

Supplementary Materials: Hydrogen Oxidation on Ni-based Electrocatalysts: The Effect of Metal Doping

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1. Experimental Part

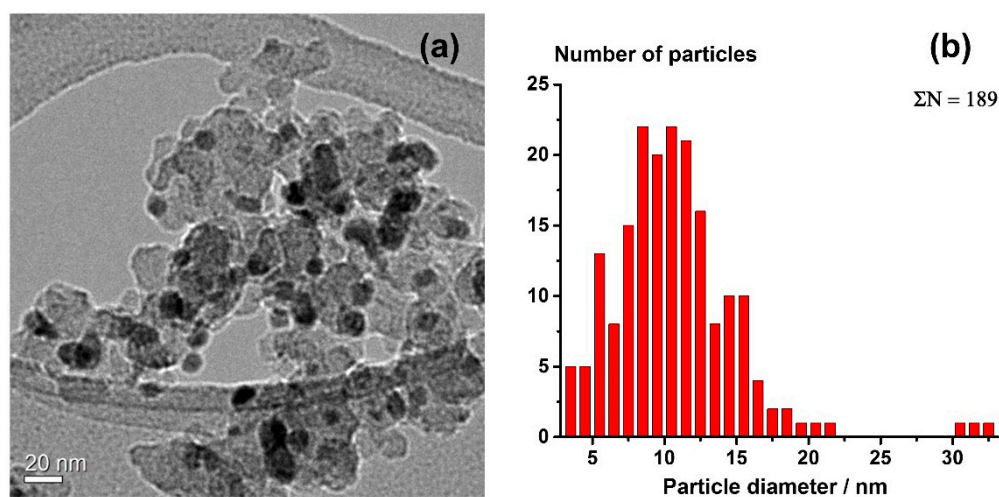


Figure S1. (a) Electron microscopy images of Ni₃Fe₁ catalyst; (b) Particles size distribution for Ni₃Fe₁ catalyst.

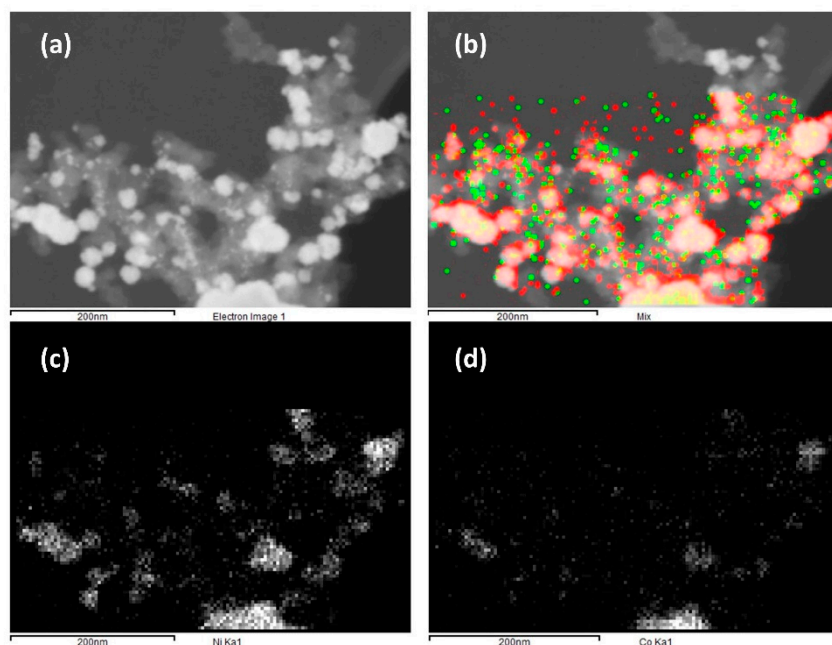


Figure S2. STEM images of Ni₃Co₁/C: (a) Electron image; (b) Element map overlapping: Ni: red; Co: green; Ni + Co: yellow/orange; (c) Element mapping of Ni; (d) Element mapping of Co.

