

Supporting Information

In silico discovery of new dopants for Fe-doped Ni oxyhydroxide (Ni_{1-x}Fe_xOOH) catalysts for oxygen evolution reaction

Hyeyoung Shin, Hai Xiao and William A. Goddard III*

Materials and Process Simulation Center (MSC) and Joint Center for Artificial Photosynthesis (JCAP), California Institute of Technology, Pasadena, California 91125, USA

*E-mail: wag@wag.caltech.edu

I. Simulation Details

In this work, the projector augmented wave (PAW) method¹ to model the valence electron-ion interactions is employed for all calculations. We use periodic (100) slab models consisting of four metal–oxygen layers with three metal sites per layer (Figure S1), which has been considered as the OER active surface in similar oxide models.^{2,3} The slabs are separated by a 15 Å vacuum region and the atomic positions of top two layers are optimized while other two layers are fixed at the optimized bulk position. The Γ -centered (3×3×1) Monkhorst–Pack K-point grids and a plane-wave energy cutoff of 400 eV are used for the slab calculations. In addition, the vibrational frequencies are computed to consider the zero-point energies, enthalpy, and entropy and ultimately to calculate the free energies at room temperature (298.15 K).

After the geometry optimization of the slab for NiOOH, we found that 1/3 of the Ni atoms (the ones close to K⁺ ions) have oxidation state of +3, probably due to the K⁺ ions donating to the nearest Ni. Thus 2/3 of the Ni atoms have 4+ oxidation states, leading to an average oxidation state of +3.67 for Ni, in agreement with previous reports.^{4,5} (see Figure S1)

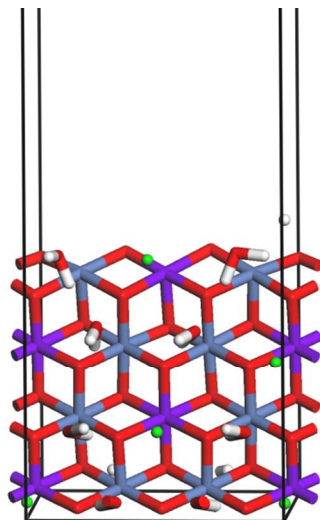
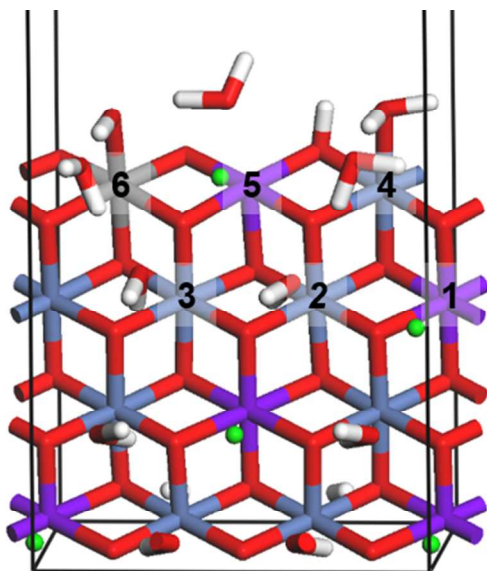


Figure S1. Model structure for the (100) surface of the pure γ -NiOOH with chemical formula $K_{1/3}(H_2O)_{2/3}NiO_2$. Blue, purple, red, white, and green atoms indicate Ni^{4+} , Ni^{3+} , O, H, and K^+ , respectively.



Site #	ΔE (eV)
1	0.45
2	0.37
3	0.47
4	0.25
5	0.53
6	0.00

Figure S2. Dopant site search of Fe dopant on γ -NiOOH surface. Here we considered six different plausible dopant sites on NiOOH (see above) and found that Fe prefers to substitute the Ni^{4+} interacting with surface OH (site 6) and it leads to the oxidation state of +4 (Fe^{4+}). Gray, blue, purple, red, white, and green atoms indicate Fe^{4+} , Ni^{4+} , Ni^{3+} , O, H, and K^+ , respectively.

II. Coordinates for all states involved in OER

Figure 2 State 1

```

K Ni O H
1.0000000000000000
  8.7372206091223994    0.0000000000000000    0.0000000000000000
  0.0000000000000000    6.9809029500783426    0.0000000000000000
  0.0000000000000000    0.0000000000000000    25.0000000000000000

  K      Ni      O      H
  4      12     35     22
Selective dynamics
Direct
0.0000000000000000    0.9295476953180497    0.0219900692777486
0.5000000000000000    0.8431778700801544    0.1149178963106294
0.0431977246227240    0.7582806340628593    0.2087123012227187
0.5427683855381095    0.6831659785942805    0.3448487673194416
0.0000000000000000    0.4295476953180497    0.0219900692777486
0.3336660000000009    0.4295476953180497    0.0219900692777486
0.6663339999999991    0.4295476953180497    0.0219900692777486
0.1663339999999991    0.3431778700801544    0.1149178963106294
0.5000000000000000    0.3431778700801544    0.1149178963106294
0.8336660000000009    0.3431778700801544    0.1149178963106294
0.9989226886732246    0.2558908428633444    0.2098439284415032
0.3333909255207630    0.2521053781339185    0.2103330282114551
0.6636181691821059    0.2545617767458928    0.2098836167092193
0.1644672719283788    0.1756692243982583    0.3061927389552984
0.5056543586010689    0.1766912594141325    0.3064125902023013
0.8337503321368842    0.1881991365673761    0.3068311318022511
0.1735150000000019    0.5955569454815901    0.0004884286588833
0.5000000000000000    0.5859389052830437    0.0000000000000000
0.8264849999999991    0.5955569454815901    0.0004884286588833
0.1735150000000019    0.2635384451545022    0.0434917098966210
0.5000000000000000    0.2731564853530557    0.0439801385555043
0.8264849999999991    0.2635384451545022    0.0434917098966210
0.0000000000000000    0.4995690800451484    0.0929278270328737
0.3264849999999991    0.5091871202437019    0.0934162556917641
0.6735150000000019    0.5091871202437019    0.0934162556917641
0.0000000000000000    0.1867866601151604    0.1369079655883780
0.3264849999999991    0.1771686199166140    0.1364195369294947
0.6735150000000019    0.1771686199166140    0.1364195369294947
0.1676638371019280    0.4119173085264791    0.1883603227241292
0.4982952510549877    0.4154071566742359    0.1876686496997411
0.8267557542931614    0.4202263032629242    0.1879581390385082
0.1719262193808487    0.0947807067571802    0.2345672007256929
0.4977790296354649    0.0883671576564856    0.2281161991225893
0.8273854263778435    0.0977690102302338    0.2337976863263437
0.0048046144425974    0.3350677021648515    0.2808386216718469
0.3380364105504263    0.3286137742396575    0.2832969013456514
0.6611420516862356    0.3390923716122154    0.2819455892616711
0.9955684382783687    0.0237391676655541    0.3219818121419502
0.3381092565193691    0.0208540097858172    0.3330612362499552
0.6664739534257762    0.0419082395470131    0.3302702346613278
0.3436370000000011    0.9295476953180497    0.0219900692777486
0.6563629999999991    0.9295476953180497    0.0219900692777486
0.1563629999999991    0.8431778700801544    0.1149178963106294
0.8436370000000011    0.8431778700801544    0.1149178963106294
0.3571129455657219    0.7223767325332665    0.2493032945012214
0.7397980783313185    0.7233582491118192    0.2552773860670580
0.2026521474386872    0.6326919716892063    0.3531156277441717
0.8888194886288273    0.6961712836277725    0.3505540434099758
0.5627595155392418    0.3674051948835708    0.4097284503997190
0.8507552094006980    0.3039852228359534    0.3754290460540963
0.1521330182340190    0.2787721224346768    0.3781160529254926
0.2777910000000006    0.8194148176612188    0.0136009167645312
0.2777910000000006    0.0396805729748735    0.0303792217909731
0.7222089999999994    0.8194148176612188    0.0136009167645312

```

0.7222089999999994	0.0396805729748735	0.0303792217909731
0.2222089999999994	0.7330449924233307	0.1065287437974050
0.2222089999999994	0.9533107477369782	0.1233070488238468
0.7777910000000006	0.7330449924233307	0.1065287437974050
0.7777910000000006	0.9533107477369782	0.1233070488238468
0.4140891298453878	0.6218942671658899	0.2300737759814150
0.4100622623992318	0.8446501488363118	0.2422901520429057
0.7536438868808700	0.6302414848894883	0.2259355701101869
0.7550516233158341	0.8558049434589091	0.2420217083844661
0.2418980922620519	0.6464502371567944	0.3162961387896417
0.0921835441368550	0.6668742264951049	0.3506834040550604
0.8473264497661512	0.6936131347602904	0.3132784213554451
0.9155880640486866	0.8348560672251958	0.3544393412179374
0.6689524571059907	0.3183324875321217	0.4023097214000433
0.5364868118109675	0.3260611220510279	0.4456612295372047
0.0352733277019890	0.2765618194976200	0.3837820712199993
0.8602994955384563	0.4428699964458778	0.3679079177556165
0.3253146876836789	0.0519525071350344	0.3711242940687646
0.1804760979163698	0.4199648646274983	0.3710118736923418

