

Water Interaction with Fe₂NiP Schreibersite (110)

Surface: a Quantum Mechanical Atomistic

Perspective

Supporting information

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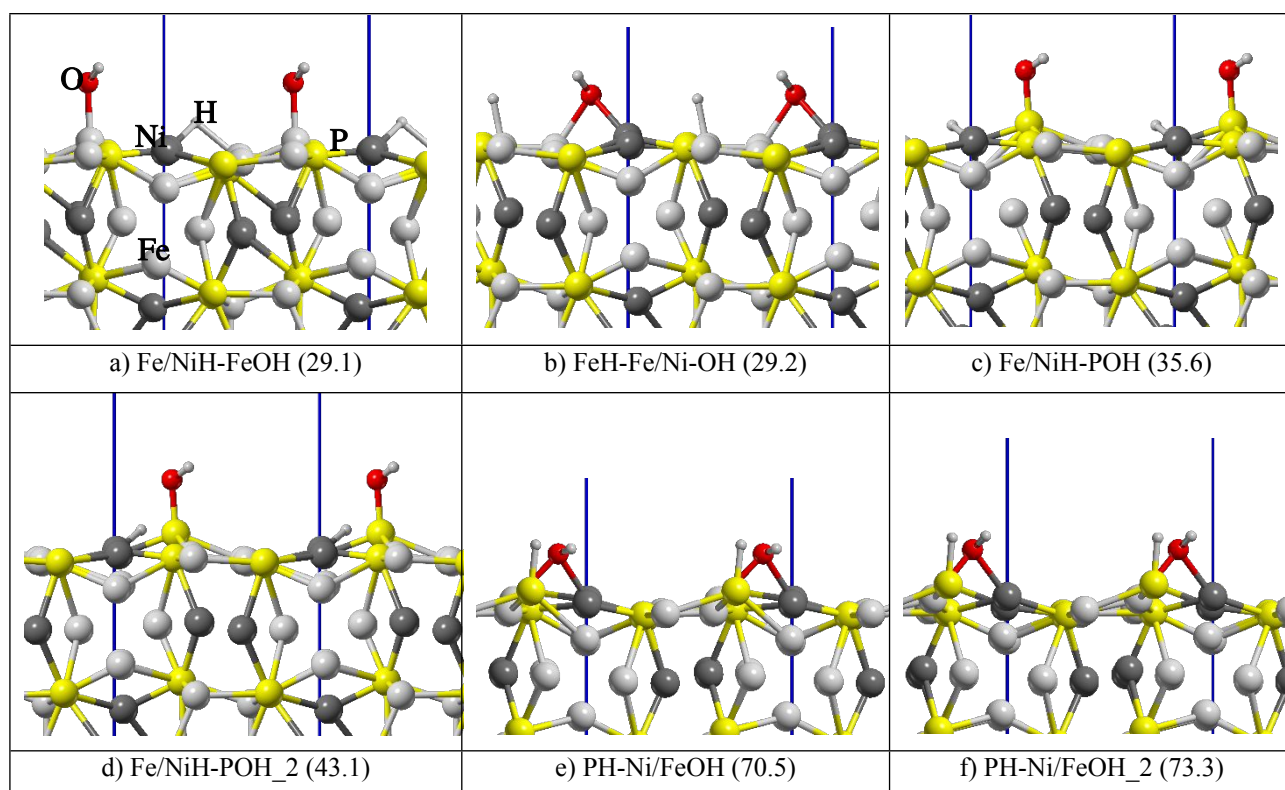


Figure S1: PBE-D*0 optimized structure of deprotonated water molecules adsorbed on the (110) schreibersite surface. H white, O red, P yellow, Fe black, Ni grey. Values in parenthesis are the binding energy per water molecule in kJ/mol.

Optimized structures in POSCAR format

H₂O-Ni

H 4 O 2 P 12 Fe 24 Ni 12

1.000000000

4.374399 0.000000 0.000000

-2.187200 6.352773 0.000000

0.000000 0.000000 40.000000

H O P Fe Ni

4 2 12 24 12

Cartesian

0.86925998	5.17132999	29.08025000	#H
0.18390999	3.81754000	29.38015000	#H
0.86925999	3.05504000	10.91975000	#H
0.18390999	4.40883000	10.61985000	#H
1.05736999	4.21388000	29.16300000	#O
1.05736999	4.01250000	10.83700000	#O
0.73699998	6.22928999	38.38620000	#P
0.85200999	2.54078000	37.90177000	#P
-1.34444002	5.71357999	35.68258000	#P
2.94794999	2.07937000	35.31145000	#P
-1.24604002	5.83021999	31.65533000	#P
3.16876999	2.27736000	31.43780000	#P
-1.20563002	5.94902999	8.56220000	#P
3.12835999	2.39616000	8.34467000	#P
-1.42645002	6.14701999	4.68855000	#P
3.02995999	2.51281000	4.31742000	#P
0.85200998	5.68559999	2.09823000	#P
0.73699999	1.99709000	1.61380000	#P
-0.39140001	2.93363000	39.84498000	#Fe
1.98456999	4.29242000	38.82216000	#Fe
0.72323000	0.23700000	37.86940000	#Fe
3.05633999	1.99862000	37.54885000	#Fe
0.84563998	6.26055999	36.01580000	#Fe
0.77174000	1.63436000	35.74982000	#Fe
-0.19231001	3.96103000	34.80420000	#Fe
1.81376998	5.24402999	33.68840000	#Fe
1.80491999	2.82847000	33.51038000	#Fe
-0.15051001	4.04999000	32.44024000	#Fe
3.13812000	0.05845000	31.63993000	#Fe
0.99552000	1.65990000	31.51552000	#Fe
3.18272000	0.21372000	8.48448000	#Fe
0.95091999	1.81516000	8.36007000	#Fe
-0.15051001	4.17639000	7.55976000	#Fe
1.80491998	5.39790999	6.48962000	#Fe
1.81376999	2.98236000	6.31160000	#Fe
-0.19231001	4.26535000	5.19580000	#Fe
2.95894000	0.23925000	4.25018000	#Fe

