184356746	0.3389491440293275	T	T	T
0.3109156493904758	0.7016052489460527	0.2392532954799645	T	T	T
0.1401250930659446	0.2803001679695279	0.3408210067396075	T	T	T
0.8993409588363310	0.1245750826383918	0.2556873129957876	T	T	T
0.5102386756372898	0.5783824422375928	0.3245240041181464	T	T	T
0.3907215067984818	0.1929768741284094	0.2467856645207453	T	T	T
0.5926420327770514	0.3586368504050159	0.3666409574348868	T	T	T
0.4470350673219419	0.4247321563979851	0.4093317287126665	T	T	T
0.2898621237225394	0.3859508479928606	0.3980182021018165	T	T	T

ReN₂ (110) + *O

Re N O

1.0000000000000000
5.5853799999999998 0.0000000000000000 0.0000000000000000
1.4576319424392254 5.4095059961960343 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.6293000000000006

Re N O
8 16 1

Selective dynamics

Direct

0.9952600000000018	0.8038200000000018	0.0037700000000029	F	F	F
0.2003500000000003	0.0179600000000022	0.0870999999999995	F	F	F
0.5982199999999978	0.4092899999999986	0.0456100000000035	F	F	F
0.80331000000000033	0.6234299999999990	0.1289400000000001	F	F	F
0.4117873896113739	0.2183033352706387	0.1713207042083083	T	T	T
0.6090694207155881	0.4431268634991717	0.2489719539593910	T	T	T
0.0030888678344999	0.8165382498864234	0.2127298325790517	T	T	T
0.1943850436736283	0.0947919430475362	0.2945469857155896	T	T	T
0.41855000000000033	0.2233200000000011	0.0858699999999999	F	F	F
0.2134599999999978	0.0091899999999967	0.0025300000000001	F	F	F
0.1070500000000010	0.5010199999999969	0.1624600000000029	F	F	F
0.9019699999999986	0.2868899999999996	0.0791299999999993	F	F	F
0.6850943098132856	0.9230203053837934	0.1619126353894227	T	T	T
0.4946500000000000	0.7062200000000018	0.0808000000000035	F	F	F
0.1814699999999974	0.99034000000000033	0.1567099999999968	F	F	F
0.9763799999999989	0.7762099999999990	0.0733800000000002	F	F	F
0.8317013955641408	0.6402849880076447	0.2480539281882629	T	T	T
0.6322614099479301	0.4393719562406692	0.1735299138356198	T	T	T
0.3764942071558273	0.8033539181874497	0.3391913906395130	T	T	T
0.3099712913263790	0.7007666820264450	0.2375606605947359	T	T	T
0.1415847964561358	0.3211771565361483	0.3385688752552511	T	T	T
0.9048902567992838	0.1236927459904100	0.2556929145504772	T	T	T
0.5007937355309854	0.6134097574201590	0.3195272159788572	T	T	T
0.3930752146267715	0.1938605008977946	0.2462476485194209	T	T	T
0.6234488001912804	0.4048345924779033	0.3367592832551249	T	T	T

ReN₂ (110) + *OH

Re N O H

1.0000000000000000
5.5853799999999998 0.0000000000000000 0.0000000000000000
1.4576319424392254 5.4095059961960343 0.0000000000000000
0.0000000000000000 0.0000000000000000 26.6293000000000006

Re N O H
8 16 1 1

Selective dynamics

Direct

0.9952600000000018	0.8038200000000018	0.0037700000000029	F	F	F
0.2003500000000003	0.0179600000000022	0.0870999999999995	F	F	F
0.5982199999999978	0.4092899999999986	0.0456100000000035	F	F	F
0.8033100000000033	0.6234299999999990	0.1289400000000001	F	F	F
0.4109898767392704	0.2219050414463382	0.1711401354913861	T	T	T
0.5949702929391465	0.4524933278018977	0.2476438405954873	T	T	T
-0.0061015359690463	0.8157825209225020	0.2118337588737423	T	T	T
0.1917034918859999	0.0760600297558157	0.2918451120897698	T	T	T
0.4185500000000033	0.2233200000000011	0.0858699999999999	F	F	F
0.2134599999999978	0.0091899999999967	0.0025300000000001	F	F	F
0.1070500000000010	0.5010199999999969	0.1624600000000029	F	F	F
0.9019699999999986	0.2868899999999996	0.0791299999999993	F	F	F
0.6851047685239618	0.9274385288980870	0.1623653653508818	T	T	T
0.4946500000000000	0.7062200000000018	0.0808000000000035	F	F	F
0.1814699999999974	0.9903400000000033	0.1567099999999968	F	F	F
0.9763799999999989	0.7762099999999990	0.0733800000000002	F	F	F
0.8265339329543943	0.6409578736223250	0.2474201535348537	T	T	T
0.6280758220718681	0.4427435999973792	0.1715420369279786	T	T	T
0.3826163910292143	0.7922125398242915	0.3391036300642212	T	T	T
0.3094762686862914	0.7033724748455108	0.2401435263124670	T	T	T
0.1108871686646469	0.2895917224122225	0.3388712398106496	T	T	T
0.8965135866585322	0.1238968843231890	0.2543931205913827	T	T	T
0.5257389149898596	0.5954315987659163	0.3268084001753765	T	T	T
0.3904122515854999	0.1963065245776527	0.2468122647228020	T	T	T
0.6364869584918769	0.4525244304866297	0.3676065082461817	T	T	T
0.8163892823410905	0.3752458947029488	0.3571156758187644	T	T	T

Ta₄N₅ (100) - Surface

Ta N

1.0000000000000000		
5.3044300000000000	0.0000000000000000	0.0000000000000000
-1.7217108756555533	10.4682601644518467	0.0000000000000000
0.0000000000000000	0.0000000000000000	29.0263999999999989

Ta N

16 20

Selective dynamics

Direct

0.4209499999999977	0.1852000000000018	0.1081599999999980	F	F	F
0.6827699999999979	0.3749899999999968	0.0316600000000022	F	F	F
0.4004100000000008	0.0834199999999967	0.0055800000000019	F	F	F

0.941499999999978	0.133580000000020	0.054070000000029	F	F	F
0.7293945299761371	0.0253256138761432	0.2248795493669699	T	T	T
0.9797561354880421	0.2337824995001521	0.1596537185260631	T	T	T
0.6843300000000028	0.444809999999968	0.1267700000000005	F	F	F
0.2270848349327307	0.4899560369975882	0.1877397014666781	T	T	T
0.420949999999977	0.685200000000018	0.108159999999980	F	F	F
0.682769999999979	0.874989999999968	0.0316600000000022	F	F	F
0.4004100000000008	0.583419999999967	0.0055800000000019	F	F	F
0.941499999999978	0.6335800000000020	0.0540700000000029	F	F	F
0.7284865580429214	0.5252959440318942	0.2246416295849823	T	T	T
0.9798648902380231	0.7341227856704416	0.1594608338086255	T	T	T
0.6871424286372603	0.9457587400216104	0.1272816820282708	T	T	T
0.2282704237497118	0.9895853888853610	0.1878484195350666	T	T	T
0.041589999999993	0.479199999999987	0.018619999999985	F	F	F
0.808259999999971	0.289409999999966	0.092649999999990	F	F	F
0.0526100000000014	0.065959999999969	0.119419999999981	F	F	F
0.309829999999981	0.252819999999998	0.0428100000000029	F	F	F
0.5541800000000023	0.0293700000000001	0.0695800000000020	F	F	F
0.3302560599278107	0.3407017770660904	0.1447578040954387	T	T	T
0.0596889098344560	0.1447416678722797	0.2165207728875129	T	T	T
0.3826484039440496	0.4603231849662598	0.2448066410449466	T	T	T
0.5940704283861260	0.1081741252086533	0.1699572647403677	T	T	T
0.8469137910579571	0.3845484746072056	0.1935415878155295	T	T	T
0.041589999999993	0.979199999999987	0.018619999999985	F	F	F
0.808259999999971	0.789409999999966	0.092649999999990	F	F	F
0.0526100000000014	0.565959999999969	0.119419999999981	F	F	F
0.309829999999981	0.752819999999998	0.0428100000000029	F	F	F
0.5541800000000023	0.5293700000000001	0.0695800000000020	F	F	F
0.3313426024605365	0.8406958754183049	0.1448369799798296	T	T	T
0.0586615641431515	0.6445739564499532	0.2164762573482146	T	T	T
0.3835494627130667	0.9601049174652603	0.2449417250790676	T	T	T
0.5936575850349639	0.6077047783871582	0.1696805552662060	T	T	T
0.8478824153304869	0.8844614534460663	0.1937895968770303	T	T	T

Ta₄N₅ (100) + *OOH

Ta N O H

1.0000000000000000		
5.3044300000000000	0.0000000000000000	0.0000000000000000
-1.7217108756555533	10.4682601644518467	0.0000000000000000
0.0000000000000000	0.0000000000000000	29.026399999999989

Ta N O H

16 20 2 1

Selective dynamics

Direct

0.4209499999999977	0.1852000000000018	0.1081599999999980	F	F	F
0.6827699999999979	0.3749899999999968	0.0316600000000022	F	F	F
0.4004100000000008	0.0834199999999967	0.0055800000000019	F	F	F
0.9414999999999978	0.1335800000000020	0.0540700000000029	F	F	F
0.7391275914174196	0.0169645030476789	0.2321435901033642	T	T	T
0.9656661388608900	0.2316897488196463	0.1597575068775549	T	T	T
0.6867299999999972	0.4461799999999982	0.1268699999999967	F	F	F
0.2292619089921453	0.4879688303568764	0.1872138564076358	T	T	T
0.4209499999999977	0.6852000000000018	0.1081599999999980	F	F	F
0.6827699999999979	0.8749899999999968	0.0316600000000022	F	F	F
0.4004100000000008	0.5834199999999967	0.0055800000000019	F	F	F
0.9414999999999978	0.6335800000000020	0.0540700000000029	F	F	F
0.7299870545739542	0.5254077399690589	0.2252735932339603	T	T	T
0.9807800323400446	0.7334556596396204	0.1605306128204050	T	T	T
0.6822900000000018	0.9438999999999993	0.1272599999999997	F	F	F
0.2216252961768428	0.0017394317349951	0.1785683635610553	T	T	T
0.0415899999999993	0.4791999999999987	0.0186199999999985	F	F	F
0.8082599999999971	0.2894099999999966	0.0926499999999990	F	F	F
0.0526100000000014	0.0659599999999969	0.1194199999999981	F	F	F
0.3098299999999981	0.2528199999999998	0.0428100000000029	F	F	F
0.5541800000000023	0.0293700000000001	0.0695800000000020	F	F	F
0.3302699999999987	0.3409100000000009	0.1444499999999991	F	F	F
0.0546379115300984	0.1369673340461500	0.2152919921894385	T	T	T
0.3839955886262167	0.4596749700412768	0.2445238471809543	T	T	T
0.5964706883950361	0.1081689283070477	0.1683835169754291	T	T	T
0.8461127965603241	0.3850740975421699	0.1936746384643554	T	T	T
0.0415899999999993	0.9791999999999987	0.0186199999999985	F	F	F
0.8082599999999971	0.7894099999999966	0.0926499999999990	F	F	F
0.0526100000000014	0.5659599999999969	0.1194199999999981	F	F	F
0.3098299999999981	0.7528199999999998	0.0428100000000029	F	F	F
0.5541800000000023	0.5293700000000001	0.0695800000000020	F	F	F
0.3295000000000030	0.8411499999999990	0.1446200000000033	F	F	F
0.0616317088539663	0.6454556483718391	0.2166960608124204	T	T	T
0.4178469790845848	0.0430634554574209	0.2627800075759736	T	T	T
0.5960981570274730	0.6077899544676212	0.1699910519334608	T	T	T
0.8472599912896808	0.8844734810486017	0.1910559217696753	T	T	T
0.2850453288344365	0.0637990999013309	0.2952591192023290	T	T	T
-0.1937208770515545	0.9236526681415153	0.2870140610204387	T	T	T
-0.2877187751473008	0.9224636274105491	0.3157681337938308	T	T	T