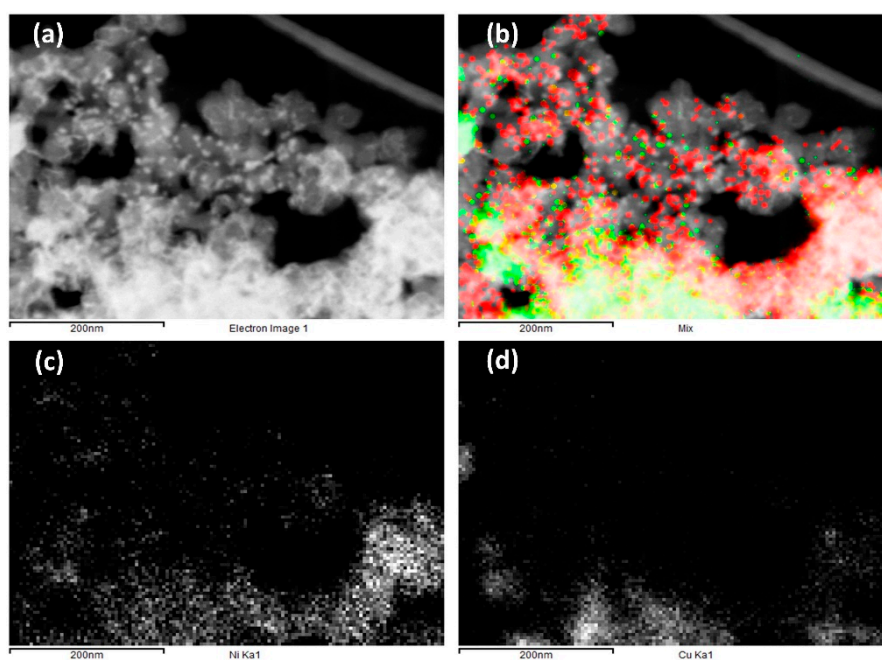


Figure S3. STEM images of Ni₃Cu₁/C: (a) Electron image; (b) Element map overlapping: Ni: red; Cu: green; Ni + Cu: yellow/orange; (c) Element mapping of Ni; (d) Element mapping of Cu.

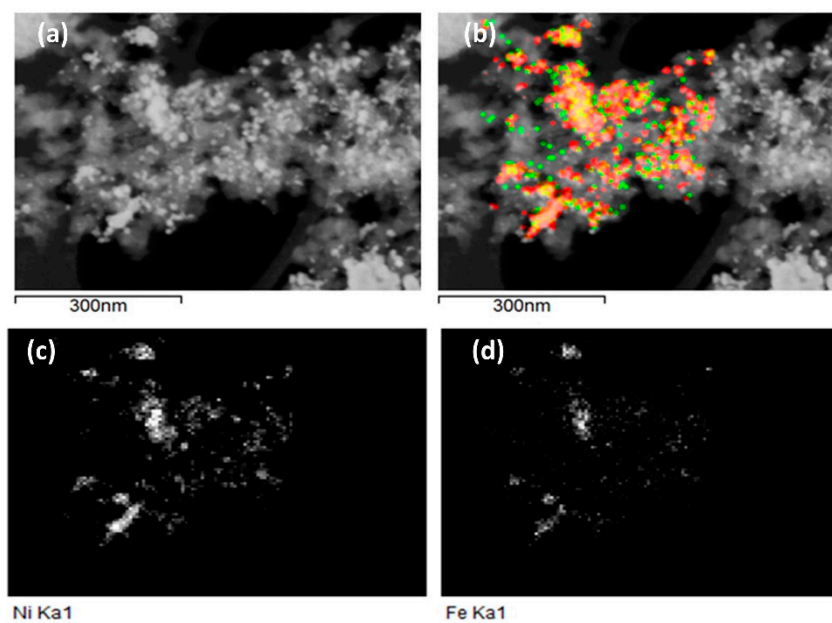


Figure S4. STEM images of Ni₃Fe₁/C: (a) Electron image; (b) Element map overlapping: Ni: red; Fe: green; Ni + Fe: yellow/orange; (c) Element mapping of Ni; (d) Element mapping of Fe.

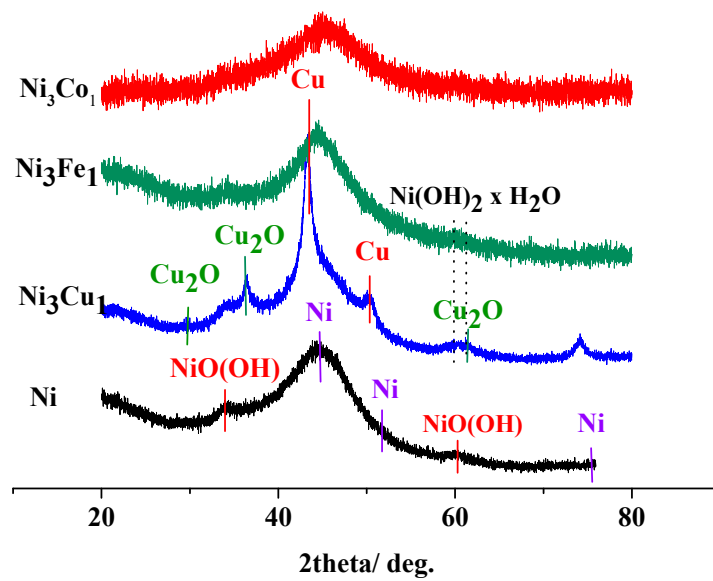


Figure S5. The main reflections of the XRD patterns for the as-synthesized monometallic Ni/C catalyst and bimetallic Ni₃TM₁/C composites.