0.84564999	1.96581000	3.98420000	#Fe
-1.31807002	6.22774999	2.45115000	#Fe
2.91043000	1.63661000	2.13060000	#Fe
1.98456999	3.93397000	1.17784000	#Fe
-0.39140002	5.29274999	0.15502000	#Fe
1.86137000	1.60418000	39.73578000	#Ni
-0.27063001	4.41288000	37.46455000	#Ni
1.90519999	3.87615000	36.17939000	#Ni
1.78391000	0.19685000	33.74391000	#Ni
-0.38749000	1.53096000	33.48869000	#Ni
1.94741999	4.06296000	31.13747000	#Ni
1.94741999	4.16341000	8.86253000	#Ni
1.79971000	0.34266000	6.51131000	#Ni
-0.40329000	1.67676000	6.25609000	#Ni
1.90519999	4.35023000	3.82061000	#Ni
-0.27063001	3.81350000	2.53545000	#Ni
4.04857000	0.26942000	0.26422000	#Ni

H₂O-Fe

H 4 O 2 P 12 Fe 24 Ni 12

1.000000000

4.374399	0.000000	0.000000
-2.187200	6.352773	0.000000
0.000000	0.000000	40.000000

H O P Fe Ni

4 2 12 24 12

Cartesian

0.87632999	4.20638000	11.13193000	#H
3.06352999	2.14640000	28.86807000	#H
0.01076998	5.41309999	10.69282000	#H
2.19797000	0.93967000	29.30718000	#H
-0.03048001	4.44258000	10.85396000	#O
2.15671999	1.91019000	29.14604000	#O
0.15830999	1.75514000	8.60257000	#P
2.24640999	4.54937000	8.24616000	#P
-0.09428001	2.07360000	4.70410000	#P
2.17008999	4.76568000	4.30270000	#P
2.18466000	1.58206000	2.10819000	#P
-0.12264001	4.24154000	1.60511000	#P
2.06454999	2.11123000	38.39489000	#P
-0.00254001	4.77072000	37.89181000	#P
-0.01711000	1.58709000	35.69730000	#P
2.09291999	4.27918000	35.29590000	#P
0.05920999	1.80340000	31.75384000	#P
2.34550999	4.59763000	31.39743000	#P
2.34929999	2.35065000	8.50617000	#Fe
0.06278999	4.00881000	8.48795000	#Fe
1.20944000	0.00733000	7.54622000	#Fe

3.10187000	1.27512000	6.43416000	#Fe
0.94454998	5.19303999	6.26739000	#Fe
1.13205000	0.16014000	5.17253000	#Fe
2.09143999	2.49854000	4.25642000	#Fe
-0.01547001	4.22729000	3.96236000	#Fe
0.01435999	2.12476000	2.45696000	#Fe
2.05143999	3.88563000	2.12496000	#Fe
1.12577998	6.17807999	1.17655000	#Fe
0.93714000	1.17976000	0.16104000	#Fe
-1.25006002	5.17301999	39.83896000	#Fe
3.31298000	0.17470000	38.82345000	#Fe
-0.13576001	2.46715000	37.87504000	#Fe
2.20155999	4.22801000	37.54304000	#Fe
2.17172999	2.12548000	36.03764000	#Fe
-0.09576001	3.85423000	35.74358000	#Fe
-1.05515002	6.19262999	34.82747000	#Fe
3.13175000	1.15973000	33.73261000	#Fe
0.91466999	5.07764999	33.56584000	#Fe
-0.97776002	6.34543999	32.45378000	#Fe
2.24998999	2.34397000	31.51205000	#Fe
0.16209999	4.00213000	31.49383000	#Fe
1.11387998	6.35264299	8.63482000	#Ni
0.92553999	2.57348000	6.56778000	#Ni
-1.24249001	3.90868000	6.23979000	#Ni
3.23477000	0.26082000	3.81936000	#Ni
-1.13129002	6.06558999	2.52316000	#Ni
3.19126999	2.50955000	0.26955000	#Ni
1.00406999	3.84323000	39.73045000	#Ni
1.05591000	0.28718000	37.47684000	#Ni
1.04756998	6.09194999	36.18064000	#Ni
0.94470999	2.44410000	33.76021000	#Ni
-1.26166001	3.77929000	33.43222000	#Ni
3.30108000	0.00013000	31.36518000	#Ni