Ta₄N₅ (100) + *O

Ta N O

1.0000000000000000		
5.3044300000000000	0.0000000000000000	0.0000000000000000
-1.7217108756555533	10.4682601644518467	0.0000000000000000
0.0000000000000000	0.0000000000000000	29.026399999999989

Ta N O

16 20 1

Selective dynamics

Direct

0.4209499999999977	0.1852000000000018	0.1081599999999980	F	F	F
0.6827699999999979	0.3749899999999968	0.0316600000000022	F	F	F
0.4004100000000008	0.0834199999999967	0.0055800000000019	F	F	F
0.9414999999999978	0.1335800000000020	0.0540700000000029	F	F	F
0.7356574971649085	0.0287723286694636	0.2247075621449405	T	T	T
0.9786921870942978	0.2356005936048593	0.1580644391246185	T	T	T
0.6867299999999972	0.4461799999999982	0.1268699999999967	F	F	F
0.2274678063399510	0.4895655656304688	0.1876465051142486	T	T	T
0.4209499999999977	0.6852000000000018	0.1081599999999980	F	F	F
0.6827699999999979	0.8749899999999968	0.0316600000000022	F	F	F
0.4004100000000008	0.5834199999999967	0.0055800000000019	F	F	F
0.9414999999999978	0.6335800000000020	0.0540700000000029	F	F	F
0.7286358621645714	0.5249627212154252	0.2247000533209170	T	T	T
0.9763440629378942	0.7339389733144378	0.1594165027586038	T	T	T
0.6822900000000018	0.9438999999999993	0.1272599999999997	F	F	F
0.2237836170648278	-0.0116009093303173	0.1887694472343969	T	T	T
0.0415899999999993	0.4791999999999987	0.0186199999999985	F	F	F
0.8082599999999971	0.2894099999999966	0.0926499999999990	F	F	F
0.0526100000000014	0.0659599999999969	0.1194199999999981	F	F	F
0.3098299999999981	0.2528199999999998	0.0428100000000029	F	F	F
0.5541800000000023	0.0293700000000001	0.0695800000000020	F	F	F
0.3302699999999987	0.3409100000000009	0.1444499999999991	F	F	F
0.0692322165270905	0.1433226309706105	0.2146463218658675	T	T	T
0.3828306477839895	0.4599040041136542	0.2447072049028186	T	T	T
0.5893083334774406	0.1075531477887974	0.1699294871517106	T	T	T
0.8476634645921665	0.3840655320816060	0.1936500490184533	T	T	T
0.0415899999999993	0.9791999999999987	0.0186199999999985	F	F	F
0.8082599999999971	0.7894099999999966	0.0926499999999990	F	F	F
0.0526100000000014	0.5659599999999969	0.1194199999999981	F	F	F
0.3098299999999981	0.7528199999999998	0.0428100000000029	F	F	F
0.5541800000000023	0.5293700000000001	0.0695800000000020	F	F	F
0.3295000000000030	0.8411499999999990	0.1446200000000033	F	F	F

0.0587658032467092	0.6444851159392119	0.2160546502980324	T	T	T
0.4094044989192641	0.9631696383655798	0.2520056475016315	T	T	T
0.5927095225688533	0.6083302408717055	0.1697823831113524	T	T	T
0.8384316835202628	0.8855527170835542	0.1910002913537962	T	T	T
0.1608889434704381	0.9216633196600977	0.2587846405294500	T	T	T

Ta₄N₅ (100) + *OH

Ta N O H

1.0000000000000000			
5.3044300000000000	0.0000000000000000	0.0000000000000000	
-1.7217108756555533	10.4682601644518467	0.0000000000000000	
0.0000000000000000	0.0000000000000000	29.0263999999999989	

Ta N O H

16 20 1 1

Selective dynamics

Direct

0.4209499999999977	0.1852000000000018	0.1081599999999980	F	F	F
0.6827699999999979	0.3749899999999968	0.0316600000000022	F	F	F
0.4004100000000008	0.0834199999999967	0.0055800000000019	F	F	F
0.9414999999999978	0.1335800000000020	0.0540700000000029	F	F	F
0.7228727967865344	0.0266212044199915	0.2235910132607347	T	T	T
0.9747088588102408	0.2333585095038778	0.1597210875117201	T	T	T
0.6867299999999972	0.4461799999999982	0.1268699999999967	F	F	F
0.2280668702357874	0.4889614211875451	0.1876535543136729	T	T	T
0.4209499999999977	0.6852000000000018	0.1081599999999980	F	F	F
0.6827699999999979	0.8749899999999968	0.0316600000000022	F	F	F
0.4004100000000008	0.5834199999999967	0.0055800000000019	F	F	F
0.9414999999999978	0.6335800000000020	0.0540700000000029	F	F	F
0.7296139963363943	0.5258707834587811	0.2247781726167916	T	T	T
0.9795023167222445	0.7347102069035228	0.1599575053670257	T	T	T
0.6822900000000018	0.9438999999999993	0.1272599999999997	F	F	F
0.2285671107882138	0.9969244713344108	0.1828651706627503	T	T	T
0.0415899999999993	0.4791999999999987	0.0186199999999985	F	F	F
0.8082599999999971	0.2894099999999966	0.0926499999999990	F	F	F
0.0526100000000014	0.0659599999999969	0.1194199999999981	F	F	F
0.3098299999999981	0.2528199999999998	0.0428100000000029	F	F	F
0.5541800000000023	0.0293700000000001	0.0695800000000020	F	F	F
0.3302699999999987	0.3409100000000009	0.1444499999999991	F	F	F
0.0566704154009080	0.1425822344184972	0.2171089676748752	T	T	T
0.3840188269301243	0.4599165090383492	0.2448889076594891	T	T	T
0.5976064401644422	0.1119853955503713	0.1687461529517850	T	T	T
0.8468473477914016	0.3848830647191715	0.1937919674651885	T	T	T

0.0415899999999993	0.9791999999999987	0.0186199999999985	F	F	F
0.8082599999999971	0.7894099999999966	0.0926499999999990	F	F	F
0.0526100000000014	0.5659599999999969	0.1194199999999981	F	F	F
0.3098299999999981	0.7528199999999998	0.0428100000000029	F	F	F
0.5541800000000023	0.5293700000000001	0.0695800000000020	F	F	F
0.3295000000000030	0.8411499999999990	0.1446200000000033	F	F	F
0.0608292600515972	0.6451444681747660	0.2165425065415855	T	T	T
0.3701276235157901	0.9705157336810309	0.2490830811757276	T	T	T
0.5943400772055381	0.6082240995307889	0.1698599845018724	T	T	T
0.8462033283956404	0.8852308002296735	0.1930551463585802	T	T	T
0.1888822037141047	0.9564095029139497	0.2862968520258027	T	T	T
0.2669174343854281	0.0150740236798149	0.3102129949893568	T	T	T

Ni₃N (110) - Surface

Ni N

1.0000000000000000					
4.3013100000000000	0.0000000000000000	0.0000000000000000			
0.0000000000000000	7.9770300000000001	0.0000000000000000			
0.0000000000000000	0.0000000000000000	27.6332999999999984			

Ni N

24 8

Selective dynamics

Direct

0.5000000000000000	0.1645299999999992	0.0131799999999984	F	F	F
0.5000000000000000	0.6645299999999992	0.0965100000000021	F	F	F
0.0000000000000000	0.3354700000000008	0.0416700000000034	F	F	F
0.0000000000000000	0.8354700000000008	0.1250000000000000	F	F	F
0.0000000000000000	0.5000000000000000	0.1239300000000014	F	F	F
0.0000000000000000	0.0000000000000000	0.0405999999999977	F	F	F
0.5000000000000000	0.8354700000000008	0.0131799999999984	F	F	F
0.5000000000000000	0.3354700000000008	0.0965100000000021	F	F	F
0.5000000000000000	0.5000000000000000	0.0142400000000009	F	F	F
0.5000000000000000	0.0000000000000000	0.0975800000000007	F	F	F
0.0000000000000000	0.6645299999999992	0.0416700000000034	F	F	F
0.0000000000000000	0.1645299999999992	0.1250000000000000	F	F	F
0.4949581033046698	0.1669037208550333	0.1794712455889469	T	T	T
0.5008518786571907	0.6642596644618823	0.2678170817950116	T	T	T
-0.0011174313860081	0.3349892439444008	0.2082360672591807	T	T	T
0.0108172445599954	0.8333265797814742	0.2905431617782624	T	T	T
0.0000320403536215	0.5002131663218148	0.2928231891180743	T	T	T
-0.0000276776375876	0.0000805893032433	0.2079867789464517	T	T	T
0.5049704638989332	0.8331270844322879	0.1794778792543936	T	T	T

0.4990066708352540	0.3361014883835530	0.2677909916262879	T	T	T
0.5000069162170692	0.5000136820083662	0.1815739450215116	T	T	T
0.5000804353788646	0.0001567489332731	0.2615986077677800	T	T	T
0.0009961339056021	0.6651106920638551	0.2082388116210723	T	T	T
0.9891839966153283	0.1671117660737502	0.2905500524374454	T	T	T
0.2500000000000000	0.6666700000000034	0.1524199999999993	F	F	F
0.2500000000000000	0.1666700000000034	0.0690900000000028	F	F	F
0.7500000000000000	0.3333299999999966	0.1524199999999993	F	F	F
0.7500000000000000	0.8333299999999966	0.0690900000000028	F	F	F
0.2250227813101537	0.6690520002751982	0.3154058777102137	T	T	T
0.2529483209374063	0.1688653218665754	0.2370155893254735	T	T	T
0.7748456788886844	0.3313833855943143	0.3153710816052658	T	T	T
0.7469977318707240	0.8313242084111646	0.2370152294413743	T	T	T

Ni₃N (110) + *OOH

Ni N O H

1.0000000000000000			
4.3013100000000000	0.0000000000000000	0.0000000000000000	
0.0000000000000000	7.9770300000000001	0.0000000000000000	
0.0000000000000000	0.0000000000000000	27.6332999999999984	

Ni N O H
24 8 2 1

Selective dynamics

Direct

0.5000000000000000	0.1645299999999992	0.0131799999999984	F	F	F
0.5000000000000000	0.6645299999999992	0.0965100000000021	F	F	F
0.0000000000000000	0.3354700000000008	0.0416700000000034	F	F	F
0.0000000000000000	0.8354700000000008	0.1250000000000000	F	F	F
0.0000000000000000	0.5000000000000000	0.1239300000000014	F	F	F
0.0000000000000000	0.0000000000000000	0.0405999999999977	F	F	F
0.5000000000000000	0.8354700000000008	0.0131799999999984	F	F	F
0.5000000000000000	0.3354700000000008	0.0965100000000021	F	F	F
0.5000000000000000	0.5000000000000000	0.0142400000000009	F	F	F
0.5000000000000000	0.0000000000000000	0.0975800000000007	F	F	F
0.0000000000000000	0.6645299999999992	0.0416700000000034	F	F	F
0.0000000000000000	0.1645299999999992	0.1250000000000000	F	F	F
0.4944496787496243	0.1681407127667426	0.1830662895641180	T	T	T
0.5128762839536036	0.6542174673252678	0.2582427276250117	T	T	T
-0.0138702358353434	0.3318678066905447	0.2080754432016668	T	T	T
-0.0038414320245991	0.7332272388789270	0.2953075404494352	T	T	T
-0.0706834573295554	0.4479674433884334	0.3279404908948116	T	T	T
-0.0034234863308174	-0.0006931123917513	0.2106997875230535	T	T	T

0.5045016881045301	0.8366098086054943	0.1800356977470821	T	T	T
0.4104459136714761	0.3594500153002616	0.2682442534414846	T	T	T
0.4950929249550052	0.4976392699795344	0.1801130895693604	T	T	T
0.4970915466054722	-0.0069507035235969	0.2628631234063192	T	T	T
0.0023782030139770	0.6728662027797404	0.2063906625463206	T	T	T
0.9422218825845845	0.1774032386579032	0.2909044821137934	T	T	T
0.2500000000000000	0.6666700000000034	0.1524199999999993	F	F	F
0.2500000000000000	0.1666700000000034	0.0690900000000028	F	F	F
0.7500000000000000	0.3333299999999966	0.1524199999999993	F	F	F
0.7500000000000000	0.8333299999999966	0.0690900000000028	F	F	F
0.2706602630107320	0.5476123243711266	0.2987366620190988	T	T	T
0.2407944127457863	0.1654603620399534	0.2406983161380738	T	T	T
0.8228014076499504	0.2436282290959134	0.3494796928329469	T	T	T
0.7672825209222609	0.8309005266909258	0.2412179083873212	T	T	T
0.7632920876568494	0.1872596776674591	0.3888237720415048	T	T	T
0.8599473718673564	0.6605152251262667	0.3604931394666552	T	T	T
0.6398126144826796	0.6838045294864898	0.3660485313582565	T	T	T