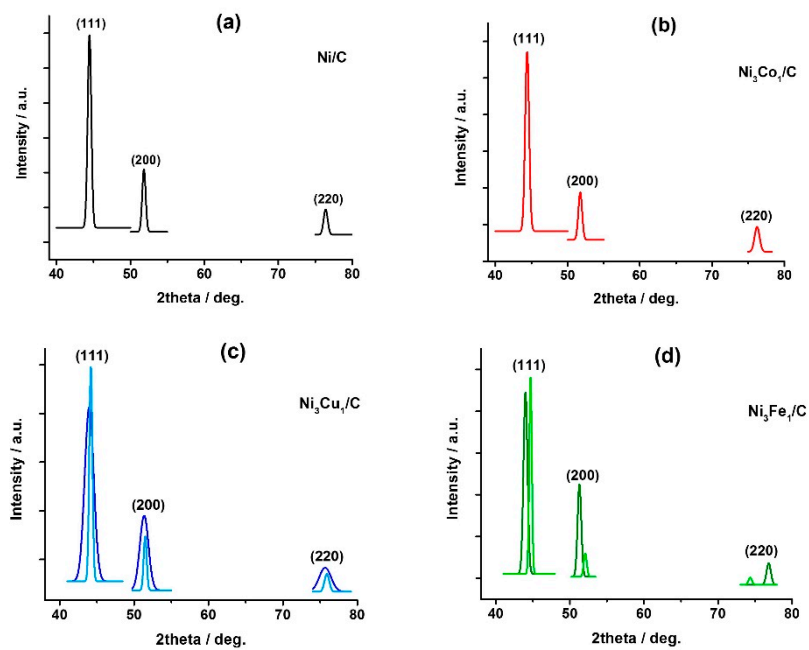


Figure S6. The main reflections of the XRD patterns for monometallic Ni/C catalyst and bimetallic Ni₃TM₁/C composites after the thermal treatment at 450 °C in the mixture of 10% H₂/Ar.

Table S1. Elemental composition of the catalysts (in at.%) based on the EDS and XPS data.

Catalyst	Method	Ni/Me atomic ratio	Element concentration/at.%			
			C	O	Ni	Me
Ni/C	XPS	-	79.40	12.07	6.36	-
	EDS	-	73.88	11.83	12.18	-
Ni ₃ Fe ₁ /C	XPS	9.0	82.49	11.84	2.79	0.31
	EDS	2.7	72.22	14.14	9.02	3.38
Ni ₃ Co ₁ /C	XPS	17.3	81.11	12.43	4.16	0.24
	EDS	3.0	72.40	8.37	12.61	4.22
Ni ₃ Cu ₁ /C	XPS	6.8	59.49	23.19	11.64	1.71
	EDS	3.1	61.63	25.28	8.63	2.82

Table S2. Elemental composition of the catalysts (in wt.%) based on the EDS data.

Catalyst	Ni/(Ni+C)	O/(Ni+Me)	Element concentration/wt.%			
			Ni	Me	C	O
Ni/C	0.43	0.12	37.45	-	48.83	10.43
Ni ₃ Fe ₁ /C	0.37	0.15	28.31	9.97	48.09	11.83
Ni ₃ Co ₁ /C	0.45	0.30	30.20	9.27	37.45	20.40
Ni ₃ Cu ₁ /C	0.47	0.11	35.35	18.84	39.12	8.01

Table S2 summarizes the relative bulk concentration of elements in the catalysts determined by EDS. All the samples comprise Ni, the second transition metal in case of the bimetallic Ni₃TM₁/C and carbon as the main catalyst components. Oxygen also appears as a component as a result of passivation during the synthetic procedure and/or samples handling in the ambient air. Relative Ni content, Ni/(Ni+C), expected to be 0.5, varies between 0.34 to 0.47. The actual wt.% of Ni presented in Table S2 was used to calculate the mass specific catalytic activity of the catalysts in HOR.

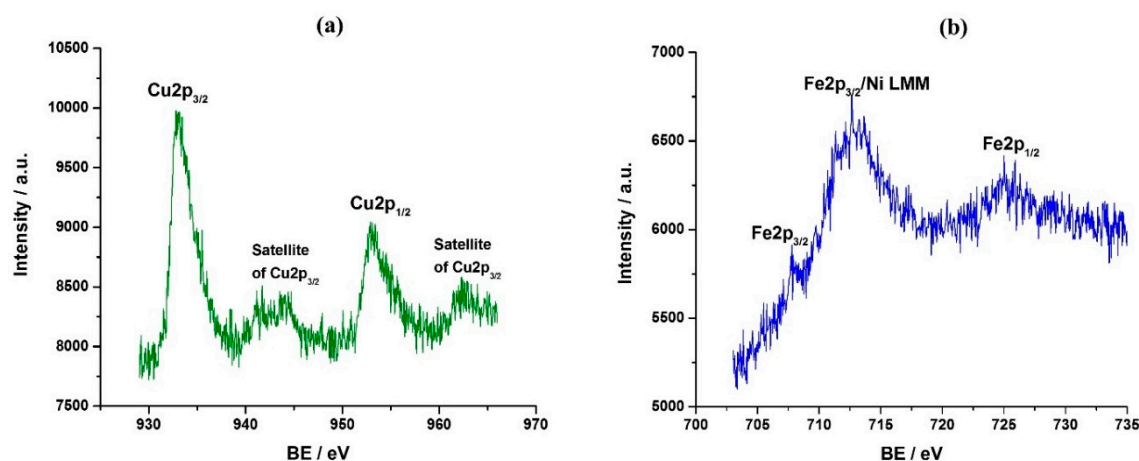


Figure S7. HR-XPS spectra for Cu of the catalyst Ni₃Cu₁/C (a) and Fe of the catalyst Ni₃Fe₁/C (b).