Figure 2 State 2

K Ni O H

1.0000000000000000		
8.7372206091223994	0.0000000000000000	0.0000000000000000
0.0000000000000000	6.9809029500783426	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000

K	Ni	O	H
4	12	35	21

Selective dynamics

Direct

0.0000000000000000	0.9295476953180497	0.0219900692777486
0.5000000000000000	0.8431778700801544	0.1149178963106294
0.0219772289370202	0.7645102671146051	0.2073713123627349
0.5221860237024207	0.7074914228743956	0.3562244311306270
0.0000000000000000	0.4295476953180497	0.0219900692777486
0.3336660000000009	0.4295476953180497	0.0219900692777486
0.6663339999999991	0.4295476953180497	0.0219900692777486
0.1663339999999991	0.3431778700801544	0.1149178963106294
0.5000000000000000	0.3431778700801544	0.1149178963106294
0.8336660000000009	0.3431778700801544	0.1149178963106294
0.0012961495535132	0.2620747623372240	0.2100919939448649
0.3338739878040317	0.2579497279349519	0.2096999214961149
0.6665967355351463	0.2580840207787507	0.2092547305870878
0.1692939666191214	0.1784601680910908	0.3054598809790290
0.5046437118072188	0.1859296112248006	0.3044913510085394
0.8338643522243194	0.1858011288887492	0.3046234629882161
0.1735150000000019	0.5955569454815901	0.0004884286588833
0.5000000000000000	0.5859389052830437	0.0000000000000000
0.8264849999999981	0.5955569454815901	0.0004884286588833
0.1735150000000019	0.2635384451545022	0.0434917098966210
0.5000000000000000	0.2731564853530557	0.0439801385555043
0.8264849999999981	0.2635384451545022	0.0434917098966210
0.0000000000000000	0.4995690800451484	0.0929278270328737
0.3264849999999981	0.5091871202437019	0.0934162556917641
0.6735150000000019	0.5091871202437019	0.0934162556917641
0.0000000000000000	0.1867866601151604	0.1369079655883780
0.3264849999999981	0.1771686199166140	0.1364195369294947
0.6735150000000019	0.1771686199166140	0.1364195369294947
0.1691898666870562	0.4193368598413515	0.1872283079217001
0.4990383888845986	0.4179591577114631	0.1869559160197237
0.8314201037809903	0.4214325861611162	0.1876862891772020
0.1683850963046782	0.1036176290417214	0.2333250331638163
0.5010110505572180	0.0994218583626602	0.2317856189735233
0.8337261680986494	0.1009108481487715	0.2336718061959445
0.0028802184543310	0.3408240500934637	0.2823107898038140
0.3349628014351718	0.3385934139889731	0.2815515727703180

0.6678090491962858	0.3429302566166438	0.2802895864778854
-0.0021592566859802	0.0273369240582836	0.3237482699476721
0.3421390782394277	0.0260519612945379	0.3228947086425956
0.6690080069204597	0.0296909286814576	0.3219748085426093
0.3436370000000011	0.9295476953180497	0.0219900692777486
0.6563629999999989	0.9295476953180497	0.0219900692777486
0.1563629999999989	0.8431778700801544	0.1149178963106294
0.8436370000000011	0.8431778700801544	0.1149178963106294
0.2901826393955977	0.7251882265176370	0.2669960749061309
0.7141654161791503	0.7150389540771965	0.2614513232919779
0.1825117422473321	0.6223710212417533	0.3624652155136454
0.8682713130434493	0.6988584525810841	0.3556330376295847
0.5182659672882968	0.3068422705051227	0.3723098325429717
0.8163151471935557	0.3054410588638692	0.3770402317591246
0.1684447072865352	0.2711739846405071	0.3784379971340407
0.2777910000000006	0.8194148176612188	0.0136009167645312
0.2777910000000006	0.0396805729748735	0.0303792217909731
0.7222089999999994	0.8194148176612188	0.0136009167645312
0.7222089999999994	0.0396805729748735	0.0303792217909731
0.2222089999999994	0.7330449924233307	0.1065287437974050
0.2222089999999994	0.9533107477369782	0.1233070488238468
0.7777910000000006	0.7330449924233307	0.1065287437974050
0.7777910000000006	0.9533107477369782	0.1233070488238468
0.3726314824845948	0.6570393507124014	0.2488556776566294
0.3253505184986785	0.8568018478598782	0.2795440111555240
0.7279945610877649	0.6320055852380001	0.2301433118383743
0.7139521032122699	0.8511764672330664	0.2513609475065818
0.2196899398360929	0.6413781537120761	0.3245356696223293
0.0735271285430832	0.6618626574595257	0.3609291166444564
0.8279943920697254	0.6901643714460757	0.3182195853715611
0.9035997392944021	0.8349247769041508	0.3566509804665735
0.6988986682796208	0.2935056087785691	0.3821029963021381
0.4427988149647655	0.2382739471841590	0.3939507100517043
0.0659055658841757	0.2320616471057814	0.3903263075071554
0.8379162148170484	0.4446625946623879	0.3732111713853560
0.1717285424510631	0.4237205116770359	0.3734403385200936

Figure 2 State 3

K Ni O H

1.0000000000000000		
8.7372206091223994	0.0000000000000000	0.0000000000000000
0.0000000000000000	6.9809029500783426	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000

K	Ni	O	H
4	12	35	20

Selective dynamics

Direct

0.0000000000000000	0.9295476953180497	0.0219900692777486
0.5000000000000000	0.8431778700801544	0.1149178963106294
-0.0002585876083442	0.7671346269876054	0.2119470605741065
0.4920874678869419	0.7640732935784272	0.3856704934546264
0.0000000000000000	0.4295476953180497	0.0219900692777486
0.3336660000000009	0.4295476953180497	0.0219900692777486
0.6663339999999991	0.4295476953180497	0.0219900692777486
0.1663339999999991	0.3431778700801544	0.1149178963106294
0.5000000000000000	0.3431778700801544	0.1149178963106294
0.8336660000000009	0.3431778700801544	0.1149178963106294
-0.0002710542514955	0.2664242251192260	0.2105550443170425
0.3318709228674441	0.2625503705611819	0.2095105682130712
0.6668782861346676	0.2623483248058537	0.2093985312789806
0.1661233570552173	0.1923548437907445	0.3063502314410516
0.4991756696965112	0.1962064736730173	0.3042122038245993
0.8314622418367428	0.1941415200201544	0.3059162802322605
0.1735150000000019	0.5955569454815901	0.0004884286588833
0.5000000000000000	0.5859389052830437	0.0000000000000000
0.8264849999999981	0.5955569454815901	0.0004884286588833

0.1735150000000019	0.2635384451545022	0.0434917098966210
0.5000000000000000	0.2731564853530557	0.0439801385555043
0.8264849999999981	0.2635384451545022	0.0434917098966210
0.0000000000000000	0.4995690800451484	0.0929278270328737
0.3264849999999981	0.5091871202437019	0.0934162556917641
0.6735150000000019	0.5091871202437019	0.0934162556917641
0.0000000000000000	0.1867866601151604	0.1369079655883780
0.3264849999999981	0.1771686199166140	0.1364195369294947
0.6735150000000019	0.1771686199166140	0.1364195369294947
0.1657455472267081	0.4217053852494989	0.1868110967820061
0.4998948051353816	0.4175420070816093	0.1864626715182205
0.8329329850135335	0.4217956761275090	0.1867969138862821
0.1651470676477415	0.1109358209718709	0.2331212718091196
0.4995501047617127	0.1065232300780866	0.2315370564485392
0.8348664805196642	0.1106279392339288	0.2338981556319769
-0.0012938298876153	0.3496783233081489	0.2824505514290350
0.3337092226391752	0.3514370133463907	0.2799479622847541
0.6639732730188800	0.3523323509055514	0.2796028938128073
-0.0010350201560570	0.0420585937432569	0.3243499714055292
0.3378549707099412	0.0370596833500826	0.3223480540523331
0.6611532199159101	0.0369697064513037	0.3224608903717315
0.3436370000000011	0.9295476953180497	0.0219900692777486
0.6563629999999989	0.9295476953180497	0.0219900692777486
0.1563629999999989	0.8431778700801544	0.1149178963106294
0.8436370000000011	0.8431778700801544	0.1149178963106294
0.2325312572812353	0.7173968892240560	0.2821801373228148
0.7663905695690288	0.7170265278813963	0.2843929167006110
0.1705189150324584	0.6652539137630783	0.3898423436505685
0.8554178212725873	0.6474939804032769	0.3849262588457468
0.5007987962219175	0.3142848060097598	0.3712980106064918
0.8110006115881979	0.2920218057158239	0.3774388099375114
0.1721586085826945	0.2848819081811843	0.3759695866751505
0.2777910000000006	0.8194148176612188	0.0136009167645312
0.2777910000000006	0.0396805729748735	0.0303792217909731
0.7222089999999994	0.8194148176612188	0.0136009167645312
0.7222089999999994	0.0396805729748735	0.0303792217909731
0.2222089999999994	0.7330449924233307	0.1065287437974050
0.2222089999999994	0.9533107477369782	0.1233070488238468
0.7777910000000006	0.7330449924233307	0.1065287437974050
0.7777910000000006	0.9533107477369782	0.1233070488238468
0.2965783907160089	0.6013467027510833	0.2788616344354599
0.2958515135278569	0.8353475238471346	0.2867317688793678
0.7008254492272276	0.6034235183613043	0.2789605384564540
0.7049456792019392	0.8371742778474196	0.2895165714773934
0.1760098750938847	0.7017414080696052	0.3513314948712162
0.1693710830475574	0.5217216293668411	0.3872328560480128
0.8378454048748837	0.6885509271366551	0.3467721183589199
0.9662821388976566	0.6743305918598087	0.3921084489399768
0.6977830392237657	0.2791440425873528	0.3836369357868094
0.3984225412429666	0.2798968939390092	0.3852321472302723
0.0900128992852268	0.2105284307955552	0.3928155015723335
0.8349618983279140	0.4415950876141634	0.3800265738487771