Ni₃N (110) + *O

Ni N O

1.0000000000000000		
4.3013100000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.9770300000000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.6332999999999984

Ni N O

24 8 1

Selective dynamics

Direct

0.5000000000000000	0.1645299999999992	0.0131799999999984	F	F	F
0.5000000000000000	0.6645299999999992	0.0965100000000021	F	F	F
0.0000000000000000	0.3354700000000008	0.0416700000000034	F	F	F
0.0000000000000000	0.8354700000000008	0.1250000000000000	F	F	F
0.0000000000000000	0.5000000000000000	0.1239300000000014	F	F	F
0.0000000000000000	0.0000000000000000	0.0405999999999977	F	F	F
0.5000000000000000	0.8354700000000008	0.0131799999999984	F	F	F
0.5000000000000000	0.3354700000000008	0.0965100000000021	F	F	F
0.5000000000000000	0.5000000000000000	0.0142400000000009	F	F	F
0.5000000000000000	0.0000000000000000	0.0975800000000007	F	F	F
0.0000000000000000	0.6645299999999992	0.0416700000000034	F	F	F
0.0000000000000000	0.1645299999999992	0.1250000000000000	F	F	F
0.4967841730553349	0.1664247347814460	0.1797893614758180	T	T	T
0.5020199775208110	0.6621162442222508	0.2669464307999522	T	T	T

0.0055608067600788	0.3389827090679488	0.2076573366250550	T	T	T
0.0045949946162819	0.8276285955697215	0.2905874561149457	T	T	T
-0.0066879283587954	0.4960205305327599	0.2913497475770457	T	T	T
-0.0008393288213491	0.0021547391256829	0.2083609096358461	T	T	T
0.5031098806434142	0.8342474158475872	0.1793081761079868	T	T	T
0.4968955348281463	0.3377896863550899	0.2682897234124147	T	T	T
0.5022416051556379	0.5006887787839054	0.1815166113467969	T	T	T
0.4936427239580387	-0.0010034425109397	0.2614687355142613	T	T	T
-0.0005811729541324	0.6663214270076623	0.2079204895306598	T	T	T
0.9733007787080673	0.1670393765775151	0.2886345158660032	T	T	T
0.2500000000000000	0.6666700000000034	0.1524199999999993	F	F	F
0.2500000000000000	0.1666700000000034	0.0690900000000028	F	F	F
0.7500000000000000	0.3333299999999966	0.1524199999999993	F	F	F
0.7500000000000000	0.8333299999999966	0.0690900000000028	F	F	F
0.2229894173886493	0.6613446305891424	0.3136718278527275	T	T	T
0.2553619626295709	0.1714106100021401	0.2370983488090063	T	T	T
0.7579755012616439	0.3287875326955583	0.3231340374342235	T	T	T
0.7447882204991546	0.8326093633710704	0.2368142454203432	T	T	T
0.6942781204168860	0.3253555725789896	0.3662696002664164	T	T	T

Ni₃N (110) + *OH

Ni N O H

1.0000000000000000			
4.3013100000000000	0.0000000000000000	0.0000000000000000	
0.0000000000000000	7.9770300000000001	0.0000000000000000	
0.0000000000000000	0.0000000000000000	27.6332999999999984	

Ni N O H

24 8 1 1

Selective dynamics

Direct

0.5000000000000000	0.1645299999999992	0.0131799999999984	F	F	F
0.5000000000000000	0.6645299999999992	0.0965100000000021	F	F	F
0.0000000000000000	0.3354700000000008	0.0416700000000034	F	F	F
0.0000000000000000	0.8354700000000008	0.1250000000000000	F	F	F
0.0000000000000000	0.5000000000000000	0.1239300000000014	F	F	F
0.0000000000000000	0.0000000000000000	0.0405999999999977	F	F	F
0.5000000000000000	0.8354700000000008	0.0131799999999984	F	F	F
0.5000000000000000	0.3354700000000008	0.0965100000000021	F	F	F
0.5000000000000000	0.5000000000000000	0.0142400000000009	F	F	F
0.5000000000000000	0.0000000000000000	0.0975800000000007	F	F	F
0.0000000000000000	0.6645299999999992	0.0416700000000034	F	F	F
0.0000000000000000	0.1645299999999992	0.1250000000000000	F	F	F

0.4970674553105374	0.1660466457497265	0.1796647292498076	T	T	T
0.5041999496548309	0.6618823700035665	0.2668360071375372	T	T	T
0.0033450593383000	0.3374410416536085	0.2074721078083312	T	T	T
0.0170898561402399	0.8257550763845281	0.2906175080977287	T	T	T
-0.0120212378685542	0.4984529966407362	0.2918151092461917	T	T	T
0.0008111055290539	-0.0005070845560223	0.2080784450910911	T	T	T
0.5050302678489786	0.8335908056469167	0.1797183874753255	T	T	T
0.4926652392156411	0.3350616909085654	0.2666362863495446	T	T	T
0.5008668009895890	0.5000560920363817	0.1815039434003253	T	T	T
0.5006635321442863	0.9993848895396387	0.2624590622694922	T	T	T
0.0010224806915443	0.6655064602947499	0.2080678877098923	T	T	T
0.9818989535137645	0.1738763560941420	0.2886332402806384	T	T	T
0.2500000000000000	0.6666700000000034	0.1524199999999993	F	F	F
0.2500000000000000	0.1666700000000034	0.0690900000000028	F	F	F
0.7500000000000000	0.3333299999999966	0.1524199999999993	F	F	F
0.7500000000000000	0.8333299999999966	0.0690900000000028	F	F	F
0.2310695146243567	0.6571947983522498	0.3150517911913603	T	T	T
0.2528930998296718	0.1669265564659271	0.2369285177972808	T	T	T
0.7508121061085316	0.3287902774310421	0.3204309932920187	T	T	T
0.7479585999371791	0.8324884647384108	0.2374668145735158	T	T	T
0.6364092520253152	0.3486313096461785	0.3669410917094529	T	T	T
0.5020193285928383	0.4494263874814571	0.3655416889381694	T	T	T

Fe₃N (110) - Surface

Fe N

1.0000000000000000		
4.3045799999999996	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0405899999999999	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.8534000000000006

Fe N

24 8

Selective dynamics

Direct

0.0000000000000000	0.5000000000000000	0.1230499999999992	F	F	F
0.0000000000000000	0.0000000000000000	0.0397200000000026	F	F	F
0.5000000000000000	0.1627799999999979	0.0125900000000030	F	F	F
0.5000000000000000	0.6627799999999979	0.0959300000000027	F	F	F
0.5000000000000000	0.8372200000000021	0.0125900000000030	F	F	F
0.5000000000000000	0.3372200000000021	0.0959300000000027	F	F	F
0.5000000000000000	0.5000000000000000	0.0145399999999967	F	F	F
0.5000000000000000	0.0000000000000000	0.0978700000000003	F	F	F
0.0000000000000000	0.3372200000000021	0.0416700000000034	F	F	F

0.0000000000000000	0.8372200000000021	0.1250000000000000	F	F	F
0.0000000000000000	0.6627799999999979	0.0416700000000034	F	F	F
0.0000000000000000	0.1627799999999979	0.1250000000000000	F	F	F
-0.0000000000000000	0.5000000000000000	0.2888700051602655	T	T	T
-0.0000000000000000	-0.0000000000000000	0.2054802011728181	T	T	T
0.5017981428864230	0.1656938597716576	0.1796844272498765	T	T	T
0.4979847119877185	0.6576511147146733	0.2651037550722578	T	T	T
0.4982018571135769	0.8343061402283426	0.1796844272498765	T	T	T
0.5020152880122816	0.3423488852853264	0.2651037550722578	T	T	T
0.5000000000000000	0.5000000000000000	0.1817955607652538	T	T	T
0.5000000000000000	-0.0000000000000000	0.2608845067861496	T	T	T
0.9990186788837607	0.3385305543598645	0.2082733088140492	T	T	T
0.9690494853425677	0.8301181593844832	0.2879324063180843	T	T	T
0.0009813211162392	0.6614694456401354	0.2082733088140492	T	T	T
0.0309505146574322	0.1698818406155169	0.2879324063180843	T	T	T
0.7500000000000000	0.6666700000000034	0.1521299999999997	F	F	F
0.7500000000000000	0.1666700000000034	0.0688000000000031	F	F	F
0.2500000000000000	0.3333299999999966	0.1521299999999997	F	F	F
0.2500000000000000	0.8333299999999966	0.0688000000000031	F	F	F
0.7698257811552646	0.6593372727642154	0.3148967478842637	T	T	T
0.7486963744355218	0.1698862295228002	0.2370542477666007	T	T	T
0.2301742188447359	0.3406627272357846	0.3148967478842637	T	T	T
0.2513036255644785	0.8301137704771997	0.2370542477666007	T	T	T

Fe₃N (110) + *OOH

Fe N O H

1.0000000000000000			
4.3045799999999996	0.0000000000000000	0.0000000000000000	
0.0000000000000000	8.0405899999999999	0.0000000000000000	
0.0000000000000000	0.0000000000000000	27.8534000000000006	

Fe N O H

24 8 2 1

Selective dynamics

Direct

0.0000000000000000	0.5000000000000000	0.1230499999999992	F	F	F
0.0000000000000000	0.0000000000000000	0.0397200000000026	F	F	F
0.5000000000000000	0.1627799999999979	0.0125900000000030	F	F	F
0.5000000000000000	0.6627799999999979	0.0959300000000027	F	F	F
0.5000000000000000	0.8372200000000021	0.0125900000000030	F	F	F
0.5000000000000000	0.3372200000000021	0.0959300000000027	F	F	F
0.5000000000000000	0.5000000000000000	0.0145399999999967	F	F	F
0.5000000000000000	0.0000000000000000	0.0978700000000003	F	F	F

0.0000000000000000	0.3372200000000021	0.0416700000000034	F	F	F
0.0000000000000000	0.8372200000000021	0.1250000000000000	F	F	F
0.0000000000000000	0.6627799999999979	0.0416700000000034	F	F	F
0.0000000000000000	0.1627799999999979	0.1250000000000000	F	F	F
0.9920297175164713	0.5041074968527681	0.2891064356886706	T	T	T
-0.0002392901227993	0.0008144743395470	0.2068465305256881	T	T	T
0.5054192428287602	0.1665113798216589	0.1794194201360668	T	T	T
0.5105821786500664	0.6651478828100837	0.2644220196042599	T	T	T
0.4964529046897394	0.8361142841282865	0.1791009777606656	T	T	T
0.5001913227744806	0.3453325530664225	0.2638179992720211	T	T	T
0.5000834530272454	0.5004311788307315	0.1809040228322491	T	T	T
0.4971048377019033	0.0015186711928710	0.2579833363456065	T	T	T
0.0037197857845217	0.3352581443252173	0.2080742258396094	T	T	T
0.9812486516778109	0.8302717024040155	0.2909303754081328	T	T	T
0.0016497192778134	0.6605637460693834	0.2083511852509863	T	T	T
0.0182114679304945	0.1775901987686708	0.2935726546214621	T	T	T
0.7500000000000000	0.6666700000000034	0.1521299999999997	F	F	F
0.7500000000000000	0.1666700000000034	0.0688000000000031	F	F	F
0.2500000000000000	0.3333299999999966	0.1521299999999997	F	F	F
0.2500000000000000	0.8333299999999966	0.0688000000000031	F	F	F
0.7556378712624656	0.6618944217485369	0.3233349674699053	T	T	T
0.7538351599259078	0.1728897118296409	0.2375330884990046	T	T	T
0.2412659130552020	0.3547658531498049	0.3141251278669030	T	T	T
0.2454690842451081	0.8288540767187564	0.2363668886907181	T	T	T
0.6752946786432340	0.6579656554447872	0.3659707857286045	T	T	T
-0.0052138728345394	0.9969253600522768	0.3413950212800085	T	T	T
0.8361525818181434	0.9931942517264338	0.3663963150145674	T	T	T