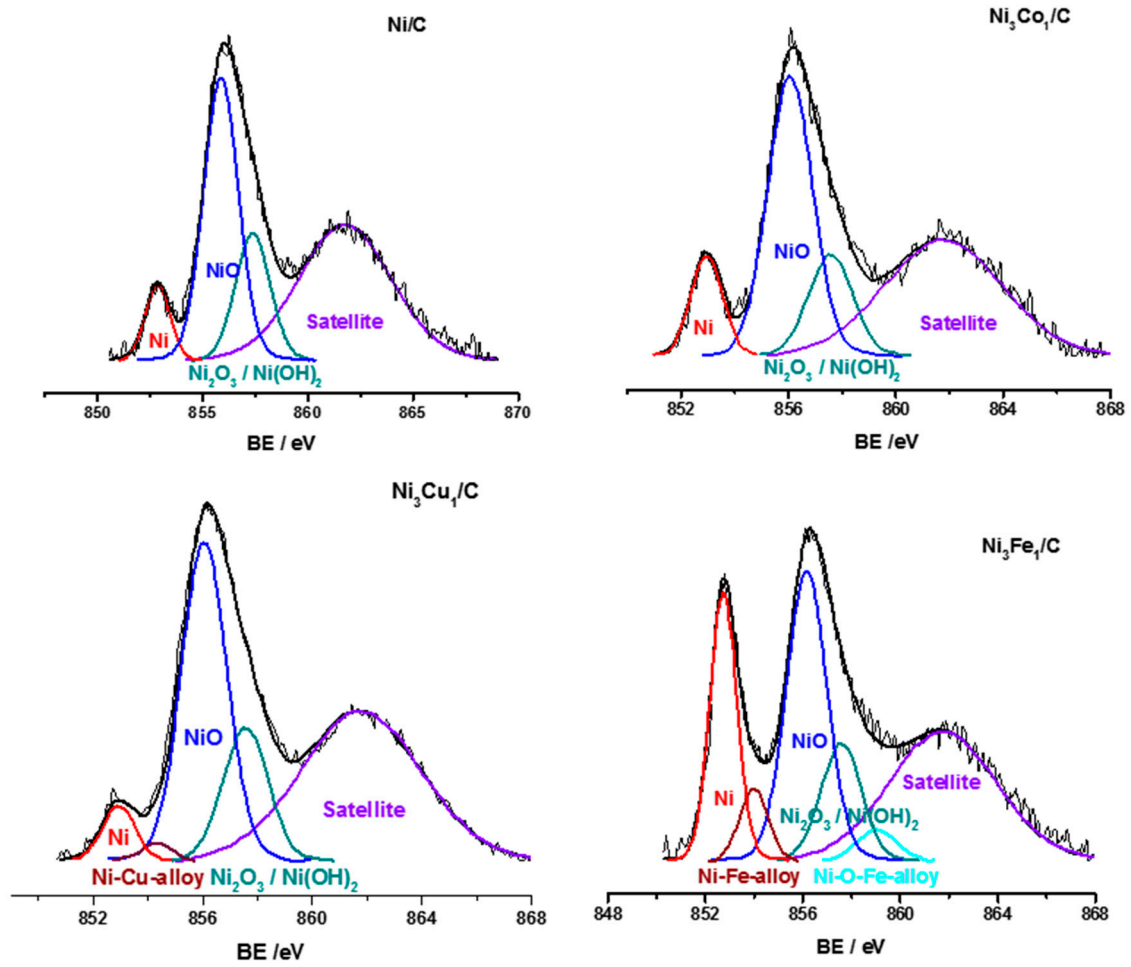


Figure S8. Deconvolution of HR-XPS spectra of Ni 2p_{3/2}.

Table S3. Elemental composition of the catalysts (in at.%) based on the HR-XPS Ni2p_{3/2} spectra deconvolution.

Catalyst	BE / eV	Ni ⁰ /Ni _±	Atomic ratio	Chemical state
Ni/C	861.76	0.065	43.84	Satellite
	857.37		15.45	Ni ₂ O ₃ and/or Ni(OH) ₂
	855.86		34.22	NiO
	852.85		6.50	Ni
Ni ₃ Fe ₁ /C	861.76	0.180	33.91	Satellite
	859.04		3.11	Ni-O-Fe-alloy
	857.57		11.54	Ni ₂ O ₃ and/or Ni(OH) ₂
	856.16		28.63	NiO
	853.98		5.11	Ni-Fe-alloy
	852.75		17.70	Ni
Ni ₃ Co ₁ /C	861.76	0.090	40.78	Satellite
	857.57		13.28	Ni ₂ O ₃ and/or Ni(OH) ₂
	856.06		36.55	NiO
	852.95		9.39	Ni
Ni ₃ Cu ₁ /C	861.76	0.045	44.11	Satellite
	857.57		14.71	Ni ₂ O ₃ and/or Ni(OH) ₂
	856.06		35.26	NiO
	854.32		1.46	Ni-Cu-alloy
	852.95		4.45	Ni