Figure 2 State 4

K Ni O H			
1.0000000000000000			
8.7372206091223994	0.0000000000000000	0.0000000000000000	
0.0000000000000000	6.9809029500783426	0.0000000000000000	
0.0000000000000000	0.0000000000000000	25.0000000000000000	
K	Ni	O	H
4	12	36	21
Selective dynamics			
Direct			
0.0000000000000000	0.9295476953180497	0.0219900692777486	
0.5000000000000000	0.8431778700801544	0.1149178963106294	
-0.0003265507281078	0.7643873458160285	0.2128119121678972	

0.4800858710527695 0.8097401443704785 0.3996833318649938
0.0000000000000000 0.4295476953180497 0.0219900692777486
0.3336660000000000 0.4295476953180497 0.0219900692777486
0.6663339999999999 0.4295476953180497 0.0219900692777486
0.1663339999999999 0.3431778700801544 0.1149178963106294
0.5000000000000000 0.3431778700801544 0.1149178963106294
0.8336660000000000 0.3431778700801544 0.1149178963106294
-0.0000293465417951 0.2644505302808114 0.2102589883507384
0.3322021799547887 0.2618777405007845 0.2098264673141764
0.6665506132320419 0.2603482198775274 0.2093063974170445
0.1651674973190403 0.1866694018668697 0.3061630999255814
0.5001928429840506 0.1936916196532949 0.3061867086191367
0.8324539410388943 0.1898070135187163 0.3051515404679754
0.1735150000000019 0.5955569454815901 0.0004884286588833
0.5000000000000000 0.5859389052830437 0.0000000000000000
0.8264849999999981 0.5955569454815901 0.0004884286588833
0.1735150000000019 0.2635384451545022 0.0434917098966210
0.5000000000000000 0.2731564853530557 0.0439801385555043
0.8264849999999981 0.2635384451545022 0.0434917098966210
0.0000000000000000 0.4995690800451484 0.0929278270328737
0.3264849999999981 0.5091871202437019 0.0934162556917641
0.6735150000000019 0.5091871202437019 0.0934162556917641
0.0000000000000000 0.1867866601151604 0.1369079655883780
0.3264849999999981 0.1771686199166140 0.1364195369294947
0.6735150000000019 0.1771686199166140 0.1364195369294947
0.1656065395612832 0.4209779587497114 0.1869475135506296
0.4999599627105746 0.4166818876329703 0.1866132603371756
0.8333163342416410 0.4205071253592820 0.1868905353952071
0.1659466431042289 0.1092447484800991 0.2327848939005392
0.4988062222135731 0.1059626139297122 0.2316355037633262
0.8345934755714975 0.1073471149327922 0.2330451169426415
-0.0004678403223323 0.3454310199419155 0.2822275129895414
0.3328615695168772 0.3481839818194692 0.2808339427454397
0.6649734879355238 0.3484284147226218 0.2794889105114542
0.9977495953155020 0.0337957308576899 0.3222817908401970
0.3383540956772948 0.0336607407240575 0.3218482422744982
0.6630483392469790 0.0334401391968365 0.3229057913912161
0.3436370000000011 0.9295476953180497 0.0219900692777486
0.6563629999999989 0.9295476953180497 0.0219900692777486
0.1563629999999989 0.8431778700801544 0.1149178963106294
0.8436370000000011 0.8431778700801544 0.1149178963106294
0.2375694929974418 0.7128389681334321 0.2813875216154132
0.7657836444896026 0.7133610451006643 0.2851399418154140
0.1807487264059690 0.6539562753050535 0.3887191807639755
0.8676517525265348 0.6423905436746836 0.3846992022839820
0.5167753321359876 0.3134382924706147 0.3683147971265053
0.8164983215098778 0.2919349965366971 0.3759894787361632
0.1601621522079057 0.2688407443127265 0.3771619108330363
0.3548807548806081 0.1078553925833144 0.4477615452303266
0.2777910000000006 0.8194148176612188 0.0136009167645312
0.2777910000000006 0.0396805729748735 0.0303792217909731
0.7222089999999994 0.8194148176612188 0.0136009167645312
0.7222089999999994 0.0396805729748735 0.0303792217909731
0.2222089999999994 0.7330449924233307 0.1065287437974050
0.2222089999999994 0.9533107477369782 0.1233070488238468
0.7777910000000006 0.7330449924233307 0.1065287437974050
0.7777910000000006 0.9533107477369782 0.1233070488238468
0.3012659873754485 0.5958686932122884 0.2795717342124203
0.3020238661095760 0.8291717541560266 0.2863135935985009
0.6997627319390590 0.5994726850109228 0.2811806835152998
0.7032671454039959 0.8319265311824177 0.2910455196887091
0.1876622146331154 0.6893891365197030 0.3500925048177075
0.1796131285178355 0.5108063112188554 0.3867813833325673
0.8441205160210088 0.6877460825664609 0.3474077730688528
0.9797916468309301 0.6670422545839867 0.3904307170023302
0.7000845382966719 0.2838423151084856 0.3809220420624476
0.0613740676147732 0.2149217919737786 0.3885781971803324
0.8444167799391566 0.4428898094221809 0.3786014285960417
0.3757936803987383 0.2093050693288025 0.4732864752613082

0.2866494768223371 0.1674293087583986 0.4197265701778259

Figure 2 State 4'

K Ni O H

1.000000000000000		
8.7372206091223994	0.000000000000000	0.000000000000000
0.000000000000000	6.9809029500783426	0.000000000000000
0.000000000000000	0.000000000000000	25.000000000000000

K	Ni	O	H
4	12	36	21

Selective dynamics

Direct

0.000000000000000	0.9295476953180497	0.0219900692777486
0.500000000000000	0.8431778700801544	0.1149178963106294
-0.0004377300953357	0.7665371236184298	0.2105854508263613
0.5474138491322136	0.7455687881253050	0.3923416178263027
0.000000000000000	0.4295476953180497	0.0219900692777486
0.333660000000009	0.4295476953180497	0.0219900692777486
0.6663339999999991	0.4295476953180497	0.0219900692777486
0.1663339999999991	0.3431778700801544	0.1149178963106294
0.500000000000000	0.3431778700801544	0.1149178963106294
0.833660000000009	0.3431778700801544	0.1149178963106294
-0.0004311046257435	0.2663482436415386	0.2098575367766323
0.3323796418749631	0.2619360737476999	0.2097581107551498
0.6668607301367893	0.2617701760985651	0.2091741604887839
0.1624911077017390	0.1922631825072682	0.3062358888968710
0.5049582479788398	0.1929044956033778	0.3049460059856989
0.8332306246869675	0.1920177598179424	0.3055177689980856
0.1735150000000019	0.5955569454815901	0.0004884286588833
0.500000000000000	0.5859389052830437	0.000000000000000
0.8264849999999991	0.5955569454815901	0.0004884286588833
0.1735150000000019	0.2635384451545022	0.0434917098966210
0.500000000000000	0.2731564853530557	0.0439801385555043
0.8264849999999991	0.2635384451545022	0.0434917098966210
0.000000000000000	0.4995690800451484	0.0929278270328737
0.3264849999999991	0.5091871202437019	0.0934162556917641
0.6735150000000019	0.5091871202437019	0.0934162556917641
0.000000000000000	0.1867866601151604	0.1369079655883780
0.3264849999999991	0.1771686199166140	0.1364195369294947
0.6735150000000019	0.1771686199166140	0.1364195369294947
0.1667657889765085	0.4220109993694590	0.1868783767633953
0.4993049858671654	0.4176933347908909	0.1865294009806717
0.8329722342571912	0.4211304375515060	0.1870198204801642
0.1646803494685877	0.1107418744382546	0.2335975568375116
0.4997236942709063	0.1049123082753331	0.2317709702404538
0.8345524612243584	0.1096407855119913	0.2338240862377764
0.9975695344444125	0.3494809165621071	0.2817770916348182
0.3351674928797359	0.3469357180142081	0.2813905326470624
0.6629498860785070	0.3501389034144798	0.2806300119058811
0.9981757789328801	0.0398160034989905	0.3235740180505027
0.3448357445373841	0.0228612621213188	0.3251520060179487
0.6648341772769689	0.0332849774472825	0.3235729487273595
0.3436370000000011	0.9295476953180497	0.0219900692777486
0.6563629999999991	0.9295476953180497	0.0219900692777486
0.1563629999999991	0.8431778700801544	0.1149178963106294
0.8436370000000011	0.8431778700801544	0.1149178963106294
0.2224623445835508	0.7001169276216017	0.2861045722622884
0.7658096124988358	0.7144890916732284	0.2853595991938105
0.1823821364547148	0.6748907493794729	0.3940268183722132
0.8651132788675195	0.6559699102779009	0.3843585585731004
0.5131462216476700	0.3137231843323461	0.3743436326985284
0.8224052495732470	0.2942080385042066	0.3780861464421761
0.1655274168235713	0.2838865739371761	0.3783749632090315
0.4300323110106986	0.2128140636874085	0.4146834809179125
0.2777910000000006	0.8194148176612188	0.0136009167645312
0.2777910000000006	0.0396805729748735	0.0303792217909731