Fe₃N (110) + *O

Fe N O

1.0000000000000000		
4.3045799999999996	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0405899999999999	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.8534000000000006

Fe N O

24 8 1

Selective dynamics

Direct

0.0000000000000000	0.5000000000000000	0.1230499999999992	F	F	F
0.0000000000000000	0.0000000000000000	0.0397200000000026	F	F	F
0.5000000000000000	0.1627799999999979	0.0125900000000030	F	F	F
0.5000000000000000	0.6627799999999979	0.0959300000000027	F	F	F

0.5000000000000000	0.8372200000000021	0.0125900000000030	F	F	F
0.5000000000000000	0.3372200000000021	0.0959300000000027	F	F	F
0.5000000000000000	0.5000000000000000	0.0145399999999967	F	F	F
0.5000000000000000	0.0000000000000000	0.0978700000000003	F	F	F
0.0000000000000000	0.3372200000000021	0.0416700000000034	F	F	F
0.0000000000000000	0.8372200000000021	0.1250000000000000	F	F	F
0.0000000000000000	0.6627799999999979	0.0416700000000034	F	F	F
0.0000000000000000	0.1627799999999979	0.1250000000000000	F	F	F
0.9910104759442934	0.5009752623201175	0.2905570989701497	T	T	T
0.9957557985432346	-0.0021969297153067	0.2055219288031717	T	T	T
0.5003124335431792	0.1648151438645509	0.1795013372598486	T	T	T
0.5017795899075560	0.6593660483759045	0.2646074197656237	T	T	T
0.4981676420924903	0.8348641670130771	0.1798810906073936	T	T	T
0.5000827515833334	0.3454847283499666	0.2642240333686457	T	T	T
0.4993950817722166	0.5000272072795997	0.1809639642629444	T	T	T
0.4938648805671084	0.0005645403706548	0.2606654818331283	T	T	T
-0.0008856673883322	0.3370658375615393	0.2079701328247942	T	T	T
0.9613072308103360	0.8326599063547341	0.2879729539275468	T	T	T
0.0020168995516820	0.6578999779377079	0.2085552446770985	T	T	T
0.0246523274518884	0.1707257058736150	0.2875968133129626	T	T	T
0.7500000000000000	0.6666700000000034	0.1521299999999997	F	F	F
0.7500000000000000	0.1666700000000034	0.0688000000000031	F	F	F
0.2500000000000000	0.3333299999999966	0.1521299999999997	F	F	F
0.2500000000000000	0.8333299999999966	0.0688000000000031	F	F	F
0.7532466160380622	0.6639339997509986	0.3226669340680450	T	T	T
0.7440616276190537	0.1700522772174456	0.2369647011966250	T	T	T
0.2311411772824479	0.3405085483921425	0.3136045264842600	T	T	T
0.2482103673467397	0.8295086547105378	0.2366967971703769	T	T	T
0.6851948507312831	0.6690753582015539	0.3658263047475626	T	T	T

Fe₃N (110) + *OH

Fe N O H

1.0000000000000000		
4.3045799999999996	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.0405899999999999	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.8534000000000006

Fe N O H

24 8 1 1

Selective dynamics

Direct

0.0000000000000000	0.5000000000000000	0.1230499999999992	F	F	F
0.0000000000000000	0.0000000000000000	0.0397200000000026	F	F	F

0.5000000000000000	0.1627799999999979	0.0125900000000030	F	F	F
0.5000000000000000	0.6627799999999979	0.0959300000000027	F	F	F
0.5000000000000000	0.8372200000000021	0.0125900000000030	F	F	F
0.5000000000000000	0.3372200000000021	0.0959300000000027	F	F	F
0.5000000000000000	0.5000000000000000	0.0145399999999967	F	F	F
0.5000000000000000	0.0000000000000000	0.0978700000000003	F	F	F
0.0000000000000000	0.3372200000000021	0.0416700000000034	F	F	F
0.0000000000000000	0.8372200000000021	0.1250000000000000	F	F	F
0.0000000000000000	0.6627799999999979	0.0416700000000034	F	F	F
0.0000000000000000	0.1627799999999979	0.1250000000000000	F	F	F
0.9910642722171278	0.4996243899146987	0.2889693372666465	T	T	T
0.9962340041824606	-0.0006635512430308	0.2059071375547173	T	T	T
0.5013711935062998	0.1650858522577551	0.1799182131051630	T	T	T
0.4988446180625848	0.6627246490991314	0.2636368978795999	T	T	T
0.4993287411969620	0.8353157344062029	0.1800936224569287	T	T	T
0.5035147674011473	0.3465446441356131	0.2637589429815653	T	T	T
0.4983089451350167	0.5005558540449838	0.1811447578298147	T	T	T
0.4965808677085045	0.0015352544392074	0.2616681048786691	T	T	T
0.9986283806512525	0.3366762837720992	0.2077721522773059	T	T	T
0.9668315380860861	0.8267842652106088	0.2892679467076404	T	T	T
0.0033502565255853	0.6593443375196699	0.2081388663736012	T	T	T
0.0337275070792764	0.1748479501723454	0.2879738919248128	T	T	T
0.7500000000000000	0.6666700000000034	0.1521299999999997	F	F	F
0.7500000000000000	0.1666700000000034	0.0688000000000031	F	F	F
0.2500000000000000	0.3333299999999966	0.1521299999999997	F	F	F
0.2500000000000000	0.8333299999999966	0.0688000000000031	F	F	F
0.7407592206252162	0.6573201575646772	0.3194952509456399	T	T	T
0.7470810491715437	0.1700885341732919	0.2376620795176407	T	T	T
0.2400013758789704	0.3478052389596273	0.3145164314495588	T	T	T
0.2482476994845020	0.8319268688694104	0.2371234290285943	T	T	T
0.6311715063815372	0.6327194872006145	0.3662469297130871	T	T	T
0.4918567463423095	0.5350512477631689	0.3634849910451782	T	T	T

Cr₃N₂ (110) - Surface

Cr N

1.0000000000000000		
5.6371200000000004	0.0000000000000000	0.0000000000000000
-1.4093135030247566	5.9627453468257468	0.0000000000000000
0.0000000000000000	0.0000000000000000	32.8644000000000034

Cr N

24 16

Selective dynamics

Direct

0.4792800000000028	0.9171100000000010	0.0618300000000005	F	F	F
0.3149349999999984	0.2597299999999976	0.0328200000000010	F	F	F
0.1715549999999979	0.6862100000000027	0.0075100000000035	F	F	F
0.4513499999999979	0.8053900000000027	0.1451599999999971	F	F	F
0.2870050000000006	0.1480099999999993	0.1161499999999975	F	F	F
0.1436250000000001	0.5744899999999973	0.0908400000000000	F	F	F
0.3963616892311532	0.6104483017640305	0.2179806546558280	T	T	T
-0.0867588400061782	-0.2162940418520518	0.2299477589194733	T	T	T
-0.2765181300828854	0.4093090238454242	0.1789861144061153	T	T	T
0.6117117009438667	0.5274571405542716	0.2933480019319651	T	T	T
0.2008971432202756	0.6719643297660028	0.2922903009587287	T	T	T
0.0156063093851228	0.2382991566015941	0.2352810763515419	T	T	T
0.3999650000000017	0.5998599999999996	0.0478299999999976	F	F	F
0.0585900000000024	0.2343699999999984	0.0758300000000034	F	F	F
0.3720349999999968	0.4881400000000014	0.1311600000000013	F	F	F
0.0306599999999975	0.1226500000000001	0.1591600000000000	F	F	F
0.3595661272698978	0.0846858221618851	0.2081051293447883	T	T	T
0.5988685480617147	-0.0124046571810642	0.2687615458216490	T	T	T
0.2505987371559207	0.1465351200519260	0.2981052799458070	T	T	T
0.4980030863481182	0.8351214840322335	0.3411869684687887	T	T	T
0.9792800000000028	0.9171100000000010	0.0618300000000005	F	F	F
0.8149349999999984	0.2597299999999976	0.0328200000000010	F	F	F
0.6715549999999979	0.6862100000000027	0.0075100000000035	F	F	F
0.9513499999999979	0.8053900000000027	0.1451599999999971	F	F	F
0.7870050000000006	0.1480099999999993	0.1161499999999975	F	F	F
0.6436250000000001	0.5744899999999973	0.0908400000000000	F	F	F
0.8027780650871743	0.4541989613870979	0.2458313818311978	T	T	T
0.2787036784574656	-0.1617700426955131	0.2428456066798803	T	T	T
0.6775132776584454	0.7160273927760435	0.1843007810163346	T	T	T
0.9440646829601136	0.6520815568148648	0.3273014091441886	T	T	T
0.4731913060102857	0.1330183580159937	0.3454519633126000	T	T	T
0.2891239489866342	0.4214438180377857	0.2658557711614157	T	T	T
0.8999650000000017	0.5998599999999996	0.0478299999999976	F	F	F
0.5585900000000024	0.2343699999999984	0.0758300000000034	F	F	F
0.8720349999999968	0.4881400000000014	0.1311600000000013	F	F	F
0.5306599999999975	0.1226500000000001	0.1591600000000000	F	F	F
0.6768993286695490	0.2458865435776578	0.2308357094394977	T	T	T
-0.0611581528458019	0.0026427774646064	0.2733033463687308	T	T	T
0.6002217089824101	0.2193683065520067	0.3122669815975709	T	T	T
0.7578426152382519	0.6864306816969967	0.3437051623365066	T	T	T

Cr₃N₂ (110) + *OOH

Cr N O H

1.0000000000000000

5.6371200000000004 0.0000000000000000 0.0000000000000000

-1.4093135030247566 5.9627453468257468 0.0000000000000000

0.0000000000000000 0.0000000000000000 32.8644000000000034

Cr N O H

24 16 2 1

Selective dynamics

Direct

0.4792800000000028 0.9171100000000010 0.0618300000000005 F F F

0.3149349999999984 0.2597299999999976 0.0328200000000010 F F F

0.1715549999999979 0.6862100000000027 0.0075100000000035 F F F

0.4513499999999979 0.8053900000000027 0.1451599999999971 F F F

0.2870050000000006 0.1480099999999993 0.1161499999999975 F F F

0.1436250000000001 0.5744899999999973 0.0908400000000000 F F F

0.5910476053743763 0.7198261803777370 0.2525802875885961 T T T

0.3791279728959400 -0.0303667067003835 0.2138670879347934 T T T

0.0306303331459393 0.5945614457511851 0.1799359885637077 T T T

0.6381204658840951 0.7417615407365185 0.3216867032113922 T T T

0.0319427642726220 0.8980893177861999 0.2800570294402702 T T T

0.1224410894717791 0.3139086487890600 0.2819135217327230 T T T

0.3999650000000017 0.5998599999999996 0.0478299999999976 F F F

0.0585900000000024 0.2343699999999984 0.0758300000000034 F F F

0.3720349999999968 0.4881400000000014 0.1311600000000013 F F F

0.0306599999999975 0.1226500000000001 0.1591600000000000 F F F

0.3292790735950367 0.3754502459035968 0.2165282470973282 T T T

0.8189937917729883 0.1629530842271798 0.2275589372980598 T T T

0.5247439987335174 0.1326859547332810 0.2848876319418022 T T T

0.2417263018612862 0.8914368286823526 0.3484326392244155 T T T

0.9119205895125182 0.1480232379226383 0.3416929624998288 T T T

0.9792800000000028 0.9171100000000010 0.0618300000000005 F F F

0.8149349999999984 0.2597299999999976 0.0328200000000010 F F F

0.6715549999999979 0.6862100000000027 0.0075100000000035 F F F

0.9513499999999979 0.8053900000000027 0.1451599999999971 F F F

0.7870050000000006 0.1480099999999993 0.1161499999999975 F F F

0.6436250000000001 0.5744899999999973 0.0908400000000000 F F F

0.9082682509525405 0.6580232364764537 0.2380609670872564 T T T

0.5847208224332413 0.2488342898667437 0.1927678311864695 T T T

0.3918375976095932 0.6748070954850257 0.1991664569720322 T T T

0.9558400437406465 0.6550475969893392 0.3261619119506496 T T T

0.5806697472595369 0.0370218035317930 0.3384019285271374 T T T

0.4685734339271114 0.4226784987134622 0.2760911668625922 T T T

0.8999650000000017	0.5998599999999996	0.0478299999999976	F	F	F
0.5585900000000024	0.2343699999999984	0.0758300000000034	F	F	F
0.8720349999999968	0.4881400000000014	0.1311600000000013	F	F	F
0.5306599999999975	0.1226500000000001	0.1591600000000000	F	F	F
0.9694368961432867	0.4620575913033646	0.2405801685120946	T	T	T
0.1167003317776060	0.0832291347457520	0.2309660859620775	T	T	T
-0.0189199886913749	0.4465981501699332	0.3219499136618054	T	T	T
0.0863257805732891	0.0616513343091730	0.3798208543006049	T	T	T
0.3880540079073676	0.6345183871991750	0.3652186338195516	T	T	T
0.4680021626035446	0.6615960856981231	0.3916910259493125	T	T	T