According to the XPS data (Table S3), the surface of the samples is composed of carbon, oxygen, nickel and corresponding doping metal, as the main components. XPS measurements show that the relative surface concentration of the dopant in the chemically reduced samples is lower than in the bulk (for instance, Ni/Me = 9 for Ni₃Fe₁/C CR), as determined by EDS, Ni tends to segregate on the surface. The bulk ratio Ni/Me is between 2.5 and 4.0 at.% which is in agreement with the expected value of 3. Deconvolution of Ni 2p_{3/2} lines (Figure S8) allows to distinguish between the contribution of metallic and oxidized Ni, which may be critical for the electroactivity of the Ni-based catalysts. The XPS analysis reveals that the concentration of zero valent Ni does not exceed 18 at.% (Table S1). The main component is NiO with 28–36 at.%, the rest (10–15 at.%) is represented by Ni₂O₃ and/or Ni(OH)₂. In TM-doped Ni catalysts, some components of alloys (for instance, Ni-O-Fe-alloy and Ni-Fe-alloy) could also be detected.

2. Computational

Bare- NiSc (25% Sc) 111 Facet supercell 2X2X1 - [Etot = -465.27421802 eV]

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-5.0134000778000001	8.6834636535000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.1868000031000001

Sc Ni

20 60

Direct

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0.6666650180000033	0.8333350420000016	0.0000000000000000
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Bare- NiTi (25% Ti) 111 Facet supercell 2X2X1 - [Etot = -498.92309867 eV]

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Ti Ni

20 60

Direct

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Bare- NiV (25% V) 111 Facet supercell 2X2X1 - [Etot = -500.71042203 eV]

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0.0000000000000000	0.0000000000000000	28.1868000031000001

V Ni

20 60

Direct

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0.7500000000000000	0.2500000000000000	0.0726099979999972
0.7500000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.0000000000000000	0.0726099979999972
0.2500000000000000	0.5000000000000000	0.0726099979999972
0.7500000000000000	0.0000000000000000	0.0726099979999972
0.7500000000000000	0.5000000000000000	0.0726099979999972

0.3326008933568641	0.4162997158953582	0.1451924426269643
0.3326008933568641	0.9162997158953582	0.1451924426269643
0.8326008933568640	0.4162997158953582	0.1451924426269643
0.8326008933568640	0.9162997158953582	0.1451924426269643
0.0837009472096972	0.4162990307903010	0.1451922482236181
0.0837009472096972	0.9162990007903056	0.1451922482236181
0.5837009402096931	0.4162990307903010	0.1451922482236181
0.5837009402096931	0.9162990007903056	0.1451922482236181
0.0837002541046465	0.1673991066431359	0.1451924426269643
0.0837002541046465	0.6673991066431360	0.1451924426269643
0.5837002841046418	0.1673991066431359	0.1451924426269643
0.5837002841046418	0.6673991066431360	0.1451924426269643
0.1657226680597641	0.0828577557348174	0.2165934147351953
0.1657226680597641	0.5828577407348197	0.2165934147351953
0.6657226530597664	0.0828577557348174	0.2165934147351953
0.6657226530597664	0.5828577407348197	0.2165934147351953
0.4171415574776942	0.0828584285223046	0.2165935077324066
0.4171415574776942	0.5828584425223058	0.2165935077324066
0.9171415574776942	0.0828584285223046	0.2165935077324066
0.9171415574776942	0.5828584425223058	0.2165935077324066
0.4171422302651814	0.3342773469402336	0.2165934147351953
0.4171422302651814	0.8342773469402336	0.2165934147351953
0.9171422592651803	0.3342773469402336	0.2165934147351953
0.9171422592651803	0.8342773469402336	0.2165934147351953
0.0006181494091921	0.2503061182045195	0.2895166766633493
0.0006181494091921	0.7503061472045184	0.2895166766633493
0.5006181564091963	0.2503061182045195	0.2895166766633493
0.5006181564091963	0.7503061472045184	0.2895166766633493
0.2496950969927762	0.2503048880072262	0.2895162705686341
0.2496950969927762	0.7503048590072273	0.2895162705686341
0.7496950819927785	0.2503048880072262	0.2895162705686341
0.7496950819927785	0.7503048590072273	0.2895162705686341
0.2496938817954805	0.4993818435908037	0.2895166766633493

0.2496938817954805 0.9993818435908037 0.2895166766633493
 0.7496938527954816 0.4993818435908037 0.2895166766633493
 0.7496938527954816 0.9993818435908037 0.2895166766633493

Bare- NiCr (25% Cr) 111 Facet supercell 2X2X1 - [Etot = -496.02028563 eV]

0.995572721824907

10.0268001556000002 0.0000000000000000 0.0000000000000000
 -5.0134000778000001 8.6834636535000005 0.0000000000000000
 0.0000000000000000 0.0000000000000000 28.1868000031000001