H₂O-mono

H 12 O 6 P 12 Fe 24 Ni 12

1.000000000

4.374399 0.000000 0.000000

-2.187200 6.352773 0.000000

0.000000 0.000000 40.000000

H O P Fe Ni

12 6 12 24 12

Cartesian

0.65768398 5.65295699 11.29907400 #H

2.84488400 0.69981600 28.70092600 #H

2.23750198 5.62605299 11.31905200 #H

0.05030300 0.72672000 28.68094800 #H

0.42482999 2.06796100 13.00708500 #H

2.61202999 4.28481200 26.99291500 #H

3.79528800	1.38868500	12.02283500	#H
1.60808899	4.96408900	27.97716500	#H
-0.74648401	4.30616100	10.51216100	#H
1.44071599	2.04661200	29.48783900	#H
-0.63839501	3.73581700	11.96265800	#H
1.54880499	2.61695600	28.03734200	#H
1.46118098	6.21272399	11.08568600	#O
3.64838100	0.14004900	28.91431400	#O
-0.46252501	2.17623800	12.62303600	#O
1.72467399	4.17653600	27.37696400	#O
-0.71975701	4.60449900	11.45985700	#O
1.46744299	1.74827400	28.54014300	#O
0.55586899	1.83875800	8.55565400	#P
2.68012699	4.63991000	8.25254300	#P
0.33767999	2.05566900	4.69594900	#P
2.61304699	4.76746300	4.30678700	#P
2.62271500	1.58096600	2.09866400	#P
0.32017799	4.24339700	1.61070100	#P
2.50737799	2.10937600	38.38929900	#P
0.43551599	4.77180800	37.90133600	#P
0.42584700	1.58531000	35.69321300	#P
2.52487999	4.29710500	35.30405100	#P
0.49292799	1.71286300	31.74745700	#P
2.74306899	4.51401600	31.44434600	#P
2.75604799	2.45671200	8.49618600	#Fe
0.50477999	4.06757900	8.34980700	#Fe
1.64161900	0.07616000	7.57225500	#Fe
3.58341000	1.29219900	6.50553500	#Fe
1.39722098	5.24121899	6.29203500	#Fe
1.57767900	0.16870300	5.19483500	#Fe
2.53500799	2.48694100	4.24703100	#Fe
0.43040599	4.22056300	3.97159700	#Fe
0.45184499	2.12213700	2.45256400	#Fe
2.49459399	3.88410100	2.12775800	#Fe
1.56764898	6.17920599	1.17801700	#Fe
1.37838000	1.17959600	0.15690100	#Fe
-0.80882002	5.17317799	39.84309900	#Fe
3.75484900	0.17356800	38.82198300	#Fe
0.30739399	2.46867200	37.87224200	#Fe
2.63904399	4.23063600	37.54743600	#Fe
2.61760599	2.13221100	36.02840300	#Fe
0.34780799	3.86583300	35.75296900	#Fe
-0.60952102	6.18406999	34.80516500	#Fe
3.58442000	1.11155400	33.70796500	#Fe
1.39621099	5.06057399	33.49446500	#Fe
-0.54558102	6.27661399	32.42774500	#Fe
2.69197899	2.28519400	31.65019300	#Fe
0.56884799	3.89606100	31.50381400	#Fe
3.71295500	0.04695500	8.89162700	#Ni
1.38923999	2.59393000	6.51512400	#Ni

-0.81227601	3.91767900	6.22526400	#Ni
3.67399700	0.25371700	3.82432200	#Ni
-0.68913802	6.06378099	2.53383200	#Ni
-0.74223901	2.51082400	0.26470900	#Ni
1.44496099	3.84195000	39.73529100	#Ni
1.49806100	0.28899200	37.46616800	#Ni
1.48679798	6.09905699	36.17567800	#Ni
1.37492399	2.43509400	33.77473600	#Ni
-0.79796001	3.75884300	33.48487600	#Ni
1.52575398	6.30581799	31.10837300	#Ni

H₂O-Ni-multi

H 38 O 19 P 12 Fe 24 Ni 12

1.000000000

4.361536 0.000000 -0.106245

-2.188342 6.337633 -0.085901

0.000000 0.000000 38.736014

H O P Fe Ni

38 19 12 24 12

Cartesian

0.70239504	4.74486630	24.61231610	#H
-0.17709625	5.91664842	23.93259747	#H
-0.15635932	2.01958554	18.21768067	#H
3.34175171	2.88032799	17.11251755	#H
0.07062041	5.04917435	20.01356949	#H
-0.78530108	4.20446206	18.97687019	#H
0.59611342	0.86618278	22.93371264	#H
4.25721393	0.04769795	23.99497411	#H
-0.99663558	4.01265721	15.14918869	#H
2.41787964	2.71281534	15.06856702	#H
-0.31559592	1.73938946	21.27097563	#H
0.16656848	0.22445953	21.09191020	#H
0.38098887	5.72673124	14.90860413	#H
-0.16349986	5.43003550	13.42840880	#H
0.24272471	2.21889272	15.03599500	#H
1.15999759	0.94900613	14.56147761	#H
1.36566621	0.10311127	18.60046397	#H
2.00720904	1.52214690	18.10574107	#H
2.72358425	2.71182675	22.43743007	#H
1.92081733	2.06306293	21.25086477	#H
1.04340600	5.05721590	22.11593403	#H
1.95857724	4.30322723	21.07580424	#H
4.26198450	0.08736587	16.67978203	#H
2.71757718	0.03667202	16.95609313	#H
-0.65485875	1.99868106	24.41061045	#H
2.14911473	1.79135454	24.33080458	#H
0.96857807	5.70410776	11.08872339	#H
2.66227053	0.28552783	27.30573336	#H
-1.80957633	5.71150416	11.18766692	#H

4.24341264	0.33276563	27.26828084 #H
0.19136914	2.21882080	13.05945466 #H
2.08940566	3.56522468	25.54434337 #H
-0.46008977	1.59247273	11.75782409 #H
1.33920778	4.55274138	26.59419738 #H
-0.42924057	4.51999108	10.38125788 #H
1.27763641	1.62009483	28.15029535 #H
-0.42433221	3.76854214	11.76917352 #H
1.14110463	2.20358416	26.71085218 #H
0.67348886	5.40326020	23.86261980 #O
3.39909971	2.59927355	18.07585783 #O
-0.71447690	5.09557835	19.40942567 #O
0.64860350	0.69449681	23.93940140 #O
3.25349453	3.11776655	15.45440158 #O
0.48776623	1.13734340	21.34281557 #O
-0.44469265	5.58317697	14.35009941 #O
1.04789702	1.93453312	14.50997418 #O
1.27297038	0.86420375	17.93514429 #O
2.68850310	2.67272568	21.44638399 #O
1.36805410	5.09333647	21.18265142 #O
1.24008637	5.99643317	16.30052666 #O
2.84648837	2.48492270	24.25425222 #O
1.75515220	6.25936346	10.81194430 #O
1.28166055	6.07426846	27.42086754 #O
-0.47726466	2.39190113	12.33829535 #O
1.21952969	3.78319171	25.96304303 #O
-0.41372420	4.72857376	11.35130054 #O
1.22867396	1.33265908	27.19586263 #O
0.84134534	1.82024614	8.46018445 #P
-1.41187283	4.60820635	8.14670626 #P
0.53677377	1.96575016	4.60148410 #P
-1.56685337	4.66098399	4.20203804 #P
2.75775032	1.44170763	1.95520174 #P
0.44784318	4.08539678	1.46403764 #P
2.55801838	1.89961166	36.97642210 #P
0.47840176	4.54344036	36.47902292 #P
0.42177185	1.32341866	34.33994071 #P
2.50242375	4.01555237	33.83908576 #P
0.39521338	1.37147090	30.39848077 #P
2.63428210	4.15873715	29.95976139 #P
3.03226782	2.43461033	8.33430814 #Fe
0.78348906	4.04019394	8.20495990 #Fe
1.89684053	0.04323796	7.48050172 #Fe
3.81910035	1.23666285	6.34971339 #Fe
1.63055354	5.17291991	6.10039916 #Fe
1.78925266	0.09196813	5.10876282 #Fe
2.71629925	2.38425139	4.08659239 #Fe
0.60982523	4.11046630	3.82127488 #Fe
0.60002638	1.98537725	2.35373025 #Fe
2.62794683	3.73863815	1.94052483 #Fe