Cr₃N₂ (110) + *O

Cr N O

1.0000000000000000

5.6371200000000004 0.0000000000000000 0.0000000000000000

-1.4093135030247566 5.9627453468257468 0.0000000000000000

0.0000000000000000 0.0000000000000000 32.8644000000000034

Cr N O

24 16 1

Selective dynamics

Direct

0.4792800000000028	0.9171100000000010	0.0618300000000005	F	F	F
0.3149349999999984	0.2597299999999976	0.0328200000000010	F	F	F
0.1715549999999979	0.6862100000000027	0.0075100000000035	F	F	F
0.4513499999999979	0.8053900000000027	0.1451599999999971	F	F	F
0.2870050000000006	0.1480099999999993	0.1161499999999975	F	F	F
0.1436250000000001	0.5744899999999973	0.0908400000000000	F	F	F
0.6297760079050954	0.7734806953980208	0.2502394793046152	T	T	T
0.2574342222532934	-0.0339495845165079	0.2275664962509299	T	T	T
0.0443026761799000	0.5957805070548921	0.1779777911406560	T	T	T
0.4013714504717608	0.6392000938463346	0.3098473674016538	T	T	T
0.0253848923055347	0.8639296022209603	0.2994678197762065	T	T	T
0.1068747752284595	0.2714757983082718	0.2739301314930943	T	T	T
0.3999650000000017	0.5998599999999996	0.0478299999999976	F	F	F
0.0585900000000024	0.2343699999999984	0.0758300000000034	F	F	F
0.3720349999999968	0.4881400000000014	0.1311600000000013	F	F	F
0.0306599999999975	0.1226500000000001	0.1591600000000000	F	F	F
0.3376425626486786	0.4068555884616934	0.2156609975042027	T	T	T
0.7115408004585686	0.2461199374413108	0.2422121164240742	T	T	T
0.2260234206494477	0.1970112354257410	0.3495453941832851	T	T	T
0.4546521258695074	0.1003082094968878	0.2971054559795090	T	T	T
0.6453535737070112	0.8753827462244352	0.3353879939071819	T	T	T

0.9792800000000028	0.9171100000000010	0.0618300000000005	F	F	F
0.8149349999999984	0.2597299999999976	0.0328200000000010	F	F	F
0.6715549999999979	0.6862100000000027	0.0075100000000035	F	F	F
0.9513499999999979	0.8053900000000027	0.1451599999999971	F	F	F
0.7870050000000006	0.1480099999999993	0.1161499999999975	F	F	F
0.6436250000000001	0.5744899999999973	0.0908400000000000	F	F	F
0.9679914869640162	0.7262389672537858	0.2456579277438029	T	T	T
0.5316385739569630	0.2108315066663632	0.1947054972667565	T	T	T
0.4061639926833477	0.7280224723481120	0.2034383574122678	T	T	T
0.0481306570434810	0.6180169398388622	0.3259900597641736	T	T	T
0.7884058391439105	0.0470414552713448	0.2845471885721890	T	T	T
0.4871279955329623	0.4261504686233258	0.2703076691433057	T	T	T
0.8999650000000017	0.5998599999999996	0.0478299999999976	F	F	F
0.5585900000000024	0.2343699999999984	0.0758300000000034	F	F	F
0.8720349999999968	0.4881400000000014	0.1311600000000013	F	F	F
0.5306599999999975	0.1226500000000001	0.1591600000000000	F	F	F
0.9786808152260510	0.5110225541621729	0.2365919109136578	T	T	T
0.0438847213807098	0.1584066218251033	0.2170881119122900	T	T	T
0.0808158226972128	0.4258543246468574	0.3344631972580971	T	T	T
0.4884103264579508	0.0796533016925433	0.3604027554239543	T	T	T

Cr₃N₂ (110) + *OH

Cr N O H

1.0000000000000000

5.6371200000000004	0.0000000000000000	0.0000000000000000
-1.4093135030247566	5.9627453468257468	0.0000000000000000
0.0000000000000000	0.0000000000000000	32.8644000000000034

Cr N O H

24 16 1 1

Selective dynamics

Direct

0.4792800000000028	0.9171100000000010	0.0618300000000005	F	F	F
0.3149349999999984	0.2597299999999976	0.0328200000000010	F	F	F
0.1715549999999979	0.6862100000000027	0.0075100000000035	F	F	F
0.4513499999999979	0.8053900000000027	0.1451599999999971	F	F	F
0.2870050000000006	0.1480099999999993	0.1161499999999975	F	F	F
0.1436250000000001	0.5744899999999973	0.0908400000000000	F	F	F
0.6748685288796330	0.7381540964431711	0.2481566766347359	T	T	T
0.3165732558525315	-0.0326317544017930	0.2212711575728539	T	T	T
0.0226649749234458	0.5937922156453033	0.1792046981948414	T	T	T
0.5150552032630201	0.7840373879826142	0.3146076476194090	T	T	T
0.0935274228579125	0.9128463044605802	0.2936652147356529	T	T	T

0.2603585300874519	0.4517524250983301	0.2838669742263996	T	T	T
0.3999650000000017	0.5998599999999996	0.0478299999999976	F	F	F
0.0585900000000024	0.2343699999999984	0.0758300000000034	F	F	F
0.3720349999999968	0.4881400000000014	0.1311600000000013	F	F	F
0.0306599999999975	0.1226500000000001	0.1591600000000000	F	F	F
0.3596278051646253	0.4090729256131996	0.2151292554329973	T	T	T
0.7990466892173373	0.2298135381117261	0.2407637426018690	T	T	T
0.4758946024957571	0.1607414587085170	0.2980111855321128	T	T	T
0.9125332787764496	0.1731016805121581	0.3347075948858493	T	T	T
0.5287194383139627	0.1239666878602702	0.3704385314961791	T	T	T
0.9792800000000028	0.9171100000000010	0.0618300000000005	F	F	F
0.8149349999999984	0.2597299999999976	0.0328200000000010	F	F	F
0.6715549999999979	0.6862100000000027	0.0075100000000035	F	F	F
0.9513499999999979	0.8053900000000027	0.1451599999999971	F	F	F
0.7870050000000006	0.1480099999999993	0.1161499999999975	F	F	F
0.6436250000000001	0.5744899999999973	0.0908400000000000	F	F	F
0.0213538121057844	0.7306039663904644	0.2407911583572714	T	T	T
0.5815044854147786	0.2243286852426950	0.1941620876783920	T	T	T
0.4864842060914299	0.7302882864065922	0.2018012765639962	T	T	T
0.1606313043488408	0.6593936658356774	0.3249735406292665	T	T	T
0.7674002737352701	0.0033970786200556	0.2858003771994044	T	T	T
0.5754757722226423	0.4287328923601504	0.2646822695345034	T	T	T
0.8999650000000017	0.5998599999999996	0.0478299999999976	F	F	F
0.5585900000000024	0.2343699999999984	0.0758300000000034	F	F	F
0.8720349999999968	0.4881400000000014	0.1311600000000013	F	F	F
0.5306599999999975	0.1226500000000001	0.1591600000000000	F	F	F
0.0604965097988997	0.5116282269410486	0.2390916597967849	T	T	T
0.0847645063652721	0.1465529645918131	0.2146305591692663	T	T	T
0.0343690588128231	0.4633815508132381	0.3324106854553848	T	T	T
0.2192066182743079	0.0872436947774798	0.3437549573302187	T	T	T
0.8299082184384102	0.1282552974835201	0.3859345226623513	T	T	T

Cr₂N (110) - Surface

Cr N

1.0000000000000000		
4.3887799999999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.2692700000000006	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.6456000000000017

Cr N

24 12

Selective dynamics

Direct

0.2528999999999968	0.1631799999999970	0.0127299999999977	F	F	F
0.2528999999999968	0.6631799999999970	0.0960600000000014	F	F	F
0.2528999999999968	0.8368200000000030	0.0127299999999977	F	F	F
0.2528999999999968	0.3368200000000030	0.0960600000000014	F	F	F
0.2528999999999968	0.5000000000000000	0.0144700000000029	F	F	F
0.2528999999999968	0.0000000000000000	0.0977999999999994	F	F	F
0.7471000000000032	0.5000000000000000	0.1232600000000019	F	F	F
0.7471000000000032	0.0000000000000000	0.0399200000000022	F	F	F
0.7471000000000032	0.3368200000000030	0.0416700000000034	F	F	F
0.7471000000000032	0.8368200000000030	0.1250000000000000	F	F	F
0.7471000000000032	0.6631799999999970	0.0416700000000034	F	F	F
0.7471000000000032	0.1631799999999970	0.1250000000000000	F	F	F
0.2498608700509189	0.1661770120456993	0.1800792533888242	T	T	T
0.2531906643399364	0.6718850682177816	0.2648917727674691	T	T	T
0.2498067271963688	0.8337787276631299	0.1800931806257774	T	T	T
0.2533352275230251	0.3280794057809672	0.2648691603780414	T	T	T
0.2555382575671817	0.4999972508696971	0.1832381563767014	T	T	T
0.2246470794759941	0.0000043063458053	0.2615120060104971	T	T	T
0.7108229590431240	0.4999972232951270	0.2897692014051046	T	T	T
0.7485800688019016	-0.0000393586493232	0.2065072254263040	T	T	T
0.7528328780549342	0.3372594005363551	0.2085649428196442	T	T	T
0.7623752939267744	0.8228090396647829	0.2893660564418405	T	T	T
0.7527570440076025	0.6626628590693836	0.2085792814682405	T	T	T
0.7624575018085429	0.1771594135207845	0.2893571800818810	T	T	T
0.0000000000000000	0.5000000000000000	0.0688600000000008	F	F	F
0.0000000000000000	0.0000000000000000	0.1522000000000006	F	F	F
0.5000000000000000	0.6666700000000034	0.1522000000000006	F	F	F
0.5000000000000000	0.1666700000000034	0.0688600000000008	F	F	F
0.5000000000000000	0.3333299999999966	0.1522000000000006	F	F	F
0.5000000000000000	0.8333299999999966	0.0688600000000008	F	F	F
0.0021839066843494	0.4999589406031261	0.2397176265681224	T	T	T
0.9547132076135708	-0.0000224178016002	0.3123807611470300	T	T	T
0.5278403747353860	0.6735098820348836	0.3173165312150559	T	T	T
0.4993601022537301	0.1644915577548668	0.2364165484835107	T	T	T
0.5279699394623332	0.3264557412662776	0.3173013798367910	T	T	T
0.4992712486271738	0.8354490565393111	0.2364312295788034	T	T	T

Cr₂N (110) + *OOH

Cr N O H

1.0000000000000000		
4.3887799999999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.2692700000000006	0.0000000000000000