Cr Ni

20 60

Direct

0.1666650029999985 0.3333350119999992 0.0000000000000000
 0.1666650029999985 0.8333350420000016 0.0000000000000000
 0.6666650180000033 0.3333350119999992 0.0000000000000000
 0.6666650180000033 0.8333350420000016 0.0000000000000000
 0.0000000000000000 0.0000000000000000 0.0726099979999972
 0.0000000000000000 0.5000000000000000 0.0726099979999972
 0.5000000000000000 0.0000000000000000 0.0726099979999972
 0.5000000000000000 0.5000000000000000 0.0726099979999972
 0.3333332074274225 0.1666668065725716 0.1453299403103543
 0.3333332074274225 0.6666668215725764 0.1453299403103543
 0.8333332374274249 0.1666668065725716 0.1453299403103543
 0.8333332374274249 0.6666668215725764 0.1453299403103543
 0.1666684834839174 0.3333315465160851 0.2221199165184728
 0.1666684834839174 0.8333315165160826 0.2221199165184728
 0.6666684834839174 0.3333315465160851 0.2221199165184728
 0.6666684834839174 0.8333315165160826 0.2221199165184728
 0.0000028796404550 0.4999971163595447 0.2921639793122779
 0.0000028796404550 0.9999971163595447 0.2921639793122779
 0.5000028836404553 0.4999971163595447 0.2921639793122779
 0.5000028836404553 0.9999971163595447 0.2921639793122779
 0.1666650029999985 0.0833349970000015 0.0000000000000000

0.1666650029999985	0.5833349819999967	0.0000000000000000
0.6666650180000033	0.0833349970000015	0.0000000000000000
0.6666650180000033	0.5833349819999967	0.0000000000000000
0.4166649880000008	0.0833349970000015	0.0000000000000000
0.4166649880000008	0.5833349819999967	0.0000000000000000
0.9166649579999984	0.0833349970000015	0.0000000000000000
0.9166649579999984	0.5833349819999967	0.0000000000000000
0.4166649880000008	0.3333350119999992	0.0000000000000000
0.4166649880000008	0.8333350420000016	0.0000000000000000
0.9166649579999984	0.3333350119999992	0.0000000000000000
0.9166649579999984	0.8333350420000016	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0726099979999972
0.0000000000000000	0.7500000000000000	0.0726099979999972
0.5000000000000000	0.2500000000000000	0.0726099979999972
0.5000000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.2500000000000000	0.0726099979999972
0.2500000000000000	0.7500000000000000	0.0726099979999972
0.7500000000000000	0.2500000000000000	0.0726099979999972
0.7500000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.0000000000000000	0.0726099979999972
0.2500000000000000	0.5000000000000000	0.0726099979999972
0.7500000000000000	0.0000000000000000	0.0726099979999972
0.7500000000000000	0.5000000000000000	0.0726099979999972
0.3327292432529703	0.4163633881598585	0.1457636164680665
0.3327292432529703	0.9163633881598585	0.1457636164680665
0.8327292432529703	0.4163633881598585	0.1457636164680665
0.8327292432529703	0.9163633881598585	0.1457636164680665
0.0836343429218616	0.4163656350781366	0.1457635424375567
0.0836343429218616	0.9163656050781412	0.1457635424375567
0.5836343359218574	0.4163656350781366	0.1457635424375567
0.5836343359218574	0.9163656050781412	0.1457635424375567
0.0836365818401461	0.1672707567470297	0.1457636164680665
0.0836365818401461	0.6672707567470297	0.1457636164680665

0.5836366118401415	0.1672707567470297	0.1457636164680665
0.5836366118401415	0.6672707567470297	0.1457636164680665
0.1667022608071989	0.0833492381847876	0.2178230715861247
0.1667022608071989	0.5833492231847899	0.2178230715861247
0.6667022458072012	0.0833492381847876	0.2178230715861247
0.6667022458072012	0.5833492231847899	0.2178230715861247
0.4166501284783664	0.0833498575216325	0.2178229868053663
0.4166501284783664	0.5833498715216336	0.2178229868053663
0.9166501284783664	0.0833498575216325	0.2178229868053663
0.9166501284783664	0.5833498715216336	0.2178229868053663
0.4166507478152113	0.3332977541927988	0.2178230715861247
0.4166507478152113	0.8332977541927988	0.2178230715861247
0.9166507768152101	0.3332977541927988	0.2178230715861247
0.9166507768152101	0.8332977541927988	0.2178230715861247
0.0017294364182305	0.2508603656883892	0.2906462910142693
0.0017294364182305	0.7508603946883881	0.2906462910142693
0.5017294434182347	0.2508603656883892	0.2906462910142693
0.5017294434182347	0.7508603946883881	0.2906462910142693
0.2491390440141572	0.2508609409858451	0.2906458196759303
0.2491390440141572	0.7508609119858463	0.2906458196759303
0.7491390290141595	0.2508609409858451	0.2906458196759303
0.7491390290141595	0.7508609119858463	0.2906458196759303
0.2491396343116108	0.4982705565817653	0.2906462910142693
0.2491396343116108	0.9982705565817653	0.2906462910142693
0.7491396053116119	0.4982705565817653	0.2906462910142693
0.7491396053116119	0.9982705565817653	0.2906462910142693

Bare- NiMn (25% Mn) 111 Facet supercell 2X2X1 - [Etot = -494.23957091 eV]

1.000000000000000

9.9196901320999995	0.0000000000000000	0.0000000000000000
-4.9598426818999997	8.5906995225999996	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.8856849669999995