0.7222089999999994	0.8194148176612188	0.0136009167645312
0.7222089999999994	0.0396805729748735	0.0303792217909731
0.2222089999999994	0.7330449924233307	0.1065287437974050
0.2222089999999994	0.9533107477369782	0.1233070488238468
0.7777910000000006	0.7330449924233307	0.1065287437974050
0.7777910000000006	0.9533107477369782	0.1233070488238468
0.2821909356653481	0.5796307896171793	0.2818135451859923
0.2932777710899658	0.8090995912442571	0.2888084670811694
0.6996126545233011	0.6025205545761321	0.2786140098671326
0.7054829963872281	0.8364436403470770	0.2894854979318623
0.1867780810768691	0.6983773525452239	0.3544786107847958
0.1769461729643742	0.5325974401798065	0.3943549031597496
0.8490137984995026	0.6920368459184347	0.3456427330094326
0.9742635045475670	0.6868905788049201	0.3926705445720761
0.7092446606014097	0.2832058929009340	0.3847393318735299
0.0751586739593916	0.2194863640645172	0.3932408966895415
0.8472889223546427	0.4406576855155719	0.3798568800360655
0.3414063387196568	0.0348420974940837	0.3644795107825679
0.3157041424711716	0.2505100011422038	0.4052567642998503

Figure 2 State 5

K Ni O H

1.0000000000000000		
8.7372206091223994	0.0000000000000000	0.0000000000000000
0.0000000000000000	6.9809029500783426	0.0000000000000000
0.0000000000000000	0.0000000000000000	25.0000000000000000

K	Ni	O	H
4	12	36	20

Selective dynamics

Direct

0.0000000000000000	0.9295476953180497	0.0219900692777486
0.5000000000000000	0.8431778700801544	0.1149178963106294
0.9961659773456399	0.7655012177568289	0.2113959230288941
0.5229931894917942	0.7638198490621904	0.3938285379396821
0.0000000000000000	0.4295476953180497	0.0219900692777486
0.3336660000000009	0.4295476953180497	0.0219900692777486
0.6663339999999991	0.4295476953180497	0.0219900692777486
0.1663339999999991	0.3431778700801544	0.1149178963106294
0.5000000000000000	0.3431778700801544	0.1149178963106294
0.8336660000000009	0.3431778700801544	0.1149178963106294
0.0001103765821653	0.2638453458332449	0.2095918479337560
0.3330942807867945	0.2609138569007995	0.2095154451296117
0.6661739164349749	0.2608379191051171	0.2093422218011749
0.1615570838642056	0.1876702331827106	0.3049228789565738
0.5036386976537968	0.1958519959049570	0.3059153684456186
0.8343268207115717	0.1892709766443590	0.3054015009329699
0.1735150000000019	0.5955569454815901	0.0004884286588833
0.5000000000000000	0.5859389052830437	0.0000000000000000
0.8264849999999981	0.5955569454815901	0.0004884286588833
0.1735150000000019	0.2635384451545022	0.0434917098966210
0.5000000000000000	0.2731564853530557	0.0439801385555043
0.8264849999999981	0.2635384451545022	0.0434917098966210
0.0000000000000000	0.4995690800451484	0.0929278270328737
0.3264849999999981	0.5091871202437019	0.0934162556917641
0.6735150000000019	0.5091871202437019	0.0934162556917641
0.0000000000000000	0.1867866601151604	0.1369079655883780
0.3264849999999981	0.1771686199166140	0.1364195369294947
0.6735150000000019	0.1771686199166140	0.1364195369294947
0.1671524631360243	0.4209717523483316	0.1869470426237301
0.4993972323635512	0.4174069441729071	0.1866201603723611
0.8330295773508914	0.4198394679444681	0.1872748494491559
0.1668543146873144	0.1071364763541585	0.2325289373428577
0.4988852155241143	0.1028822786643025	0.2313278031012242
0.8325967355017949	0.1082006537858232	0.2337298429256991
0.0010014905503377	0.3444422193315810	0.2817654754735706
0.3348746414156488	0.3469605621835795	0.2809322426202909

0.6636266912429652	0.3496488083073174	0.2806261149829786
0.9980601760982211	0.0303625876975265	0.3204955375712085
0.3401846871149712	0.0345016326910342	0.3309245419273318
0.6640234774814704	0.0376679253129891	0.3249935288814750
0.3436370000000011	0.9295476953180497	0.0219900692777486
0.6563629999999989	0.9295476953180497	0.0219900692777486
0.1563629999999989	0.8431778700801544	0.1149178963106294
0.8436370000000011	0.8431778700801544	0.1149178963106294
0.2262867207143615	0.7026682897857541	0.2849514337149569
0.7652197462656244	0.7116048754416511	0.2903866168554922
0.1918257893069207	0.6524807341322846	0.3930840949903345
0.8689446776170778	0.6407735392636144	0.3874177463140046
0.5051428507750290	0.3287901415079888	0.3736041557973436
0.8426308794544474	0.2844310063941932	0.3787240737772771
0.1659386653119621	0.2668321895398668	0.3763038287382296
0.5448962659578567	0.2285300190581974	0.4157619589666053
0.2777910000000006	0.8194148176612188	0.0136009167645312
0.2777910000000006	0.0396805729748735	0.0303792217909731
0.7222089999999994	0.8194148176612188	0.0136009167645312
0.7222089999999994	0.0396805729748735	0.0303792217909731
0.2222089999999994	0.7330449924233307	0.1065287437974050
0.2222089999999994	0.9533107477369782	0.1233070488238468
0.7777910000000006	0.7330449924233307	0.1065287437974050
0.7777910000000006	0.9533107477369782	0.1233070488238468
0.2851399174456115	0.5820047441274545	0.2798663564359116
0.2968947557472137	0.8110634846865179	0.2865523054329942
0.6987018846508255	0.6007709668750466	0.2823818977319483
0.7063959519310745	0.8349889622042328	0.2936991660915796
0.1929411018835334	0.6858879117317970	0.3541990512735000
0.1899346093579414	0.5093861447375417	0.3913213795036150
0.8465907171164678	0.6816017367252369	0.3493211472000469
0.9797153150641394	0.6677797975495519	0.3939537059987890
0.7480388602868200	0.2401103355413346	0.3965943980506987
0.0653440391340271	0.2237894374002945	0.3893635890711898
0.8518256051430478	0.4367576989707015	0.3826239314193518
0.3083696870342585	0.0878429210093814	0.3665982542843826

Figure 3 State 1

K	Ni	O	H	Fe
1.00000000000000				
8.7372206091223994	0.00000000000000	0.00000000000000		
0.00000000000000	6.9809029500783426	0.00000000000000		
0.00000000000000	0.00000000000000	25.00000000000000		
K	Ni	O	H	Fe
4	11	35	22	1

Selective dynamics

Direct

0.00000000000000	0.9295476953180497	0.0219900692777486
0.50000000000000	0.8431778700801544	0.1149178963106294
0.0456172516317765	0.7603924818685465	0.2074506794813830
0.5409594686324396	0.6908385238927409	0.3379369486402265
0.00000000000000	0.4295476953180497	0.0219900692777486
0.33366600000000	0.4295476953180497	0.0219900692777486
0.66633399999999	0.4295476953180497	0.0219900692777486
0.16633399999999	0.3431778700801544	0.1149178963106294
0.50000000000000	0.3431778700801544	0.1149178963106294
0.83366600000000	0.3431778700801544	0.1149178963106294
0.0001882631107049	0.2590405342296531	0.2098602570020885
0.3330139409673090	0.2543032099467442	0.2101669821209445
0.6634556167051613	0.2553271576283597	0.2098105677314869
0.1628653062705149	0.1815269226551374	0.3066670008572200
0.5049302662659991	0.1868140857707309	0.3083179885780539
0.1735150000000019	0.5955569454815901	0.0004884286588833
0.50000000000000	0.5859389052830437	0.00000000000000
0.8264849999999981	0.5955569454815901	0.0004884286588833
0.1735150000000019	0.2635384451545022	0.0434917098966210