0.0000000000000000 0.0000000000000000 28.645600000000017

Cr N O H

24 12 2 1

Selective dynamics

Direct

0.2528999999999968	0.1631799999999970	0.0127299999999977	F	F	F
0.2528999999999968	0.6631799999999970	0.0960600000000014	F	F	F
0.2528999999999968	0.8368200000000030	0.0127299999999977	F	F	F
0.2528999999999968	0.3368200000000030	0.0960600000000014	F	F	F
0.2528999999999968	0.5000000000000000	0.0144700000000029	F	F	F
0.2528999999999968	0.0000000000000000	0.0977999999999994	F	F	F
0.7471000000000032	0.5000000000000000	0.1232600000000019	F	F	F
0.7471000000000032	0.0000000000000000	0.0399200000000022	F	F	F
0.7471000000000032	0.3368200000000030	0.0416700000000034	F	F	F
0.7471000000000032	0.8368200000000030	0.1250000000000000	F	F	F
0.7471000000000032	0.6631799999999970	0.0416700000000034	F	F	F
0.7471000000000032	0.1631799999999970	0.1250000000000000	F	F	F
0.2498707187993779	0.1660986295472615	0.1800604798179030	T	T	T
0.2539200717384268	0.6676758588043756	0.2651885396045890	T	T	T
0.2515981494727913	0.8342465433829337	0.1798754411711121	T	T	T
0.2502797025959701	0.3295115518093036	0.2653712729761749	T	T	T
0.2531814033622209	0.5003612512226530	0.1824167931436021	T	T	T
0.2237914551408157	-0.0011797960994516	0.2614438115083276	T	T	T
0.7211724395738019	0.4987045020039212	0.2899202160894959	T	T	T
0.7459126696612108	-0.0004327705775992	0.2063663302722401	T	T	T
0.7516295678640513	0.3367173913607909	0.2084147235287022	T	T	T
0.7647465751305494	0.8219629968625469	0.2906894893624302	T	T	T
0.7517740180673387	0.6637406860963502	0.2086439413016049	T	T	T
0.7595741433719623	0.1793624366149650	0.2895707848352572	T	T	T
0.0000000000000000	0.5000000000000000	0.0688600000000008	F	F	F
0.0000000000000000	0.0000000000000000	0.1522000000000006	F	F	F
0.5000000000000000	0.6666700000000034	0.1522000000000006	F	F	F
0.5000000000000000	0.1666700000000034	0.0688600000000008	F	F	F
0.5000000000000000	0.3333299999999966	0.1522000000000006	F	F	F
0.5000000000000000	0.8333299999999966	0.0688600000000008	F	F	F
0.0033035142339655	0.4997889666546532	0.2387324595772111	T	T	T
0.9544779269636270	0.0013963514921233	0.3120769177248275	T	T	T
0.5044408414991024	0.6689127760439749	0.3214697777763325	T	T	T
0.4960918369929578	0.1645458858500053	0.2367345121216842	T	T	T
0.5231635731935146	0.3280271583428458	0.3181222675046607	T	T	T
0.5000405037790058	0.8349384486039184	0.2372359135002161	T	T	T
0.4053424522247958	0.6645427756767787	0.3671830364502500	T	T	T
0.6155725674803021	0.5607278879876797	0.3949379804876632	T	T	T
0.5448402945638422	0.4530739056795887	0.3843613282449769	T	T	T

Cr₂N (110) + *O

Cr N O

1.0000000000000000
4.3887799999999997 0.0000000000000000 0.0000000000000000
0.0000000000000000 8.2692700000000006 0.0000000000000000
0.0000000000000000 0.0000000000000000 28.6456000000000017

Cr N O

24 12 1

Selective dynamics

Direct

0.25289999999999968	0.16317999999999970	0.01272999999999977	F	F	F
0.25289999999999968	0.66317999999999970	0.09606000000000014	F	F	F
0.25289999999999968	0.83682000000000030	0.01272999999999977	F	F	F
0.25289999999999968	0.33682000000000030	0.09606000000000014	F	F	F
0.25289999999999968	0.50000000000000000	0.01447000000000029	F	F	F
0.25289999999999968	0.00000000000000000	0.09779999999999994	F	F	F
0.74710000000000032	0.50000000000000000	0.12326000000000019	F	F	F
0.74710000000000032	0.00000000000000000	0.03992000000000022	F	F	F
0.74710000000000032	0.33682000000000030	0.04167000000000034	F	F	F
0.74710000000000032	0.83682000000000030	0.12500000000000000	F	F	F
0.74710000000000032	0.66317999999999970	0.04167000000000034	F	F	F
0.74710000000000032	0.16317999999999970	0.12500000000000000	F	F	F
0.2488266692477185	0.1665455204012431	0.1801744422527417	T	T	T
0.2592965140265013	0.6667596898034810	0.2642508466748235	T	T	T
0.2506014565963030	0.8333343593723774	0.1801545043196957	T	T	T
0.2521383612652472	0.3299953372183558	0.2649174895457802	T	T	T
0.2543276060354946	0.5013376804066864	0.1826027966177365	T	T	T
0.2259656187881823	0.9978377867672906	0.2611894738436396	T	T	T
0.7161988922458399	0.4996331813912989	0.2897561913554917	T	T	T
0.7464486207957882	-0.0001568078091057	0.2061141755807707	T	T	T
0.7522368071857769	0.3370749181973809	0.2081462628443243	T	T	T
0.7647602651262763	0.8222942238969251	0.2905484349167440	T	T	T
0.7564936433128137	0.6638014972061881	0.2082634441763712	T	T	T
0.7627924631874493	0.1796728246440260	0.2891056303426323	T	T	T
0.00000000000000000	0.50000000000000000	0.06886000000000008	F	F	F
0.00000000000000000	0.00000000000000000	0.15220000000000006	F	F	F
0.50000000000000000	0.66667000000000034	0.15220000000000006	F	F	F
0.50000000000000000	0.16667000000000034	0.06886000000000008	F	F	F
0.50000000000000000	0.33332999999999966	0.15220000000000006	F	F	F
0.50000000000000000	0.83332999999999966	0.06886000000000008	F	F	F
0.0019399245880059	0.4991544654843994	0.2391170872562835	T	T	T
0.9552069731352844	0.0004681708148152	0.3117089659382726	T	T	T
0.5296480202157325	0.6763167730029438	0.3255030190512919	T	T	T

0.4971865769077080	0.1646953723792734	0.2364875618946858	T	T	T
0.5241954339887246	0.3279834102736333	0.3169772293901422	T	T	T
0.5038493484477365	0.8342048849120641	0.2373557664415823	T	T	T
0.4345652501646105	0.6707619004632702	0.3661975627898459	T	T	T

Cr₂N (110) + *OH

Cr N O H

1.0000000000000000		
4.3887799999999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	8.2692700000000006	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.6456000000000017

Cr N O H

24 12 1 1

Selective dynamics

Direct

0.2528999999999968	0.1631799999999970	0.0127299999999977	F	F	F
0.2528999999999968	0.6631799999999970	0.0960600000000014	F	F	F
0.2528999999999968	0.8368200000000030	0.0127299999999977	F	F	F
0.2528999999999968	0.3368200000000030	0.0960600000000014	F	F	F
0.2528999999999968	0.5000000000000000	0.0144700000000029	F	F	F
0.2528999999999968	0.0000000000000000	0.0977999999999994	F	F	F
0.7471000000000032	0.5000000000000000	0.1232600000000019	F	F	F
0.7471000000000032	0.0000000000000000	0.0399200000000022	F	F	F
0.7471000000000032	0.3368200000000030	0.0416700000000034	F	F	F
0.7471000000000032	0.8368200000000030	0.1250000000000000	F	F	F
0.7471000000000032	0.6631799999999970	0.0416700000000034	F	F	F
0.7471000000000032	0.1631799999999970	0.1250000000000000	F	F	F
0.2499090220838680	0.1659152840396333	0.1801737866929979	T	T	T
0.2536282827903947	0.6686820092922634	0.2651786038316635	T	T	T
0.2516998561525991	0.8343645182919344	0.1799727888573852	T	T	T
0.2498762070260354	0.3300412274722104	0.2654419609930884	T	T	T
0.2537756763779985	0.5003643079882374	0.1823190337243655	T	T	T
0.2220711876071988	0.9986156535114874	0.2615810901781139	T	T	T
0.7208256397985188	0.4983393322307712	0.2891069606704186	T	T	T
0.7458480655678327	0.0001227898308991	0.2063934405606389	T	T	T
0.7512656303926974	0.3363839351220383	0.2083957597660184	T	T	T
0.7611821775096211	0.8211646997119549	0.2911969635595796	T	T	T
0.7524746560271810	0.6643844923543416	0.2085276500967981	T	T	T
0.7570450473124115	0.1797045466938871	0.2901025080338331	T	T	T
0.0000000000000000	0.5000000000000000	0.0688600000000008	F	F	F
0.0000000000000000	0.0000000000000000	0.1522000000000006	F	F	F
0.5000000000000000	0.6666700000000034	0.1522000000000006	F	F	F

0.5000000000000000	0.1666700000000034	0.0688600000000008	F	F	F
0.5000000000000000	0.3333299999999966	0.1522000000000006	F	F	F
0.5000000000000000	0.8333299999999966	0.0688600000000008	F	F	F
0.0048874679469553	0.5002508222303962	0.2384245036870959	T	T	T
0.9516150036326289	0.0005282180882565	0.3121388667080364	T	T	T
0.5107771298156877	0.6675805289154561	0.3216235677574477	T	T	T
0.4953525915574331	0.1645756942294330	0.2370108443525848	T	T	T
0.5238670525941618	0.3308895970940173	0.3184365886251559	T	T	T
0.5003119754894964	0.8353237874682941	0.2373630863379476	T	T	T
0.4321637683874576	0.6561108550924081	0.3689905762980165	T	T	T
0.4150780588350791	0.5384968959996830	0.3743042256156489	T	T	T

MnN (100) - Surface

Mn N

1.0000000000000000		
6.0279400000000001	0.0000000000000000	0.0000000000000000
3.0139700000000009	5.2203491724883690	0.0000000000000000
0.0000000000000000	0.0000000000000000	29.530699999999995

Mn N

16 16

Selective dynamics

Direct

0.0625000000000000	0.3750000000000000	0.0312500000000000	F	F	F
0.2291700000000034	0.0416700000000034	0.1145799999999966	F	F	F
0.3956497321636986	0.2080340142002631	0.1986476916777432	T	T	T
0.0621698111750416	0.3745804846071749	0.2832881121319949	T	T	T
0.0625000000000000	0.8750000000000000	0.0312500000000000	F	F	F
0.2291700000000034	0.5416699999999963	0.1145799999999966	F	F	F
0.3956064927255862	0.7079726994700108	0.1986577974769688	T	T	T
0.0621732047782275	0.8745631384327724	0.2833022345277099	T	T	T
0.5625000000000000	0.3750000000000000	0.0312500000000000	F	F	F
0.7291700000000034	0.0416700000000034	0.1145799999999966	F	F	F
0.8955582196586434	0.2080110455178228	0.1986572814364621	T	T	T
0.5621816828780907	0.3745484336974884	0.2833336823519791	T	T	T
0.5625000000000000	0.8750000000000000	0.0312500000000000	F	F	F
0.7291700000000034	0.5416699999999963	0.1145799999999966	F	F	F
0.8956174027568589	0.7080289293849250	0.1986427236355116	T	T	T
0.5621922255391792	0.8745592887035829	0.2832968345264285	T	T	T
0.2291700000000034	0.0416700000000034	0.0520799999999966	F	F	F
0.3958299999999966	0.2083299999999966	0.1354200000000034	F	F	F
0.0622234995056851	0.3748135625342278	0.2216783316641276	T	T	T
0.2288678964433882	0.0412539424102866	0.3007002516696603	T	T	T

0.2291700000000034	0.5416699999999963	0.0520799999999966	F	F	F
0.3958299999999966	0.7083299999999966	0.1354200000000034	F	F	F
0.0621605387788026	0.8746625019787686	0.2216961247756039	T	T	T
0.2287884874751957	0.5412407530827172	0.3007216032150401	T	T	T
0.7291700000000034	0.0416700000000034	0.0520799999999966	F	F	F
0.8958299999999966	0.2083299999999966	0.1354200000000034	F	F	F
0.5622877107754570	0.3746516383271398	0.2217362346474535	T	T	T
0.7288479884919136	0.0411720070584419	0.3007317781010664	T	T	T
0.7291700000000034	0.5416699999999963	0.0520799999999966	F	F	F
0.8958299999999966	0.7083299999999966	0.1354200000000034	F	F	F
0.5624172959862987	0.8746651654216518	0.2216898371021870	T	T	T
0.7288758241496834	0.5412680762443289	0.3007052889354681	T	T	T