Mn Ni

20 60

Direct

0.1666650029999985	0.3333350119999992	0.0000000000000000
0.1666650029999985	0.8333350420000016	0.0000000000000000
0.6666650180000033	0.3333350119999992	0.0000000000000000
0.6666650180000033	0.8333350420000016	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0726099979999972
0.0000000000000000	0.5000000000000000	0.0726099979999972
0.5000000000000000	0.0000000000000000	0.0726099979999972
0.5000000000000000	0.5000000000000000	0.0726099979999972
0.3332655297792186	0.1666153471837717	0.1475653398308197
0.3332655297792186	0.6666153771837671	0.1475653398308197
0.8332655297792186	0.1666153471837717	0.1475653398308197
0.8332655297792186	0.6666153771837671	0.1475653398308197
0.1665489000084364	0.3332417222975437	0.2214153618003110
0.1665489000084364	0.8332417522975462	0.2214153618003110
0.6665489300084388	0.3332417222975437	0.2214153618003110
0.6665489300084388	0.8332417522975462	0.2214153618003110
0.4998042605921995	0.4998180188418289	0.2989863608164285
0.4998042605921995	0.9998180188418289	0.2989863608164285
0.9998042605921995	0.4998180188418289	0.2989863608164285
0.9998042605921995	0.9998180188418289	0.2989863608164285
0.1666650029999985	0.0833349970000015	0.0000000000000000
0.1666650029999985	0.5833349819999967	0.0000000000000000
0.6666650180000033	0.0833349970000015	0.0000000000000000
0.6666650180000033	0.5833349819999967	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0726099979999972
0.0000000000000000	0.7500000000000000	0.0726099979999972
0.5000000000000000	0.2500000000000000	0.0726099979999972
0.5000000000000000	0.7500000000000000	0.0726099979999972
0.4166649880000008	0.0833349970000015	0.0000000000000000
0.4166649880000008	0.5833349819999967	0.0000000000000000
0.9166649579999984	0.0833349970000015	0.0000000000000000

0.9166649579999984	0.5833349819999967	0.0000000000000000
0.2500000000000000	0.2500000000000000	0.0726099979999972
0.2500000000000000	0.7500000000000000	0.0726099979999972
0.7500000000000000	0.2500000000000000	0.0726099979999972
0.7500000000000000	0.7500000000000000	0.0726099979999972
0.4166649880000008	0.3333350119999992	0.0000000000000000
0.4166649880000008	0.8333350420000016	0.0000000000000000
0.9166649579999984	0.3333350119999992	0.0000000000000000
0.9166649579999984	0.8333350420000016	0.0000000000000000
0.2500000000000000	0.0000000000000000	0.0726099979999972
0.2500000000000000	0.5000000000000000	0.0726099979999972
0.7500000000000000	0.0000000000000000	0.0726099979999972
0.7500000000000000	0.5000000000000000	0.0726099979999972
0.3333865505946747	0.4166793897176788	0.1471594019476044
0.3333865505946747	0.9166794197176813	0.1471594019476044
0.8333865805946701	0.4166793897176788	0.1471594019476044
0.8333865805946701	0.9166794197176813	0.1471594019476044
0.1655331831062412	0.0827304573798884	0.2218632412338550
0.1655331831062412	0.5827304503798914	0.2218632412338550
0.6655331981062389	0.0827304573798884	0.2218632412338550
0.6655331981062389	0.5827304503798914	0.2218632412338550
0.4997703596160292	0.2498009190038673	0.2946061984893120
0.4997703596160292	0.7498009050038732	0.2946061984893120
0.9997703296160338	0.2498009190038673	0.2946061984893120
0.9997703296160338	0.7498009050038732	0.2946061984893120
0.0832032256285586	0.4166769875853618	0.1471597890047533
0.0832032256285586	0.9166769875853618	0.1471597890047533
0.5832032406285563	0.4166769875853618	0.1471597890047533
0.5832032406285563	0.9166769875853618	0.1471597890047533
0.4170602786834294	0.0827236536617448	0.2218613870855037
0.4170602786834294	0.5827236756617467	0.2218613870855037
0.9170602786834294	0.0827236536617448	0.2218613870855037
0.9170602786834294	0.5827236756617467	0.2218613870855037

0.2498345674826226	0.2497942679548117	0.2946056206265979
0.2498345674826226	0.7497942379548093	0.2946056206265979
0.7498345974826179	0.2497942679548117	0.2946056206265979
0.7498345974826179	0.7497942379548093	0.2946056206265979
0.0832041910890169	0.1664848653155246	0.1471606587475449
0.0832041910890169	0.6664848803155223	0.1471606587475449
0.5832042130890187	0.1664848653155246	0.1471606587475449
0.5832042130890187	0.6664848803155223	0.1471606587475449
0.4170608262194406	0.3342549782214732	0.2218627604183112
0.4170608262194406	0.8342549782214732	0.2218627604183112
0.9170608262194406	0.3342549782214732	0.2218627604183112
0.9170608262194406	0.8342549782214732	0.2218627604183112
0.2498333110093185	0.9998693950860940	0.2946083798932975
0.2498333110093185	0.4998693940860974	0.2946083798932975
0.7498333110093185	0.9998693950860940	0.2946083798932975
0.7498333110093185	0.4998693940860974	0.2946083798932975