0.5000000000000000	0.2731564853530557	0.0439801385555043
0.8264849999999981	0.2635384451545022	0.0434917098966210
0.0000000000000000	0.4995690800451484	0.0929278270328737
0.3264849999999981	0.5091871202437019	0.0934162556917641
0.6735150000000019	0.5091871202437019	0.0934162556917641
0.0000000000000000	0.1867866601151604	0.1369079655883780
0.3264849999999981	0.1771686199166140	0.1364195369294947
0.6735150000000019	0.1771686199166140	0.1364195369294947
0.1691415743561835	0.4165385758065359	0.1876618681946938
0.4971950471293527	0.4162219312889739	0.1874452701641842
0.8295909391909274	0.4197182842871572	0.1880539414342748
0.1687044335050434	0.0996391756759152	0.2330329395143918
0.4971217234246310	0.0909371877151724	0.2288695555243115
0.8294641043591722	0.1003274106840883	0.2342128816456880
0.0042073263890282	0.3401867584932245	0.2812402995170368
0.3372353138089630	0.3333952163447290	0.2828135283900369
0.6617724430422767	0.3424816245229905	0.2810166708350539
0.9896354329012630	0.0312415488339658	0.3247020776974170
0.3356199361483611	0.0269525737305644	0.3331325721303772
0.6724594733895295	0.0422913698601346	0.3287420024342198
0.3436370000000011	0.9295476953180497	0.0219900692777486
0.6563629999999989	0.9295476953180497	0.0219900692777486
0.1563629999999989	0.8431778700801544	0.1149178963106294
0.8436370000000011	0.8431778700801544	0.1149178963106294
0.3593086604783626	0.7284501786891305	0.2459797046349141
0.7435323058715448	0.7264219773380390	0.2527860344157993
0.2064128645757743	0.63694560884659251	0.3509498683876970
0.8932251685906335	0.6942679094821449	0.3473955916427335
0.5452677842436462	0.3481552297938087	0.3917465674599510
0.8385076655179257	0.3203564344481081	0.3746415289969871
0.1527714952653410	0.2885380817979053	0.3811919024235467
0.2777910000000006	0.8194148176612188	0.0136009167645312
0.2777910000000006	0.0396805729748735	0.0303792217909731
0.7222089999999994	0.8194148176612188	0.0136009167645312
0.7222089999999994	0.0396805729748735	0.0303792217909731
0.2222089999999994	0.7330449924233307	0.1065287437974050
0.2222089999999994	0.9533107477369782	0.1233070488238468
0.7777910000000006	0.7330449924233307	0.1065287437974050
0.7777910000000006	0.9533107477369782	0.1233070488238468
0.4156259418892387	0.6276399836928521	0.2265313610870462
0.4118405703378513	0.8515904092551209	0.2390856023752957
0.7583474465021852	0.6303592925658109	0.2241472979562953
0.7597015011408415	0.8579154220733991	0.2388256595337933
0.2446743803005780	0.6385993363377089	0.3138424433169881
0.0956757817179621	0.6686931118855554	0.3476327393943727
0.8505493405374949	0.6918198407760574	0.3102245774600376
0.9192803337042649	0.8332612639904678	0.3514054302173265
0.6613219097769089	0.3242574919205487	0.3913584147675148
0.5045596215486338	0.2905230825559570	0.4241697307703531
0.0392625451111155	0.2880181611791243	0.3877954844837160
0.8589206440206119	0.4572760507903416	0.3664901895153683
0.3199283990571293	0.0488170043838753	0.3714620280050874
0.1811415471151581	0.4282322340665290	0.3725557130144490
0.8334980958430774	0.1839499246661483	0.3082018969284069

Figure 3 State 2

K	Ni	O	H	Fe
1.0000000000000000				
8.7372206091223994	0.0000000000000000	0.0000000000000000		
0.0000000000000000	6.9809029500783426	0.0000000000000000		
0.0000000000000000	0.0000000000000000	25.0000000000000000		
K	Ni	O	H	Fe
4	11	35	21	1
Selective dynamics				
Direct				
0.0000000000000000	0.9295476953180497	0.0219900692777486		

0.5000000000000000 0.8431778700801544 0.1149178963106294
0.0235833671848832 0.7610896156373953 0.2060604780785119
0.5169731789877821 0.7025250247669598 0.3559084647638948
0.0000000000000000 0.4295476953180497 0.0219900692777486
0.3336660000000009 0.4295476953180497 0.0219900692777486
0.6663339999999991 0.4295476953180497 0.0219900692777486
0.1663339999999991 0.3431778700801544 0.1149178963106294
0.5000000000000000 0.3431778700801544 0.1149178963106294
0.8336660000000009 0.3431778700801544 0.1149178963106294
0.0013214901205111 0.2601607355242959 0.2101236345407043
0.3335679120572116 0.2566583581952009 0.2097465313841758
0.6656605376723471 0.2554206745009699 0.2093906948664923
0.1675914118489314 0.1761576124255569 0.3061190896520535
0.5042509046903018 0.1839488092304573 0.3050782211915273
0.1735150000000019 0.5955569454815901 0.0004884286588833
0.5000000000000000 0.5859389052830437 0.0000000000000000
0.8264849999999981 0.5955569454815901 0.0004884286588833
0.1735150000000019 0.2635384451545022 0.0434917098966210
0.5000000000000000 0.2731564853530557 0.0439801385555043
0.8264849999999981 0.2635384451545022 0.0434917098966210
0.0000000000000000 0.4995690800451484 0.0929278270328737
0.3264849999999981 0.5091871202437019 0.0934162556917641
0.6735150000000019 0.5091871202437019 0.0934162556917641
0.0000000000000000 0.1867866601151604 0.1369079655883780
0.3264849999999981 0.1771686199166140 0.1364195369294947
0.6735150000000019 0.1771686199166140 0.1364195369294947
0.1705263197099375 0.4197842669129754 0.1870616280080769
0.4983593844039415 0.4165474725039077 0.1871381683296095
0.8316037875144306 0.4184398777448762 0.1882232789532759
0.1676498120591235 0.1027597391300749 0.2325876086425917
0.5002654853694666 0.0972779614707206 0.2317165823166309
0.8314154699902981 0.0946834877826348 0.2336374102488543
0.0013210893465529 0.3358690036569651 0.2828523046984399
0.3354699137758174 0.3347727264821717 0.2816173252656241
0.6682356395428170 0.3387600885288264 0.2805558094752640
0.989297107991894 0.0241681759341360 0.3258067765790533
0.3408412966624032 0.025006440165839 0.3233195287794225
0.6728768568215672 0.0289074307152311 0.3249328644709922
0.3436370000000011 0.9295476953180497 0.0219900692777486
0.6563629999999989 0.9295476953180497 0.0219900692777486
0.1563629999999989 0.8431778700801544 0.1149178963106294
0.8436370000000011 0.8431778700801544 0.1149178963106294
0.2882160419188426 0.7235180003648963 0.2674844668763399
0.7118808673201048 0.7171872865743100 0.2590370651925053
0.1809129351504202 0.6236117531314204 0.3626695016544608
0.8598853990184218 0.6894075584384126 0.3544336575849882
0.5183996541328608 0.3073225857241580 0.3733362477652067
0.8147526331856771 0.3099840320492664 0.3771601909908951
0.1665579100468836 0.2706813820806821 0.3805331341816133
0.2777910000000006 0.8194148176612188 0.0136009167645312
0.2777910000000006 0.0396805729748735 0.0303792217909731
0.7222089999999994 0.8194148176612188 0.0136009167645312
0.7222089999999994 0.0396805729748735 0.0303792217909731
0.2222089999999994 0.7330449924233307 0.1065287437974050
0.2222089999999994 0.9533107477369782 0.1233070488238468
0.7777910000000006 0.7330449924233307 0.1065287437974050
0.7777910000000006 0.9533107477369782 0.1233070488238468
0.3694989510549683 0.6538625655215428 0.2491281741882700
0.3242769524446285 0.8549412455215030 0.2797256590959246
0.7280569250559341 0.6216626412821418 0.2306947213991578
0.7247800838674674 0.8469788219084714 0.2443563377769645
0.2176404748491191 0.6411841034706365 0.3246269994050054
0.0716060774433610 0.6588123612378232 0.3607915548868896
0.8201003039481086 0.6859021232388686 0.3168195973055712
0.8963178190612828 0.8241250070044970 0.3570622345735869
0.6970015745895752 0.3003777124361198 0.3827182655995697
0.4440721563692720 0.2388189253788066 0.3954325208998931
0.0635606429086364 0.2393375371797126 0.3934033707671934
0.8381155716407938 0.4486021688480463 0.3720225863804202

0.1722026452975610 0.4206726306163923 0.3751103880389295
0.8330159136527805 0.1706184616630597 0.3055510036950725