1.67907466	6.01050817	0.95910497	#Fe
1.47545312	1.00371098	0.05314074	#Fe
-0.71670353	4.98193093	38.44076705	#Fe
1.62620214	6.31301815	37.33426486	#Fe
0.35118740	2.24547372	36.50189516	#Fe
2.66658206	3.99830466	36.08075496	#Fe
2.61388691	1.87240996	34.61535917	#Fe
0.34233910	3.59890413	34.35481681	#Fe
-0.63660274	5.89219324	33.37861849	#Fe
3.52768158	0.81124909	32.29460537	#Fe
1.33706298	4.74725586	32.04271917	#Fe
-0.62938331	5.93821649	31.00097199	#Fe
2.58507656	1.94084559	30.23016652	#Fe
0.46596893	3.54280449	30.09508753	#Fe
3.99247673	0.03813565	8.76246943	#Ni
1.63128372	2.53741238	6.38380637	#Ni
-0.57087020	3.85030091	6.11188751	#Ni
3.84723150	0.14851813	3.68397679	#Ni
-0.53937191	5.92273361	2.37395080	#Ni
-0.63642493	2.33407292	0.18513766	#Ni
1.53074058	3.65236032	38.30764770	#Ni
1.53308004	0.06237674	36.11512202	#Ni
1.48680275	5.83499936	34.70093363	#Ni
1.32843386	2.13640179	32.38483340	#Ni
-0.84784143	3.45108897	32.11029456	#Ni
1.40200634	5.93830419	29.63946663	#Ni

H₂O-Ni_2x1

H 2 O 1 P 24 Fe 48 Ni 24

1.000000000

8.748798 0.000000 0.000000

-2.187200 6.352773 0.000000

0.000000 0.000000 40.000000

H O P Fe Ni

2 1 24 48 24

Cartesian

0.91868999 3.09588000 11.01956000 #H

0.14351999 4.38256000 10.63377000 #H

1.04674999 4.04621000 10.82713000 #O

0.73460998 6.22564999 38.38395000 #P

0.85170999 2.53616000 37.89541000 #P

-1.34621002 5.70703999 35.68088000 #P

2.95313999 2.07022000 35.30873000 #P

-1.22166002 5.83094999 31.60580000 #P

3.18850999 2.28745000 31.42219000 #P

-1.18329002 5.93467999 8.59001000 #P

3.11658999 2.40951000 8.35307000 #P

-1.42070002 6.15146999 4.67773000 #P

3.03106999 2.51470000 4.32349000 #P

0.85435998	5.68401999	2.09977000 #P
0.73817999	1.99655000	1.61097000 #P
5.10870998	6.22563999	38.38238000 #P
5.22561999	2.53628000	37.89457000 #P
3.02794998	5.70705999	35.68075000 #P
7.32742999	2.07020000	35.30838000 #P
3.15263998	5.83093999	31.60601000 #P
7.56298999	2.28738000	31.42208000 #P
3.15385998	5.96349999	8.55023000 #P
7.52297999	2.39054000	8.39460000 #P
2.95234998	6.14837999	4.69394000 #P
7.40647999	2.51761000	4.30412000 #P
5.22701998	5.68602999	2.09805000 #P
5.11093999	1.99595000	1.61068000 #P
-0.39162001	2.93052000	39.84110000 #Fe
1.98371999	4.28901000	38.82028000 #Fe
0.72072000	0.23288000	37.86731000 #Fe
3.05545999	1.99202000	37.54470000 #Fe
0.84212998	6.25326999	36.00546000 #Fe
0.77285000	1.62125000	35.74055000 #Fe
-0.20058001	3.95834000	34.80755000 #Fe
1.79904998	5.25417999	33.70109000 #Fe
1.77868999	2.80941000	33.54423000 #Fe
-0.12780001	4.05133000	32.42896000 #Fe
3.15404000	0.04816000	31.59681000 #Fe
1.01189000	1.67741000	31.50141000 #Fe
3.18485000	0.22942000	8.48583000 #Fe
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1.80174998	5.40962999	6.49375000 #Fe
1.81041999	2.97910000	6.31757000 #Fe
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0.84825999	1.96805000	3.98805000 #Fe
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7.43005999	1.99237000	37.54402000 #Fe
5.21650998	6.25329999	36.00507000 #Fe
5.14718000	1.62097000	35.74097000 #Fe
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6.15302999	2.80939000	33.54413000 #Fe
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5.38628000	1.67748000	31.50138000 #Fe