MnN (100) + *OOH

Mn N O H

1.0000000000000000					
6.0279400000000001	0.0000000000000000	0.0000000000000000			
3.0139700000000009	5.2203491724883690	0.0000000000000000			
0.0000000000000000	0.0000000000000000	29.5306999999999995			

Mn N O H

16 16 2 1

Selective dynamics

Direct

0.0625000000000000	0.3750000000000000	0.0312500000000000	F	F	F
0.2291700000000034	0.0416700000000034	0.1145799999999966	F	F	F
0.3990200146371193	0.2117446812272784	0.1985969615288428	T	T	T
0.0592572223477269	0.3711324294149964	0.2827491695513143	T	T	T
0.0625000000000000	0.8750000000000000	0.0312500000000000	F	F	F
0.2291700000000034	0.5416699999999963	0.1145799999999966	F	F	F
0.3964201211860431	0.6969667457867866	0.1992643929251691	T	T	T
0.0590582433489687	0.8715872711071007	0.2842543742199514	T	T	T
0.5625000000000000	0.3750000000000000	0.0312500000000000	F	F	F
0.7291700000000034	0.0416700000000034	0.1145799999999966	F	F	F
0.8837924854484902	0.2097421630586975	0.1993459352950824	T	T	T
0.5578221486778880	0.3704414259590640	0.3041995963100344	T	T	T
0.5625000000000000	0.8750000000000000	0.0312500000000000	F	F	F
0.7291700000000034	0.5416699999999963	0.1145799999999966	F	F	F
0.8925620601031892	0.7058608215043609	0.1985686085396865	T	T	T
0.5575628725297045	0.8724730772897105	0.2828888987799252	T	T	T
0.2291700000000034	0.0416700000000034	0.0520799999999966	F	F	F
0.3958299999999966	0.2083299999999966	0.1354200000000034	F	F	F
0.0677884431864767	0.3725233242723804	0.2200619911380297	T	T	T

0.2248760943046501	0.0402150681116007	0.2984198580655251	T	T	T
0.2291700000000034	0.5416699999999963	0.0520799999999966	F	F	F
0.3958299999999966	0.7083299999999966	0.1354200000000034	F	F	F
0.0575485872298238	0.8707734155908186	0.2221257097152390	T	T	T
0.2009837974312994	0.5494787771070292	0.3012014320069993	T	T	T
0.7291700000000034	0.0416700000000034	0.0520799999999966	F	F	F
0.8958299999999966	0.2083299999999966	0.1354200000000034	F	F	F
0.5550971623010581	0.3682588495731493	0.2240125417935697	T	T	T
0.7360382616286582	0.0145936784968355	0.3013982494792374	T	T	T
0.7291700000000034	0.5416699999999963	0.0520799999999966	F	F	F
0.8958299999999966	0.7083299999999966	0.1354200000000034	F	F	F
0.5599150650968727	0.8803937800749970	0.2202482737080604	T	T	T
0.7361793180655828	0.5497443926001117	0.2996997429832357	T	T	T
0.5798508415564080	0.3390464268051438	0.3659438613575232	T	T	T
0.4484327958397713	0.5883989825958809	0.3870425605328729	T	T	T
0.5931509551482727	0.6120806109971242	0.3953635819314024	T	T	T

MnN (100) + *O

Mn N O

1.0000000000000000		
6.0279400000000001	0.0000000000000000	0.0000000000000000
3.0139700000000009	5.2203491724883690	0.0000000000000000
0.0000000000000000	0.0000000000000000	29.5306999999999995

Mn N O

16 16 1

Selective dynamics

Direct

0.0625000000000000	0.3750000000000000	0.0312500000000000	F	F	F
0.2291700000000034	0.0416700000000034	0.1145799999999966	F	F	F
0.3962756139423267	0.2068968012587030	0.1983801896876437	T	T	T
0.0593756138210473	0.3739803313265689	0.2850674430370555	T	T	T
0.0625000000000000	0.8750000000000000	0.0312500000000000	F	F	F
0.2291700000000034	0.5416699999999963	0.1145799999999966	F	F	F
0.3961439246856540	0.7041292146060647	0.1985252693064009	T	T	T
0.0594231128964083	0.8694945275543978	0.2851533338123668	T	T	T
0.5625000000000000	0.3750000000000000	0.0312500000000000	F	F	F
0.7291700000000034	0.0416700000000034	0.1145799999999966	F	F	F
0.8923061548829438	0.2074132879570140	0.1986576262646243	T	T	T
0.5574800231637743	0.3724013942732468	0.3223968939683223	T	T	T
0.5625000000000000	0.8750000000000000	0.0312500000000000	F	F	F
0.7291700000000034	0.5416699999999963	0.1145799999999966	F	F	F
0.8938542912441509	0.7061827857636158	0.1996072823210741	T	T	T

0.5629336970031424	0.8698860342964551	0.2856570473853138	T	T	T
0.2291700000000034	0.0416700000000034	0.0520799999999966	F	F	F
0.3958299999999966	0.2083299999999966	0.1354200000000034	F	F	F
0.0628032172745105	0.3741465737119820	0.2223867525916950	T	T	T
0.2222821021805211	0.0406448552984905	0.3001796255612025	T	T	T
0.2291700000000034	0.5416699999999963	0.0520799999999966	F	F	F
0.3958299999999966	0.7083299999999966	0.1354200000000034	F	F	F
0.0614240310444401	0.8703649930429390	0.2224882266450699	T	T	T
0.2123867007766755	0.5447243729339268	0.3041351492991631	T	T	T
0.7291700000000034	0.0416700000000034	0.0520799999999966	F	F	F
0.8958299999999966	0.2083299999999966	0.1354200000000034	F	F	F
0.5591247731707677	0.3734074874498684	0.2160603877152402	T	T	T
0.7340121415110242	0.0277154731586536	0.3039068056171276	T	T	T
0.7291700000000034	0.5416699999999963	0.0520799999999966	F	F	F
0.8958299999999966	0.7083299999999966	0.1354200000000034	F	F	F
0.5612513436524629	0.8736259896916552	0.2221687621047350	T	T	T
0.7339986676546927	0.5402581412443727	0.3035114155988689	T	T	T
0.5585090759452203	0.3724811752013087	0.3764405371398035	T	T	T

MnN (100) + *OH

Mn N O H

1.0000000000000000			
6.0279400000000001	0.0000000000000000	0.0000000000000000	
3.0139700000000009	5.2203491724883690	0.0000000000000000	
0.0000000000000000	0.0000000000000000	29.530699999999995	

Mn N O H

16 16 1 1

Selective dynamics

Direct

0.0625000000000000	0.3750000000000000	0.0312500000000000	F	F	F
0.2291700000000034	0.0416700000000034	0.1145799999999966	F	F	F
0.4002637591347539	0.2100672286284000	0.1985612534881924	T	T	T
0.0625150799228883	0.3672934970335930	0.2818374229335431	T	T	T
0.0625000000000000	0.8750000000000000	0.0312500000000000	F	F	F
0.2291700000000034	0.5416699999999963	0.1145799999999966	F	F	F
0.3998575103157916	0.6948589718350511	0.1991140333278018	T	T	T
0.0613748899876811	0.8706473996190298	0.2830199736125829	T	T	T
0.5625000000000000	0.3750000000000000	0.0312500000000000	F	F	F
0.7291700000000034	0.0416700000000034	0.1145799999999966	F	F	F
0.8842342240126699	0.2103043053726535	0.1987933908181013	T	T	T
0.5603160938018124	0.3689173968367283	0.3035623040025305	T	T	T
0.5625000000000000	0.8750000000000000	0.0312500000000000	F	F	F

0.7291700000000034	0.5416699999999963	0.1145799999999966	F	F	F
0.8947528963057197	0.7059203499009683	0.1980781928642319	T	T	T
0.5603398026304250	0.8705272506839594	0.2827085604368276	T	T	T
0.2291700000000034	0.0416700000000034	0.0520799999999966	F	F	F
0.3958299999999966	0.2083299999999966	0.1354200000000034	F	F	F
0.0635714948588926	0.3726647648580779	0.2188925939807206	T	T	T
0.2280641585158758	0.0371441624897603	0.2982660642285725	T	T	T
0.2291700000000034	0.5416699999999963	0.0520799999999966	F	F	F
0.3958299999999966	0.7083299999999966	0.1354200000000034	F	F	F
0.0570006136861757	0.8733298665520888	0.2205885559391607	T	T	T
0.2019513694778732	0.5488695798148842	0.2992626637935538	T	T	T
0.7291700000000034	0.0416700000000034	0.0520799999999966	F	F	F
0.8958299999999966	0.2083299999999966	0.1354200000000034	F	F	F
0.5617534174277827	0.3662016006685250	0.2236376825200938	T	T	T
0.7404750997271755	0.0113299636279256	0.3010852391116551	T	T	T
0.7291700000000034	0.5416699999999963	0.0520799999999966	F	F	F
0.8958299999999966	0.7083299999999966	0.1354200000000034	F	F	F
0.5638895154009026	0.8759222683829938	0.2200211867051662	T	T	T
0.7405705469552141	0.5477751414552949	0.2987193533770164	T	T	T
0.5558605535300672	0.3697620420761830	0.3649036904416826	T	T	T
0.6684624491807328	0.1991586358304858	0.3772893392690580	T	T	T

Nb₄N₅ (100) - Surface

Nb N

1.0000000000000000		
5.3445200000000002	0.0000000000000000	0.0000000000000000
-1.7272543693964146	10.5485218558526483	0.0000000000000000
0.0000000000000000	0.0000000000000000	29.2037000000000013

Nb N

16 20

Selective dynamics

Direct

0.4208900000000000	0.1857100000000003	0.1081700000000012	F	F	F
0.4004699999999985	0.0837300000000027	0.0056799999999981	F	F	F
0.6826200000000000	0.3747200000000035	0.0316499999999991	F	F	F
0.9404299999999992	0.1336399999999998	0.0541600000000031	F	F	F
0.7343229421803670	0.0251660989309214	0.2250791268382200	T	T	T
0.6901403948268173	0.4470567350261742	0.1270876068686638	T	T	T
0.9812984146436868	0.2332140986823324	0.1604535515290029	T	T	T
0.2324130842917316	0.4879178366680899	0.1885315569223498	T	T	T
0.4208900000000000	0.6857100000000003	0.1081700000000012	F	F	F

0.4004699999999985	0.5837300000000027	0.0056799999999981	F	F	F
0.6826200000000000	0.8747200000000035	0.0316499999999991	F	F	F
0.9404299999999992	0.6336399999999998	0.0541600000000031	F	F	F
0.7341520360854594	0.5251998339830238	0.2250692206568394	T	T	T
0.6902435434310774	0.9470836650134447	0.1270903645021745	T	T	T
0.9812560656902699	0.7332369453983228	0.1604290835106227	T	T	T
0.2325448631003520	0.9878635859491803	0.1885245104550515	T	T	T
0.0415399999999977	0.4792300000000012	0.0186700000000002	F	F	F
0.0536699999999968	0.0664599999999993	0.1193200000000019	F	F	F
0.8081099999999992	0.2907399999999996	0.0928299999999993	F	F	F
0.5531999999999968	0.0285999999999973	0.0694999999999979	F	F	F
0.3076399999999992	0.2528799999999976	0.0430100000000024	F	F	F
0.3334830127335220	0.3396503513677391	0.1449684825481490	T	T	T
0.3857548932415856	0.4591681851941633	0.2448261796435686	T	T	T
0.0621190688643090	0.1449414759682376	0.2168522303210031	T	T	T
0.8494688650556982	0.3845994500695953	0.1944356479671060	T	T	T
0.5955583993056931	0.1072631654311149	0.1707223621816994	T	T	T
0.0415399999999977	0.9792300000000012	0.0186700000000002	F	F	F
0.0536699999999968	0.5664599999999993	0.1193200000000019	F	F	F
0.8081099999999992	0.7907399999999996	0.0928299999999993	F	F	F
0.5531999999999968	0.5285999999999973	0.0694999999999979	F	F	F
0.3076399999999992	0.7528799999999976	0.0430100000000024	F	F	F
0.3335122221387922	0.8396335931058801	0.1449725637721258	T	T	T
0.3859134097948910	0.9590250094111598	0.2448248635866055	T	T	T
0.0619372834046460	0.6449665575349792	0.2168491926632551	T	T	T
0.8495485548719025	0.8845876410304756	0.1944375596452295	T	T	T
0.5954780976439416	0.6072825961044815	0.1707031200499467	T	T	T