Figure 3 State 3

K Ni O H Fe
1.00000000000000
8.7372206091223994 0.000000000000000 0.000000000000000
0.000000000000000 6.9809029500783426 0.000000000000000
0.000000000000000 0.000000000000000 25.000000000000000

K Ni O H Fe
4 11 35 20 1

Selective dynamics

Direct
0.000000000000000 0.9295476953180497 0.0219900692777486
0.500000000000000 0.8431778700801544 0.1149178963106294
-0.0146916122734514 0.7637991030135463 0.2150514658032828
0.5695522313363484 0.7027411476933257 0.3599287341706607
0.000000000000000 0.4295476953180497 0.0219900692777486
0.3336660000000009 0.4295476953180497 0.0219900692777486
0.6663339999999991 0.4295476953180497 0.0219900692777486
0.1663339999999991 0.3431778700801544 0.1149178963106294
0.500000000000000 0.3431778700801544 0.1149178963106294
0.8336660000000009 0.3431778700801544 0.1149178963106294
0.0002150316937926 0.2652377656613481 0.2102207168140497
0.3320268592735747 0.2638813130185980 0.2099832341887780
0.6679477358076837 0.2630912485820907 0.2098184152149979
0.1636495566960492 0.1955145874867258 0.3069249466198768
0.5022013320818653 0.2015685296920332 0.3061175411488680
0.1735150000000019 0.5955569454815901 0.0004884286588833
0.500000000000000 0.5859389052830437 0.000000000000000
0.8264849999999981 0.5955569454815901 0.0004884286588833
0.1735150000000019 0.2635384451545022 0.0434917098966210
0.500000000000000 0.2731564853530557 0.0439801385555043
0.8264849999999981 0.2635384451545022 0.0434917098966210
0.000000000000000 0.4995690800451484 0.0929278270328737
0.3264849999999981 0.5091871202437019 0.0934162556917641
0.6735150000000019 0.5091871202437019 0.0934162556917641
0.000000000000000 0.1867866601151604 0.1369079655883780
0.3264849999999981 0.1771686199166140 0.1364195369294947
0.6735150000000019 0.1771686199166140 0.1364195369294947
0.1666231120400849 0.4221376418737470 0.1869590429630182
0.4993990512409480 0.4192035435743851 0.1867976978359263
0.8337148328441522 0.4217135852309898 0.1867574751223445
0.1669917047838033 0.1111942277236303 0.2338876136442866
0.4997214060112287 0.1092036233579269 0.2328740025021355
0.8338496179408927 0.1106226777239731 0.2329410907017381
-0.0002339012924240 0.3510812978342219 0.2811403514749847
0.3337348910639306 0.3541774362745931 0.2804317111169258
0.6672691093766905 0.3537409878420632 0.2797252697940449
0.9868062241989306 0.0350738162700492 0.3238132058623439
0.3366981909638091 0.0477354106003138 0.3258546811814951
0.6716725420974088 0.0477828944682916 0.3257631223270521
0.3436370000000011 0.9295476953180497 0.0219900692777486
0.6563629999999989 0.9295476953180497 0.0219900692777486
0.1563629999999989 0.8431778700801544 0.1149178963106294
0.8436370000000011 0.8431778700801544 0.1149178963106294
0.2223748278043693 0.7195799264075785 0.2924252181982880
0.5986413342585424 0.7389224109250734 0.2479760487032575
0.2129680228817904 0.6442678930181568 0.3974469076902230
0.8883275969555103 0.7277274673675578 0.3914269131265964
0.5099207880313885 0.3198914969535283 0.3730986769809062
0.8334117497573571 0.3315903112216387 0.3709440367241829
0.1451689609579249 0.2888991615151777 0.3809837435313763
0.2777910000000006 0.8194148176612188 0.0136009167645312
0.2777910000000006 0.0396805729748735 0.0303792217909731
0.7222089999999994 0.8194148176612188 0.0136009167645312

0.7222089999999994	0.0396805729748735	0.0303792217909731
0.2222089999999994	0.7330449924233307	0.1065287437974050
0.2222089999999994	0.9533107477369782	0.1233070488238468
0.7777910000000006	0.7330449924233307	0.1065287437974050
0.7777910000000006	0.9533107477369782	0.1233070488238468
0.2864883511016142	0.6083912753134018	0.2825372034971648
0.2853865510818064	0.8394184277692954	0.2948345037800985
0.5491888651434245	0.6364786341916869	0.2272268234427269
0.5492961891912915	0.8621168660210530	0.2391913288549913
0.2093117625312526	0.6865044680015767	0.3588662459915325
0.1162794943908329	0.6945267617266658	0.4121183992461215
0.8882452080396459	0.5997392350475370	0.3746440198265442
0.9235641171536564	0.8221350162294581	0.3646292448818720
0.7297192189232391	0.3100358472823987	0.3860383260644960
0.4321373657069144	0.2501807708907224	0.3934970240582581
0.0327198915727584	0.2867756572952054	0.3876912325247631
0.1776569769695109	0.4300877381375622	0.3870606683406559
0.8324012363519289	0.1887562960057956	0.3083375963869681

Figure 3 State 4

K	Ni	O	H	Fe
1.000000000000000				
8.7372206091223994	0.000000000000000	0.000000000000000		
0.000000000000000	6.9809029500783426	0.000000000000000		
0.000000000000000	0.000000000000000	25.000000000000000		

K	Ni	O	H	Fe
4	11	36	21	1

Selective dynamics

Direct

0.000000000000000	0.9295476953180497	0.0219900692777486
0.500000000000000	0.8431778700801544	0.1149178963106294
0.9810561718816594	0.7665505108314633	0.2132263917082290
0.5437097876716795	0.7532715337305980	0.3970406713408514
0.000000000000000	0.4295476953180497	0.0219900692777486
0.3336660000000009	0.4295476953180497	0.0219900692777486
0.6663339999999991	0.4295476953180497	0.0219900692777486
0.1663339999999991	0.3431778700801544	0.1149178963106294
0.500000000000000	0.3431778700801544	0.1149178963106294
0.8336660000000009	0.3431778700801544	0.1149178963106294
0.9989570327764271	0.2656214016395726	0.2102726462104375
0.3311984983106453	0.2628804541707555	0.2099898668514323
0.6672352501562534	0.2630345664806379	0.2098901794176269
0.1626592156717402	0.1943916926081247	0.3060743671683359
0.4998266427400375	0.2033036222231715	0.3061470662140889
0.1735150000000019	0.5955569454815901	0.0004884286588833
0.500000000000000	0.5859389052830437	0.000000000000000
0.8264849999999981	0.5955569454815901	0.0004884286588833
0.1735150000000019	0.2635384451545022	0.0434917098966210
0.500000000000000	0.2731564853530557	0.0439801385555043
0.8264849999999981	0.2635384451545022	0.0434917098966210
0.000000000000000	0.4995690800451484	0.0929278270328737
0.3264849999999981	0.5091871202437019	0.0934162556917641
0.6735150000000019	0.5091871202437019	0.0934162556917641
0.000000000000000	0.1867866601151604	0.1369079655883780
0.3264849999999981	0.1771686199166140	0.1364195369294947
0.6735150000000019	0.1771686199166140	0.1364195369294947
0.1665509337734901	0.4219470621178407	0.1867575887754920
0.4973067367233813	0.4162780134924038	0.1869156074832171
0.8341107127112670	0.4203865259357460	0.1866227207562040
0.1651931669207395	0.1106887351950656	0.2343313855563812
0.4982112813872639	0.1102607203179267	0.2337321676946654
0.8330245208200164	0.1130826123810981	0.2326078035048271
0.9974979081295816	0.3529194009541952	0.2806086441393817
0.3303293525090423	0.3535711034153565	0.2811209884963613
0.6657147108060655	0.3571231497323984	0.2794927390839390
0.9894682189002425	0.0344320918128573	0.3218113458248258