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H₂O-Ni_2x2

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H O P Fe Ni

2 1 48 96 48

Cartesian

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H₂O-Fe_2x1

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0.000000 0.000000 40.000000

H O P Fe Ni
2 1 24 48 24

Cartesian

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H₂O-Fe_2x2

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H O P Fe Ni

2 1 48 96 48

Cartesian

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Fe/NiH-FeOH

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0.000000 0.000000 40.000000

H O P Fe Ni

2 1 24 48 24

Cartesian

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FeH-Fe/Ni-OH

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-2.187200 6.352773 0.000000

0.000000 0.000000 40.000000

H O P Fe Ni

2 1 24 48 24

Cartesian

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4.33821999	3.88322000	35.74914000 #Fe

3.36273998	6.21810999	34.81772000	#Fe
7.54798000	1.15498000	33.71202000	#Fe
5.33919999	5.06208999	33.55346000	#Fe
3.43277998	6.30230999	32.43926000	#Fe
6.71408999	2.29782000	31.60691000	#Fe
4.57078999	3.92674000	31.51311000	#Fe
1.15140998	6.34885299	8.90675000	#Ni
0.96288999	2.65082000	6.59627000	#Ni
-1.19972001	3.97311000	6.26016000	#Ni
3.27848000	0.30361000	3.83374000	#Ni
-1.08604002	6.10517999	2.53151000	#Ni
3.23663999	2.54454000	0.27448000	#Ni
1.04909999	3.88102000	39.74163000	#Ni
1.10542000	0.32754000	37.47168000	#Ni
1.08942998	6.13154999	36.18554000	#Ni
0.95581999	2.43226000	33.72610000	#Ni
-1.21711001	3.77871000	33.47938000	#Ni
1.13837998	6.31155999	31.30762000	#Ni
7.69521000	0.06580000	8.66211000	#Ni
5.36746999	2.63465000	6.53710000	#Ni
3.18050999	3.94224000	6.19242000	#Ni
7.65660000	0.30908000	3.82819000	#Ni
3.28903998	6.10453999	2.53070000	#Ni
7.61141999	2.54534000	0.27383000	#Ni
5.42483999	3.88095000	39.73793000	#Ni
5.47948000	0.32760000	37.47208000	#Ni
5.46345998	6.13148999	36.18454000	#Ni
5.33020999	2.43260000	33.72611000	#Ni
3.15692999	3.77875000	33.47954000	#Ni
5.51271998	6.31170999	31.30787000	#Ni

Fe/NiH-POH

H 2 O 1 P 24 Fe 48 Ni 24

1.000000000

8.748798 0.000000 0.000000

-2.187200 6.352773 0.000000

0.000000 0.000000 40.000000

H O P Fe Ni

2 1 24 48 24

Cartesian

1.05955999 2.25964000 11.21837000 #H

4.24411998 5.77720999 9.14774000 #H

0.34196000 1.70509000 10.85314000 #O

0.26470999 1.81935000 9.18573000 #P

2.22382999 4.63129000 8.24366000 #P

-0.05215001 2.08421000 4.66099000 #P

2.21356999 4.79981000 4.30041000 #P

2.22884000 1.60677000 2.09127000 #P

-0.07877001 4.26984000 1.59671000 #P

4.49756999	1.87238000	8.54276000 #P
6.72453999	4.61672000	8.29955000 #P
4.32637999	2.09423000	4.69717000 #P
6.58902999	4.79832000	4.28335000 #P
6.59817000	1.60898000	2.09030000 #P
4.29585999	4.26933000	1.59811000 #P
2.10928999	2.12955000	38.37450000 #P
0.03892999	4.79252000	37.88343000 #P
0.02762000	1.60063000	35.67295000 #P
2.13843999	4.31824000	35.29916000 #P
0.14525999	1.71561000	31.59726000 #P
2.36927999	4.52459000	31.41231000 #P
6.48236999	2.12876000	38.37318000 #P
4.41306999	4.79270000	37.88312000 #P
4.40191000	1.60057000	35.67314000 #P
6.51278999	4.31794000	35.29883000 #P
4.51963999	1.71561000	31.59744000 #P
6.74353999	4.52458000	31.41223000 #P
2.32332999	2.45897000	8.44301000 #Fe
0.11747999	3.95929000	8.37874000 #Fe
1.21889000	0.16996000	7.58294000 #Fe
3.14885000	1.32284000	6.43285000 #Fe
0.97863998	5.25561999	6.26154000 #Fe
1.16257000	0.19199000	5.18739000 #Fe
2.14258999	2.52597000	4.23661000 #Fe
0.02647999	4.25101000	3.96795000 #Fe
0.05774999	2.15344000	2.43198000 #Fe
2.09701999	3.91413000	2.11616000 #Fe
1.17122998	6.20291999	1.16932000 #Fe
0.98070000	1.20336000	0.14335000 #Fe
6.79355999	2.39276000	8.51155000 #Fe
4.48111999	4.15131000	8.41588000 #Fe
5.59099000	0.08233000	7.61485000 #Fe
7.50484000	1.34152000	6.42672000 #Fe
5.36165998	5.24508999	6.25644000 #Fe
5.54952000	0.19340000	5.20585000 #Fe
6.50742999	2.52656000	4.24733000 #Fe
4.40407999	4.25116000	3.96864000 #Fe
4.42984999	2.15266000	2.44898000 #Fe
6.46945999	3.90981000	2.11424000 #Fe
5.54405998	6.20441999	1.16524000 #Fe
5.35440000	1.20316000	0.14611000 #Fe
-1.20767002	5.19568999	39.82957000 #Fe
3.35705000	0.19577000	38.81084000 #Fe
-0.09074001	2.48939000	37.85927000 #Fe
2.24344999	4.24479000	37.53507000 #Fe
2.21698999	2.14997000	35.99433000 #Fe
-0.04136001	3.86786000	35.72898000 #Fe
-1.01572002	6.20283999	34.79772000 #Fe
3.16951000	1.14189000	33.69181000 #Fe