Nb₄N₅ (100) + *OOH

Nb N O H

1.0000000000000000		
5.3445200000000002	0.0000000000000000	0.0000000000000000
-1.7272543693964146	10.5485218558526483	0.0000000000000000
0.0000000000000000	0.0000000000000000	29.2037000000000013

Nb N O H

16 20 2 1

Selective dynamics

Direct

0.4208900000000000	0.1857100000000003	0.1081700000000012	F	F	F
0.4004699999999985	0.0837300000000027	0.0056799999999981	F	F	F
0.6826200000000000	0.3747200000000035	0.0316499999999991	F	F	F
0.9404299999999992	0.1336399999999998	0.0541600000000031	F	F	F

0.7163181388510456	0.0238320651609883	0.2237464516167240	T	T	T
0.6885369478678811	0.4468022330814647	0.1267643158387591	T	T	T
0.9770969065481362	0.2297303308541261	0.1617891291588134	T	T	T
0.2323056751401142	0.4865307511608434	0.1883255463088837	T	T	T
0.4208900000000000	0.6857100000000003	0.1081700000000012	F	F	F
0.4004699999999985	0.5837300000000027	0.0056799999999981	F	F	F
0.6826200000000000	0.8747200000000035	0.0316499999999991	F	F	F
0.9404299999999992	0.6336399999999998	0.0541600000000031	F	F	F
0.7337856731209379	0.5244194485282918	0.2255295798853229	T	T	T
0.6788480271180177	0.9436809706610872	0.1271005071487916	T	T	T
0.9795127327713030	0.7325351008972903	0.1610917018312269	T	T	T
0.2277167068677745	-0.0049310869164746	0.1836044037615311	T	T	T
0.0415399999999977	0.4792300000000012	0.0186700000000002	F	F	F
0.0536699999999968	0.0664599999999993	0.1193200000000019	F	F	F
0.8081099999999992	0.2907399999999996	0.0928299999999993	F	F	F
0.5531999999999968	0.0285999999999973	0.0694999999999979	F	F	F
0.3076399999999992	0.2528799999999976	0.0430100000000024	F	F	F
0.3313465512369319	0.3384088851428221	0.1450645522839729	T	T	T
0.3852834889296692	0.4569871739477135	0.2445348833583798	T	T	T
0.0593211298388339	0.1407570857656422	0.2175887327574900	T	T	T
0.8472076760510320	0.3846627465419054	0.1944536550410728	T	T	T
0.5963607649348590	0.1109630534508437	0.1689646166210853	T	T	T
0.0415399999999977	0.9792300000000012	0.0186700000000002	F	F	F
0.0536699999999968	0.5664599999999993	0.1193200000000019	F	F	F
0.8081099999999992	0.7907399999999996	0.0928299999999993	F	F	F
0.5531999999999968	0.5285999999999973	0.0694999999999979	F	F	F
0.3076399999999992	0.7528799999999976	0.0430100000000024	F	F	F
0.3275928692112289	0.8394607907418965	0.1446433974031412	T	T	T
0.3708894300335723	0.9545812116326198	0.2498668147778195	T	T	T
0.0623239908723385	0.6448675802225143	0.2169185608120039	T	T	T
0.8423539886442021	0.8846557866452767	0.1929214922527229	T	T	T
0.5957742878242869	0.6061942781415710	0.1709781799082385	T	T	T
0.2195074576243115	-0.0667145171162948	0.2837475793647850	T	T	T
0.3969067390763558	0.9467247751585516	0.3335990576327225	T	T	T
0.2796940820925904	0.9894484050596652	0.3512811128631382	T	T	T

Nb₄N₅ (100) + *O

Nb N O

1.0000000000000000		
5.3445200000000002	0.0000000000000000	0.0000000000000000
-1.7272543693964146	10.5485218558526483	0.0000000000000000
0.0000000000000000	0.0000000000000000	29.2037000000000013

Nb N O
16 20 1

Selective dynamics

Direct

0.4208900000000000	0.1857100000000003	0.1081700000000012	F	F	F
0.4004699999999985	0.0837300000000027	0.0056799999999981	F	F	F
0.6826200000000000	0.3747200000000035	0.0316499999999991	F	F	F
0.9404299999999992	0.1336399999999998	0.0541600000000031	F	F	F
0.7383645686720500	0.0262671114771996	0.2256547585679100	T	T	T
0.6899721396112597	0.4475053275845584	0.1273893556824144	T	T	T
0.9762986952999168	0.2352033745882747	0.1591817619569046	T	T	T
0.2316547004029085	0.4880911717399149	0.1882769568603462	T	T	T
0.4208900000000000	0.6857100000000003	0.1081700000000012	F	F	F
0.4004699999999985	0.5837300000000027	0.0056799999999981	F	F	F
0.6826200000000000	0.8747200000000035	0.0316499999999991	F	F	F
0.9404299999999992	0.6336399999999998	0.0541600000000031	F	F	F
0.7333027897616060	0.5256356861920457	0.2252162877759325	T	T	T
0.6863519799387950	0.9465271608018947	0.1267157165089524	T	T	T
0.9817352812177859	0.7336694727606089	0.1604757184722456	T	T	T
0.2280635801998085	0.9903588514704446	0.1867854235090814	T	T	T
0.0415399999999977	0.4792300000000012	0.0186700000000002	F	F	F
0.0536699999999968	0.0664599999999993	0.1193200000000019	F	F	F
0.8081099999999992	0.2907399999999996	0.0928299999999993	F	F	F
0.5531999999999968	0.0285999999999973	0.0694999999999979	F	F	F
0.3076399999999992	0.2528799999999976	0.0430100000000024	F	F	F
0.3313842525353773	0.3395974189226461	0.1449513604838141	T	T	T
0.3849508491768920	0.4589464530876905	0.2445571010598268	T	T	T
0.0544930671661718	0.1447395316138991	0.2167603845833023	T	T	T
0.8479708257814166	0.3847762261974752	0.1946762576768622	T	T	T
0.5929802705493630	0.1070959590154853	0.1698072178932943	T	T	T
0.0415399999999977	0.9792300000000012	0.0186700000000002	F	F	F
0.0536699999999968	0.5664599999999993	0.1193200000000019	F	F	F
0.8081099999999992	0.7907399999999996	0.0928299999999993	F	F	F
0.5531999999999968	0.5285999999999973	0.0694999999999979	F	F	F
0.3076399999999992	0.7528799999999976	0.0430100000000024	F	F	F
0.3340398794908512	0.8392303203165270	0.1443628907014814	T	T	T
0.3513102325079335	0.9504916295596010	0.2449493785204011	T	T	T
0.0617114962712763	0.6458240156563374	0.2166943914359842	T	T	T
0.8440320768283872	0.8859581014555424	0.1942449356601190	T	T	T
0.5950722548155473	0.6078773000455212	0.1706759722609849	T	T	T
0.5093072439628666	0.9494480829187685	0.2802061725536973	T	T	T

Nb₄N₅ (100) + *OH

Nb N O H

1.0000000000000000

5.3445200000000002 0.0000000000000000 0.0000000000000000
-1.7272543693964146 10.5485218558526483 0.0000000000000000
0.0000000000000000 0.0000000000000000 29.2037000000000013

Nb N O H

16 20 1 1

Selective dynamics

Direct

0.4208900000000000	0.1857100000000003	0.1081700000000012	F	F	F
0.4004699999999985	0.0837300000000027	0.0056799999999981	F	F	F
0.6826200000000000	0.3747200000000035	0.0316499999999991	F	F	F
0.9404299999999992	0.1336399999999998	0.0541600000000031	F	F	F
0.7562776393134356	0.0066486306107195	0.2356917768950653	T	T	T
0.6854112956277624	0.4453827526750507	0.1268094955044115	T	T	T
0.9720847686795725	0.2238790105858421	0.1631972985673429	T	T	T
0.2319988658383439	0.4850613630392339	0.1876398175262503	T	T	T
0.4208900000000000	0.6857100000000003	0.1081700000000012	F	F	F
0.4004699999999985	0.5837300000000027	0.0056799999999981	F	F	F
0.6826200000000000	0.8747200000000035	0.0316499999999991	F	F	F
0.9404299999999992	0.6336399999999998	0.0541600000000031	F	F	F
0.7326669283428748	0.5228336352352579	0.2254283477388365	T	T	T
0.6899102105290997	0.9481986116009468	0.1272566773405666	T	T	T
0.9876010044427874	0.7308914505819910	0.1615734105943761	T	T	T
0.2522386198332166	-0.0105459625443417	0.1886874689702871	T	T	T
0.0415399999999977	0.4792300000000012	0.0186700000000002	F	F	F
0.0536699999999968	0.0664599999999993	0.1193200000000019	F	F	F
0.8081099999999992	0.2907399999999996	0.0928299999999993	F	F	F
0.5531999999999968	0.0285999999999973	0.0694999999999979	F	F	F
0.3076399999999992	0.2528799999999976	0.0430100000000024	F	F	F
0.3267288948705981	0.3361999811528668	0.1451732113531517	T	T	T
0.3842870877742560	0.4555443404512730	0.2440254378773252	T	T	T
0.0645479647903641	0.1389743624741508	0.2168975875152666	T	T	T
0.8455658982875720	0.3833595337076253	0.1938976112761827	T	T	T
0.5956875672805360	0.1069177974026983	0.1690759970109553	T	T	T
0.0415399999999977	0.9792300000000012	0.0186700000000002	F	F	F
0.0536699999999968	0.5664599999999993	0.1193200000000019	F	F	F
0.8081099999999992	0.7907399999999996	0.0928299999999993	F	F	F
0.5531999999999968	0.5285999999999973	0.0694999999999979	F	F	F
0.3076399999999992	0.7528799999999976	0.0430100000000024	F	F	F
0.3376447228239370	0.8383809598582619	0.1456220230513298	T	T	T
0.3894427675586512	0.9519210360704272	0.2447265530144065	T	T	T

```
0.0619687466766987 0.6436742552792930 0.2173152844142565 T T T
0.8559296523973982 0.8839519712792553 0.1936138877267705 T T T
0.5978371349201463 0.6050882753074152 0.1709510204913924 T T T
-0.1172631478976279 -0.0328151451668470 0.2951064412269214 T T T
0.0667563703483702 0.9697653848758621 0.2973279151701939 T T T
```

The calculations have been performed with VASP with PAW pseudopotentials and with the following parameters: ¹⁻⁵

INCAR

```
ALGO = Fast
IALGO = 38
ISTART=1
ICHARG=0
EDIFF = 2e-06
ENCUT = 520
IBRION = 2
ISIF = 2
ISMEAR = 0
ISPIN = 2
LREAL = Auto
LWAVE = True
NELM = 100
NELMIN = 3
NCORE = 8
KPAR = 8
PREC = Accurate
SIGMA = 0.2
NSW=1000
```

KPOINTS

```
Regular 2 x 2 x 2 mesh centered at Gamma
0
Gamma
2 2 2
```

References

- [1] G. Kresse and J. Hafner, Phys. Rev. B 47, 558 (1993); *ibid.* 49, 14 251 (1994).
- [2] G. Kresse and J. Furthmüller, Comput. Mat. Sci. 6, 15 (1996).
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- [4] G. Kresse and J. Hafner, J. Phys.: Condens. Matt. 6, 8245 (1994).
- [5] G. Kresse and D. Joubert, Phys. Rev. 59, 1758 (1999).