0.3348642478278114	0.0447828993890028	0.3242380755067834
0.6667290438571934	0.0436224833327085	0.3237522866651032
0.3436370000000011	0.9295476953180497	0.0219900692777486
0.6563629999999989	0.9295476953180497	0.0219900692777486
0.1563629999999989	0.8431778700801544	0.1149178963106294
0.8436370000000011	0.8431778700801544	0.1149178963106294
0.2247241028075757	0.7178566963331352	0.2909348162559784
0.6404539544864337	0.7622850908548313	0.2159855097653078
0.2075520714672231	0.6371490496758436	0.3951366199678385
0.8842590478270111	0.7197670274474655	0.3906283707277999
0.5097460964126754	0.3197082828278719	0.3731008316296531
0.8374759303504421	0.3278767666658081	0.3679532687211396
0.1430045764404770	0.2824498613421088	0.3790271353063638
0.4195521920316622	0.0528306588656853	0.4477085852695903
0.2777910000000006	0.8194148176612188	0.0136009167645312
0.2777910000000006	0.0396805729748735	0.0303792217909731
0.7222089999999994	0.8194148176612188	0.0136009167645312
0.7222089999999994	0.0396805729748735	0.0303792217909731
0.2222089999999994	0.7330449924233307	0.1065287437974050
0.2222089999999994	0.9533107477369782	0.1233070488238468
0.7777910000000006	0.7330449924233307	0.1065287437974050
0.7777910000000006	0.9533107477369782	0.1233070488238468
0.2893339195784263	0.6065744139810623	0.2817865474167817
0.2873769068436561	0.8381030040974253	0.2936704944444049
0.59251262088574608	0.6427451147253623	0.2275063294997489
0.5939562490561849	0.8657167711559839	0.2370196651941686
0.2080146699149137	0.6786499214057933	0.3563386643078931
0.1061240818676232	0.6808126556579638	0.4077471499360476
0.8743411862083631	0.5935812810430623	0.3728724415991748
0.9145102872644720	0.8141835008125223	0.3632320297950346
0.4461000659922282	0.1550464464654824	0.4212778460352202
0.0277962607579768	0.2924123707869622	0.3823823567216417
0.1813535854649554	0.4220961409396303	0.3853033311532358
0.6217301114170369	0.3159149238044864	0.3799696344881119
0.3083403494215963	0.0480389238689440	0.4455987503362017
0.8305968504488523	0.1946196129204482	0.3104545716530560

Figure 3 State 4'-Ni

K Ni O H Fe
1.00000000000000
8.7372206091223994 0.000000000000000 0.000000000000000
0.000000000000000 6.9809029500783426 0.000000000000000
0.000000000000000 0.000000000000000 25.000000000000000

K Ni O H Fe
4 11 36 21 1

Selective dynamics
Direct

0.000000000000000	0.9295476953180497	0.0219900692777486
0.500000000000000	0.8431778700801544	0.1149178963106294
0.9882673081805069	0.7633688577663066	0.2097507022145051
0.6036238997352193	0.6759294211858190	0.3513119120352852
0.000000000000000	0.4295476953180497	0.0219900692777486
0.3336660000000009	0.4295476953180497	0.0219900692777486
0.6663339999999991	0.4295476953180497	0.0219900692777486
0.1663339999999991	0.3431778700801544	0.1149178963106294
0.500000000000000	0.3431778700801544	0.1149178963106294
0.8336660000000009	0.3431778700801544	0.1149178963106294
0.0018052882977446	0.2626032273260687	0.2096215766088663
0.3334023329266524	0.2591259255021907	0.2098231304688948
0.6694235906433273	0.2605563626260091	0.2096888080141786
0.1634805974744891	0.1849082043911068	0.3060634832275422
0.5091917139318071	0.1890070345928628	0.3063723283785824
0.1735150000000019	0.5955569454815901	0.0004884286588833
0.500000000000000	0.5859389052830437	0.000000000000000
0.8264849999999981	0.5955569454815901	0.0004884286588833
0.1735150000000019	0.2635384451545022	0.0434917098966210

0.5000000000000000	0.2731564853530557	0.0439801385555043
0.8264849999999981	0.2635384451545022	0.0434917098966210
0.0000000000000000	0.4995690800451484	0.0929278270328737
0.3264849999999981	0.5091871202437019	0.0934162556917641
0.6735150000000019	0.5091871202437019	0.0934162556917641
0.0000000000000000	0.1867866601151604	0.1369079655883780
0.3264849999999981	0.1771686199166140	0.1364195369294947
0.6735150000000019	0.1771686199166140	0.1364195369294947
0.1678480045256359	0.4204356913025482	0.1870550773916224
0.4990652625910704	0.4172662018619963	0.1870343232833228
0.8353076578726617	0.4196771600526228	0.1873129005348674
0.1678279032557842	0.1044634331426821	0.2328303157037404
0.5030520621479688	0.1021931708845414	0.2321822270269187
0.8362459728568236	0.1070460962563056	0.2332606475329962
0.0044362572684044	0.3441438933036653	0.2811554921591658
0.3363881094139226	0.3413917202294710	0.2815393013343868
0.6667010552735921	0.3464228760823493	0.2812923853778592
0.9922849088456647	0.0279228646939732	0.3233307702296488
0.3433158088254744	0.0211620427683478	0.3256787662916428
0.6789727373728294	0.0398079701095045	0.3263867246322492
0.3436370000000011	0.9295476953180497	0.0219900692777486
0.6563629999999989	0.9295476953180497	0.0219900692777486
0.1563629999999989	0.8431778700801544	0.1149178963106294
0.8436370000000011	0.8431778700801544	0.1149178963106294
0.2203986357325146	0.6942810605292733	0.2879798012985542
0.6106756754912503	0.7358475453499698	0.2435769932476090
0.2193672874834342	0.6402543208239748	0.3929064122432440
0.9082384623223092	0.7244242096152547	0.3904202370658001
0.5149949611675820	0.3054518869105255	0.3756112733967337
0.8483893800269287	0.3279162964483885	0.3712996037856246
0.1513083707533093	0.2861462553449561	0.3816863332685193
0.4451372366421666	0.1937970821264577	0.4167379771429414
0.2777910000000006	0.8194148176612188	0.0136009167645312
0.2777910000000006	0.0396805729748735	0.0303792217909731
0.7222089999999994	0.8194148176612188	0.0136009167645312
0.7222089999999994	0.0396805729748735	0.0303792217909731
0.2222089999999994	0.7330449924233307	0.1065287437974050
0.2222089999999994	0.9533107477369782	0.1233070488238468
0.7777910000000006	0.7330449924233307	0.1065287437974050
0.7777910000000006	0.9533107477369782	0.1233070488238468
0.2794770050447467	0.5754600461281304	0.2799426693887185
0.2899315323627471	0.8053289738996208	0.2885502299540511
0.5586347040628897	0.6348737419010473	0.2228553072063684
0.5626256812700768	0.8609399317083263	0.2356331193717824
0.2145477078058639	0.6722803698130907	0.3533652388969745
0.1205102437804303	0.6904282211311367	0.4064121610496148
0.9053869038015716	0.5957767826623199	0.3739952888870889
0.9382383949066235	0.8196358021171520	0.3628205218998205
0.3476436056929383	0.0168698898329438	0.3650867850305131
0.0373256683812834	0.2817052193034779	0.3882122734638469
0.1800055288113000	0.4314681154261726	0.3853197184613440
0.7547138654692322	0.2937802218567969	0.3908922067847296
0.3366731338976689	0.2389357076737733	0.4160212678064288
0.8378533674822164	0.1825980218410728	0.3075039130396380

Figure 3 State 4'-Fe

```

K Ni O H Fe
1.0000000000000000
  8.7372206091223994  0.0000000000000000  0.0000000000000000
  0.0000000000000000  6.9809029500783426  0.0000000000000000
  0.0000000000000000  0.0000000000000000  25.0000000000000000
  K      Ni      O      H      Fe
  4      11     36     21     1
Selective dynamics
Direct
0.0000000000000000  0.9295476953180497  0.0219900692777486