0.96048999	5.04926999	33.53351000	#Fe
-0.94718002	6.28960999	32.41918000	#Fe
2.33444999	2.28508000	31.58716000	#Fe
0.19218999	3.91441000	31.49169000	#Fe
3.16726998	5.19596999	39.83021000	#Fe
7.73130000	0.19608000	38.80852000	#Fe
4.28271999	2.48931000	37.86012000	#Fe
6.61818999	4.24475000	37.53468000	#Fe
6.59134999	2.14984000	35.99436000	#Fe
4.33291999	3.86779000	35.72947000	#Fe
3.35879998	6.20298999	34.79792000	#Fe
7.54405000	1.14182000	33.69157000	#Fe
5.33490999	5.04918999	33.53343000	#Fe
3.42740998	6.28957999	32.41918000	#Fe
6.70872999	2.28509000	31.58686000	#Fe
4.56655999	3.91431000	31.49184000	#Fe
3.27716000	0.06850000	8.68871000	#Ni
0.95716999	2.60332000	6.49919000	#Ni
-1.22450001	3.96241000	6.24000000	#Ni
3.27322000	0.28594000	3.82247000	#Ni
-1.08650002	6.09075999	2.51940000	#Ni
3.23393999	2.53101000	0.25491000	#Ni
7.78463000	0.09798000	8.62286000	#Ni
5.34206999	2.64657000	6.55549000	#Ni
3.15622999	3.95512000	6.23537000	#Ni
7.64299000	0.28527000	3.80714000	#Ni
3.28690998	6.09125999	2.52818000	#Ni
7.60581999	2.53231000	0.24915000	#Ni
1.04564999	3.86529000	39.72223000	#Ni
1.10115000	0.31141000	37.45266000	#Ni
1.08462998	6.11579999	36.16497000	#Ni
0.95238999	2.41951000	33.70779000	#Ni
-1.22117001	3.76658000	33.45747000	#Ni
1.13248998	6.29907999	31.28553000	#Ni
5.41925999	3.86689000	39.72148000	#Ni
5.47475000	0.31136000	37.45274000	#Ni
5.45931998	6.11557999	36.16479000	#Ni
5.32686999	2.41939000	33.70782000	#Ni
3.15317999	3.76685000	33.45783000	#Ni
5.50688998	6.29909999	31.28526000	#Ni

Fe/NiH-POH_2

H 2 O 1 P 24 Fe 48 Ni 24

1.000000000

8.748798 0.000000 0.000000

-2.187200 6.352773 0.000000

0.000000 0.000000 40.000000

H O P Fe Ni

2 1 24 48 24

Cartesian

-0.03316002	5.55894999	9.33815000 #H
0.02831999	2.37050000	11.28451000 #H
0.43491000	1.63080000	10.79192000 #O
0.21049999	1.81649000	9.13135000 #P
2.32600999	4.58394000	8.26053000 #P
-0.03283001	2.07445000	4.68250000 #P
2.21987999	4.77345000	4.28066000 #P
2.23485000	1.58666000	2.09273000 #P
-0.06904001	4.24978000	1.59508000 #P
2.11579999	2.11359000	38.37346000 #P
0.04666999	4.77698000	37.88230000 #P
0.03320000	1.58844000	35.67046000 #P
2.14397999	4.30585000	35.29707000 #P
0.14889999	1.70912000	31.59599000 #P
2.37232999	4.51802000	31.41075000 #P
4.57198999	1.80830000	8.54768000 #P
6.66831999	4.57885000	8.24616000 #P
4.32573999	2.06919000	4.68578000 #P
6.60948999	4.78000000	4.28725000 #P
6.61085000	1.58697000	2.08955000 #P
4.30419999	4.24501000	1.59285000 #P
6.48987999	2.11335000	38.37290000 #P
4.42082999	4.77706000	37.88161000 #P
4.40750000	1.58844000	35.67061000 #P
6.51843999	4.30556000	35.29680000 #P
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6.74669999	4.51814000	31.41081000 #P
2.34789999	2.39337000	8.48609000 #Fe
0.12896999	4.03122000	8.43478000 #Fe
1.24924000	0.12707000	7.68357000 #Fe
3.16029000	1.28502000	6.45346000 #Fe
0.99607998	5.21596999	6.26398000 #Fe
1.17717000	0.17092000	5.23347000 #Fe
2.14509999	2.49897000	4.24378000 #Fe
0.03977999	4.22951000	3.95899000 #Fe
0.06602999	2.13165000	2.44008000 #Fe
2.10364999	3.88754000	2.11502000 #Fe
1.17640998	6.18395999	1.16570000 #Fe
0.98967000	1.18295000	0.14430000 #Fe
-1.19786002	5.17646999	39.82813000 #Fe
3.36438000	0.17967000	38.80916000 #Fe
-0.08467001	2.47340000	37.85732000 #Fe
2.25083999	4.22982000	37.53293000 #Fe
2.22200999	2.13666000	35.99238000 #Fe
-0.03589001	3.85585000	35.72738000 #Fe
-1.00960002	6.19156999	34.79620000 #Fe
3.17465000	1.13293000	33.69006000 #Fe
0.96562999	5.04075999	33.53168000 #Fe
-0.94339002	6.28241999	32.41748000 #Fe

2.33804999	2.27825000	31.58500000	#Fe
0.19558999	3.90784000	31.48882000	#Fe
6.81224999	2.38734000	8.47575000	#Fe
4.50567999	4.04972000	8.36130000	#Fe
5.60781000	0.04496000	7.51896000	#Fe
7.52182000	1.29893000	6.41082000	#Fe
5.37764998	5.21306999	6.23959000	#Fe
5.55365000	0.16728000	5.15751000	#Fe
6.52511999	2.50720000	4.23639000	#Fe
4.41595999	4.23166000	3.95935000	#Fe
4.43898999	2.12952000	2.44355000	#Fe
6.47978999	3.89152000	2.10996000	#Fe
5.55491998	6.18237999	1.16533000	#Fe
5.36419000	1.18415000	0.14476000	#Fe
3.17455998	5.17717999	39.82769000	#Fe
7.73968000	0.17912000	38.80790000	#Fe
4.28947999	2.47332000	37.85708000	#Fe
6.62565999	4.22976000	37.53236000	#Fe
6.59627999	2.13638000	35.99239000	#Fe
4.33829999	3.85576000	35.72757000	#Fe
3.36473998	6.19161999	34.79644000	#Fe
7.54914000	1.13287000	33.68999000	#Fe
5.34005999	5.04073999	33.53174000	#Fe
3.43099998	6.28230999	32.41763000	#Fe
6.71245999	2.27838000	31.58499000	#Fe
4.57002999	3.90787000	31.48905000	#Fe
3.38946000	0.00438000	8.73996000	#Ni
0.97111999	2.58131000	6.54923000	#Ni
-1.19453001	3.91867000	6.23754000	#Ni
3.27591000	0.26293000	3.81839000	#Ni
-1.07767002	6.07076999	2.52835000	#Ni
3.24208999	2.51147000	0.25244000	#Ni
1.05471999	3.84630000	39.71988000	#Ni
1.10868000	0.29634000	37.45114000	#Ni
1.09181998	6.10327999	36.16457000	#Ni
0.95789999	2.41075000	33.70644000	#Ni
-1.21561001	3.75793000	33.45500000	#Ni
1.13612998	6.29264999	31.28426000	#Ni
7.72141000	0.06374000	8.58352000	#Ni
5.36078999	2.59057000	6.51965000	#Ni
3.16926999	3.92552000	6.21398000	#Ni
7.66231000	0.26667000	3.80833000	#Ni
3.29515998	6.06837999	2.51065000	#Ni
7.61689999	2.51184000	0.25025000	#Ni
5.42910999	3.84739000	39.71824000	#Ni
5.48266000	0.29614000	37.45219000	#Ni
5.46616998	6.10305999	36.16408000	#Ni
5.33241999	2.41063000	33.70648000	#Ni
3.15871999	3.75792000	33.45521000	#Ni
5.51038998	6.29269999	31.28428000	#Ni