```

0.5000000000000000 0.8431778700801544 0.1149178963106294
0.9871853159801064 0.7629460070523416 0.2104704530387418
0.5993884707173889 0.6670747236050891 0.3515356045912202
0.0000000000000000 0.4295476953180497 0.0219900692777486
0.3336660000000009 0.4295476953180497 0.0219900692777486
0.6663339999999991 0.4295476953180497 0.0219900692777486
0.1663339999999991 0.3431778700801544 0.1149178963106294
0.5000000000000000 0.3431778700801544 0.1149178963106294
0.8336660000000009 0.3431778700801544 0.1149178963106294
0.0008079771225791 0.2620981437086433 0.2096735729128670
0.3322166500024268 0.2586930873249491 0.2097032624102168
0.6686317279409221 0.2603902081869811 0.2096023314188251
0.1634953413852174 0.1833667144331252 0.3058030889060605
0.5073611287861243 0.1914494913583536 0.3059557207978190
0.1735150000000019 0.5955569454815901 0.0004884286588833
0.5000000000000000 0.5859389052830437 0.0000000000000000
0.8264849999999981 0.5955569454815901 0.0004884286588833
0.1735150000000019 0.2635384451545022 0.0434917098966210
0.5000000000000000 0.2731564853530557 0.0439801385555043
0.8264849999999981 0.2635384451545022 0.0434917098966210
0.0000000000000000 0.4995690800451484 0.0929278270328737
0.3264849999999981 0.5091871202437019 0.0934162556917641
0.6735150000000019 0.5091871202437019 0.0934162556917641
0.0000000000000000 0.1867866601151604 0.1369079655883780
0.3264849999999981 0.1771686199166140 0.1364195369294947
0.6735150000000019 0.1771686199166140 0.1364195369294947
0.1670434709142308 0.4198984300261953 0.1873397759804933
0.4993487113388134 0.4166517454285923 0.1870638637894567
0.8347131167701218 0.4194175277332862 0.1875824121464579
0.1660610928776394 0.1025778485667670 0.2326366584651116
0.5017801226575476 0.1025239239840338 0.2325637057018618
0.8346622133490925 0.1058035711838586 0.2335485603528120
0.0034551541512891 0.3414577115190375 0.2820992527515050
0.3336995914468384 0.3426422253463365 0.2809202867560672
0.6667972919442420 0.3460936151709199 0.2810866100881347
0.9910990762362137 0.0252674235714446 0.3229745124379891
0.3399418513895341 0.0262475797246574 0.3278153740019498
0.6748739809325544 0.0408042466389678 0.3262231981474243
0.3436370000000011 0.9295476953180497 0.0219900692777486
0.6563629999999989 0.9295476953180497 0.0219900692777486
0.1563629999999989 0.8431778700801544 0.1149178963106294
0.8436370000000011 0.8431778700801544 0.1149178963106294
0.2149484140702585 0.6926612607614173 0.2922896644627918
0.6076514125643108 0.7359483782958166 0.2434578817288728
0.2364675610403056 0.6354964491745804 0.3979888485490251
0.9080685650961364 0.7333993745520745 0.3921370727967077
0.4981674252484716 0.2997283047041238 0.3735224701499421
0.8516796712882319 0.3292684949685590 0.3712197010972662
0.1534641712375055 0.2746873377034084 0.3810214875497088
0.7909853695335066 0.2299845616850498 0.4187702413412414
0.2777910000000006 0.8194148176612188 0.0136009167645312
0.2777910000000006 0.0396805729748735 0.0303792217909731
0.7222089999999994 0.8194148176612188 0.0136009167645312
0.7222089999999994 0.0396805729748735 0.0303792217909731
0.2222089999999994 0.7330449924233307 0.1065287437974050
0.2222089999999994 0.9533107477369782 0.1233070488238468
0.7777910000000006 0.7330449924233307 0.1065287437974050
0.7777910000000006 0.9533107477369782 0.1233070488238468
0.2738839649386548 0.5758270834990481 0.2822731398533713
0.2837231067579348 0.8041676419871276 0.2926240680575486
0.5553979865072536 0.6345472302184211 0.2229431802779817
0.5586843038437914 0.8607504322667197 0.2359125120389656
0.2218392492823233 0.6679275392902729 0.3589841379801365
0.1438793585417239 0.6885229414807530 0.4146440726115714
0.9223719764174564 0.6162259969242483 0.3712959023333709
0.9410185696164765 0.8403571211437940 0.3684083748569986
0.3401381076044930 0.0524085115505927 0.3666330287307558
0.0397185373602111 0.2951859670085281 0.3833608350909500
0.2012271282327434 0.4060102999344387 0.3880299410473002

0.8159330973586905	0.3247337325156625	0.4465104421268410
0.5887720935371478	0.2515803547640478	0.3928502715503701
0.8363622089296316	0.1802511419272971	0.3069523568536060

Figure 3 State 5

K Ni O H Fe		
1.000000000000000		
8.7372206091223994	0.000000000000000	0.000000000000000
0.000000000000000	6.9809029500783426	0.000000000000000
0.000000000000000	0.000000000000000	25.000000000000000

K	Ni	O	H	Fe
4	11	36	20	1

Selective dynamics

Direct

0.000000000000000	0.9295476953180497	0.0219900692777486
0.500000000000000	0.8431778700801544	0.1149178963106294
0.9857444321261102	0.7634320715986770	0.2114316810784531
0.6092485568508154	0.6832337958494101	0.3518474616469796
0.000000000000000	0.4295476953180497	0.0219900692777486
0.333666000000000	0.4295476953180497	0.0219900692777486
0.666333999999999	0.4295476953180497	0.0219900692777486
0.166333999999999	0.3431778700801544	0.1149178963106294
0.500000000000000	0.3431778700801544	0.1149178963106294
0.833666000000000	0.3431778700801544	0.1149178963106294
0.9998817733660644	0.2628280076509055	0.2096278377181260
0.3313074227336404	0.2584036270978591	0.2098622998640508
0.6669186822294950	0.2606410833212151	0.2095748726413049
0.1607072028948470	0.1833057917815024	0.3062449584889774
0.5071155177701762	0.1889765160861706	0.3066174435171459
0.173515000000000	0.5955569454815901	0.0004884286588833
0.500000000000000	0.5859389052830437	0.000000000000000
0.826484999999998	0.5955569454815901	0.0004884286588833
0.173515000000000	0.2635384451545022	0.0434917098966210
0.500000000000000	0.2731564853530557	0.0439801385555043
0.826484999999998	0.2635384451545022	0.0434917098966210
0.000000000000000	0.4995690800451484	0.0929278270328737
0.326484999999998	0.5091871202437019	0.0934162556917641
0.673515000000000	0.5091871202437019	0.0934162556917641
0.000000000000000	0.1867866601151604	0.1369079655883780
0.326484999999998	0.1771686199166140	0.1364195369294947
0.673515000000000	0.1771686199166140	0.1364195369294947
0.1665087210642062	0.4201497692577152	0.1872148641659812
0.4980882247104562	0.4166444992779245	0.1873129073916197
0.8336162204855335	0.4202627561301256	0.1870585907963996
0.1646192345871748	0.1044597256543119	0.2322039983778454
0.5000502718431817	0.1010750053819366	0.2315033114219200
0.8329774765862643	0.1076353732740477	0.2329142642835800
0.9968715984965016	0.3484777257027003	0.2802141438966202
0.3328328481816189	0.3382016887949957	0.2816713556533973
0.6630553055696377	0.3482040152953090	0.2805514915899591
0.9885098596157874	0.0279087672936519	0.3223590903886427
0.3460230746060142	0.0188083683823314	0.3279780048058347
0.6775034218584595	0.0428475792992372	0.3271200218069797
0.343637000000001	0.9295476953180497	0.0219900692777486
0.656362999999998	0.9295476953180497	0.0219900692777486
0.156362999999998	0.8431778700801544	0.1149178963106294
0.843637000000001	0.8431778700801544	0.1149178963106294
0.2170795846648520	0.6949316155888429	0.2888254475951947
0.6105779360330140	0.7375513011490320	0.2431961405945169
0.2337902480159657	0.6368201922337512	0.3950946043559159
0.9111681900573719	0.7296567039035825	0.3916767694647711
0.5078229550502236	0.3102451124433598	0.3759298982440785
0.8480525074710418	0.3306292989509884	0.3711231480787335
0.1478514509877658	0.2745739871387189	0.3816130340308239
0.4946423277045554	0.2009714296407594	0.4170801333616143
0.277791000000000	0.8194148176612188	0.0136009167645312

0.2777910000000006	0.0396805729748735	0.0303792217909731
0.7222089999999994	0.8194148176612188	0.0136009167645312
0.7222089999999994	0.0396805729748735	0.0303792217909731
0.2222089999999994	0.7330449924233307	0.1065287437974050
0.2222089999999994	0.9533107477369782	0.1233070488238468
0.7777910000000006	0.7330449924233307	0.1065287437974050
0.7777910000000006	0.9533107477369782	0.1233070488238468
0.2758321034747961	0.5766149890996753	0.2803799904467260
0.2875137464901121	0.8049843847279882	0.2912647384546041
0.5571076310328470	0.6345204622094913	0.2237991969409262
0.5589897907027238	0.8608675485589403	0.2357393212431491
0.2181563379906646	0.6665797336643695	0.3560383048323068
0.1397784819983969	0.6877435707863224	0.4115397759624868
0.9130029919655345	0.6009107126034229	0.3757144061006243
0.9441415452350503	0.8234972565464204	0.3641082429934809
0.3417559844656622	0.0173771364894207	0.3673145866600057
0.0332144224164553	0.2901762492711112	0.3851486839305525
0.1910478651683542	0.4081296957405738	0.3879000938388386
0.7857930463943281	0.2667906084774587	0.3982136459079292
0.8355375169717228	0.1849106462755564	0.3069580794318858

References

- (1) Kresse, G.; Joubert, D. *Phys. Rev. B* **1999**, *59*, 1758.
- (2) Bajdich, M.; García-Mota, M.; Vojvodic, A.; Nørskov, J. K.; Bell, A. T. *J. Am. Chem. Soc.* **2013**, *135*, 13521.
- (3) Lu, Z.; Chen, G.; Li, Y.; Wang, H.; Xie, J.; Liao, L.; Liu, C.; Liu, Y.; Wu, T.; Li, Y.; Luntz, A. C.; Bajdich, M.; Cui, Y. *J. Am. Chem. Soc.* **2017**, *139*, 6270.
- (4) Friebel, D.; Louie, M. W.; Bajdich, M.; Sanwald, K. E.; Cai, Y.; Wise, A. M.; Cheng, M. J.; Sokaras, D.; Weng, T. C.; Alonso-Mori, R.; Davis, R. C.; Bargar, J. R.; Nørskov, J. K.; Nilsson, A.; Bell, A. T. *J. Am. Chem. Soc.* **2015**, *137*, 1305.
- (5) Goldsmith, Z. K.; Harshan, A. K.; Gerken, J. B.; Voros, M.; Galli, G.; Stahl, S. S.; Hammes-Schiffer, S. *P Natl Acad Sci USA* **2017**, *114*, 3050.