PH-Ni/FeOH

H 2 O 1 P 24 Fe 48 Ni 24

1.000000000

8.748798 0.000000 0.000000

-2.187200 6.352773 0.000000

0.000000 0.000000 40.000000

H O P Fe Ni

2 1 24 48 24

Cartesian

0.42198000 1.57548000 10.48850000 #H

5.85116000 0.48752000 10.36752000 #H

6.73266000 0.88286000 10.21762000 #O

0.34361999 1.72991000 9.05910000 #P

2.28132999 4.59882000 8.30269000 #P

-0.05401001 2.05728000 4.68227000 #P

2.22970999 4.77263000 4.28957000 #P

2.23911000 1.58606000 2.09357000 #P

-0.06935001 4.24686000 1.59618000 #P

4.46975999 1.78349000 8.48431000 #P

6.68055999 4.50574000 8.27698000 #P

4.33982999 2.08909000 4.71543000 #P

6.59688999 4.77405000 4.28927000 #P

6.60913000 1.58866000 2.09740000 #P

4.30727999 4.24502000 1.59841000 #P

2.11422999 2.11704000 38.37731000 #P

0.04421999 4.78016000 37.88449000 #P

0.02926000 1.59101000 35.67359000 #P

2.14005999 4.30812000 35.29933000 #P

0.14547999 1.71026000 31.59741000 #P

2.36902999 4.51923000 31.41233000 #P

6.48719999 2.11600000 38.37638000 #P

4.41860999 4.77980000 37.88482000 #P

4.40360000 1.59097000 35.67378000 #P

6.51439999 4.30793000 35.29935000 #P

4.51994999 1.71027000 31.59756000 #P

6.74334999 4.51934000 31.41206000 #P

2.35679999 2.42835000 8.40971000 #Fe

0.11716999 3.91379000 8.36201000 #Fe

1.16535000 0.05685000 7.57182000 #Fe

3.16293000 1.26851000 6.41899000 #Fe

0.99835998 5.20332999 6.26107000 #Fe

1.17953000 0.16639000 5.18687000 #Fe

2.15097999 2.49302000 4.22873000 #Fe

0.04175999 4.22399000 3.96401000 #Fe

0.06574999 2.12778000 2.44074000 #Fe

2.10467999 3.89184000 2.11776000 #Fe

1.17825998 6.18332999 1.16881000 #Fe

0.98990000 1.18580000 0.14767000 #Fe

6.72177999	2.25554000	8.76512000	#Fe
4.47900999	4.03273000	8.39421000	#Fe
5.60010000	0.01853000	7.50014000	#Fe
7.56170000	1.30763000	6.53058000	#Fe
5.39374998	5.22242999	6.29667000	#Fe
5.56664000	0.17456000	5.16888000	#Fe
6.52244999	2.49820000	4.25827000	#Fe
4.41893999	4.23198000	3.95492000	#Fe
4.44111999	2.12846000	2.45651000	#Fe
6.48018999	3.88654000	2.11833000	#Fe
5.55433998	6.18475999	1.16686000	#Fe
5.36323000	1.18547000	0.14986000	#Fe
-1.20001002	5.17882999	39.83132000	#Fe
3.36300000	0.18246000	38.81227000	#Fe
-0.08699001	2.47655000	37.86012000	#Fe
2.24895999	4.23296000	37.53505000	#Fe
2.21811999	2.13918000	35.99515000	#Fe
-0.03986001	3.85793000	35.72962000	#Fe
-1.01403002	6.19409999	34.79844000	#Fe
3.17024000	1.13498000	33.69235000	#Fe
0.96128999	5.04235999	33.53387000	#Fe
-0.94700002	6.28373999	32.41937000	#Fe
2.33448999	2.27955000	31.58776000	#Fe
0.19194999	3.90902000	31.49113000	#Fe
3.17492998	5.17859999	39.83112000	#Fe
7.73651000	0.18235000	38.81112000	#Fe
4.28679999	2.47618000	37.86062000	#Fe
6.62314999	4.23290000	37.53513000	#Fe
6.59247999	2.13931000	35.99567000	#Fe
4.33450999	3.85805000	35.73047000	#Fe
3.36064998	6.19423999	34.79874000	#Fe
7.54469000	1.13511000	33.69232000	#Fe
5.33573999	5.04237999	33.53396000	#Fe
3.42758998	6.28371999	32.41939000	#Fe
6.70878999	2.27968000	31.58757000	#Fe
4.56643999	3.90898000	31.49134000	#Fe
1.08821998	6.34373999	8.66142000	#Ni
1.00163999	2.57074000	6.48487000	#Ni
-1.19347001	3.92172000	6.21136000	#Ni
3.28971000	0.26319000	3.82021000	#Ni
-1.07573002	6.06848999	2.52120000	#Ni
3.24353999	2.51369000	0.25873000	#Ni
5.52444998	6.31513999	8.78932000	#Ni
5.40899999	2.58210000	6.57694000	#Ni
3.18580999	3.91794000	6.22209000	#Ni
7.66098000	0.26345000	3.81077000	#Ni
3.29674998	6.07038999	2.51515000	#Ni
7.61590999	2.51398000	0.25342000	#Ni
1.05410999	3.84876000	39.72137000	#Ni
1.10570000	0.29957000	37.45459000	#Ni

1.08770998	6.10564999	36.16640000	#Ni
0.95318999	2.41279000	33.70854000	#Ni
-1.22017001	3.76041000	33.45720000	#Ni
1.13262998	6.29382999	31.28626000	#Ni
5.42875999	3.84951000	39.72178000	#Ni
5.47987000	0.29908000	37.45442000	#Ni
5.46252998	6.10563999	36.16639000	#Ni
5.32773999	2.41279000	33.70869000	#Ni
3.15436999	3.76034000	33.45753000	#Ni
5.50694998	6.29386999	31.28595000	#Ni

PH-Ni/FeOH_2

H 2 O 1 P 24 Fe 48 Ni 24

1.000000000

8.748798 0.000000 0.000000

-2.187200 6.352773 0.000000

0.000000 0.000000 40.000000

H O P Fe Ni

2 1 24 48 24

Cartesian

0.07047999	1.70901000	10.66061000	#H
1.86112000	0.67219000	10.71809000	#H
2.64772000	1.06996000	10.29924000	#O
2.10704999	2.16888000	38.36601000	#P
0.03700999	4.83248000	37.87529000	#P
0.02323000	1.65097000	35.66230000	#P
2.13464999	4.36705000	35.28998000	#P
0.14278999	1.77440000	31.59050000	#P
2.36647999	4.58275000	31.40493000	#P
0.03818999	1.82609000	9.21962000	#P
2.25120999	4.54608000	8.25564000	#P
-0.03394001	2.12754000	4.69989000	#P
2.20330999	4.80954000	4.28045000	#P
2.22336000	1.62793000	2.08601000	#P
-0.07693001	4.28773000	1.58796000	#P
6.48212999	2.16980000	38.36564000	#P
4.41104999	4.83306000	37.87393000	#P
4.39741000	1.65106000	35.66241000	#P
6.50914999	4.36705000	35.28936000	#P
4.51724999	1.77435000	31.59058000	#P
6.74078999	4.58281000	31.40506000	#P
4.53728999	1.84979000	8.35688000	#P
6.68403999	4.62379000	8.31104000	#P
4.30735999	2.08811000	4.66308000	#P
6.60298999	4.81786000	4.27377000	#P
6.60498000	1.62501000	2.07900000	#P
4.29351999	4.28366000	1.58138000	#P
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3.35551000	0.23234000	38.80246000	#Fe

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2.24102999	4.28849000	37.52517000	#Fe
2.21193999	2.19746000	35.98745000	#Fe
-0.04487001	3.91784000	35.72191000	#Fe
-1.01810002	6.25452999	34.79018000	#Fe
3.16688000	1.19664000	33.68360000	#Fe
0.95822999	5.10538999	33.52512000	#Fe
-0.94898002	6.34743299	32.41113000	#Fe
2.33154999	2.34333000	31.57873000	#Fe
0.18951999	3.97343000	31.48262000	#Fe
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1.23663000	0.15396000	7.60518000	#Fe
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0.99266998	5.27102999	6.29722000	#Fe
1.16823000	0.21662000	5.21302000	#Fe
2.13090999	2.53344000	4.24373000	#Fe
0.02894999	4.26904000	3.95282000	#Fe
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0.98050000	1.23181000	0.13655000	#Fe
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7.73138000	0.23246000	38.80074000	#Fe
4.27945999	2.52858000	37.84796000	#Fe
6.61660999	4.28833000	37.52388000	#Fe
6.58628999	2.19717000	35.98659000	#Fe
4.32938999	3.91757000	35.72145000	#Fe
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6.73446999	2.41732000	8.43272000	#Fe
4.46901999	4.08937000	8.33316000	#Fe
5.54750000	0.02988000	7.49778000	#Fe
7.50523000	1.33866000	6.39519000	#Fe
5.36048998	5.25171999	6.21858000	#Fe
5.54732000	0.20637000	5.14109000	#Fe
6.52946999	2.54230000	4.21298000	#Fe
4.40978999	4.26096000	3.95450000	#Fe
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6.46832999	3.93274000	2.10013000	#Fe
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1.10055000	0.35253000	37.44457000	#Ni
1.08360998	6.16503999	36.15785000	#Ni
0.95087999	2.47535000	33.70068000	#Ni

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1.00760999	2.60444000	6.58265000	#Ni
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7.61070999	2.55867000	0.24520000	#Ni