Bare- NiFe (25% Fe) 111 Facet supercell 2X2X1 - [Etot = -479.68023055 eV]

1.0000000000000000

10.0268001556000002	0.0000000000000000	0.0000000000000000
-5.0134000778000001	8.6834636535000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.1868000031000001

Fe Ni

20 60

Direct

0.1666650029999985	0.3333350119999992	0.0000000000000000
0.1666650029999985	0.8333350420000016	0.0000000000000000
0.6666650180000033	0.3333350119999992	0.0000000000000000
0.6666650180000033	0.8333350420000016	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0726099979999972
0.0000000000000000	0.5000000000000000	0.0726099979999972
0.5000000000000000	0.0000000000000000	0.0726099979999972
0.5000000000000000	0.5000000000000000	0.0726099979999972

0.3333360210443530	0.1666639929556410	0.1447816711106995
0.3333360210443530	0.6666640079556458	0.1447816711106995
0.8333360510443555	0.1666639929556410	0.1447816711106995
0.8333360510443555	0.6666640079556458	0.1447816711106995
0.1666694936690902	0.3333305363309123	0.2193817578125845
0.1666694936690902	0.8333305063309098	0.2193817578125845
0.6666694936690902	0.3333305363309123	0.2193817578125845
0.6666694936690902	0.8333305063309098	0.2193817578125845
0.0000040302016373	0.4999959657983624	0.2885585145670859
0.0000040302016373	0.9999959657983624	0.2885585145670859
0.5000040342016376	0.4999959657983624	0.2885585145670859
0.5000040342016376	0.9999959657983624	0.2885585145670859
0.1666650029999985	0.0833349970000015	0.0000000000000000
0.1666650029999985	0.5833349819999967	0.0000000000000000
0.6666650180000033	0.0833349970000015	0.0000000000000000
0.6666650180000033	0.5833349819999967	0.0000000000000000
0.4166649880000008	0.0833349970000015	0.0000000000000000
0.4166649880000008	0.5833349819999967	0.0000000000000000
0.9166649579999984	0.0833349970000015	0.0000000000000000
0.9166649579999984	0.5833349819999967	0.0000000000000000
0.4166649880000008	0.3333350119999992	0.0000000000000000
0.4166649880000008	0.8333350420000016	0.0000000000000000
0.9166649579999984	0.3333350119999992	0.0000000000000000
0.9166649579999984	0.8333350420000016	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0726099979999972
0.0000000000000000	0.7500000000000000	0.0726099979999972
0.5000000000000000	0.2500000000000000	0.0726099979999972
0.5000000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.2500000000000000	0.0726099979999972
0.2500000000000000	0.7500000000000000	0.0726099979999972
0.7500000000000000	0.2500000000000000	0.0726099979999972
0.7500000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.0000000000000000	0.0726099979999972

0.2500000000000000	0.5000000000000000	0.0726099979999972
0.7500000000000000	0.0000000000000000	0.0726099979999972
0.7500000000000000	0.5000000000000000	0.0726099979999972
0.3330025544636754	0.4164974464143967	0.1452001606008508
0.3330025544636754	0.9164974464143967	0.1452001606008508
0.8330025544636754	0.4164974464143967	0.1452001606008508
0.8330025544636754	0.9164974464143967	0.1452001606008508
0.0835002407555834	0.4164997372444148	0.1451997975413732
0.0835002407555834	0.9164997072444194	0.1451997975413732
0.5835002337555792	0.4164997372444148	0.1451997975413732
0.5835002337555792	0.9164997072444194	0.1451997975413732
0.0835025235856079	0.1669974455363246	0.1452001606008508
0.0835025235856079	0.6669974455363246	0.1452001606008508
0.5835025535856033	0.1669974455363246	0.1452001606008508
0.5835025535856033	0.6669974455363246	0.1452001606008508
0.1669313964638022	0.0834601952999705	0.2172782882973081
0.1669313964638022	0.5834601802999728	0.2172782882973081
0.6669313814638045	0.0834601952999705	0.2172782882973081
0.6669313814638045	0.5834601802999728	0.2172782882973081
0.4165397231218151	0.0834602628781838	0.2172779930189321
0.4165397231218151	0.5834602768781849	0.2172779930189321
0.9165397231218151	0.0834602628781838	0.2172779930189321
0.9165397231218151	0.5834602768781849	0.2172779930189321
0.4165397907000283	0.3330686185361955	0.2172782882973081
0.4165397907000283	0.8330686185361955	0.2172782882973081
0.9165398197000272	0.3330686185361955	0.2172782882973081
0.9165398197000272	0.8330686185361955	0.2172782882973081
0.0011359679369107	0.2505585176516618	0.2889156470911729
0.0011359679369107	0.7505585466516607	0.2889156470911729
0.5011359749369149	0.2505585176516618	0.2889156470911729
0.5011359749369149	0.7505585466516607	0.2889156470911729
0.2494434796382308	0.2505565053617715	0.2889157699769100
0.2494434796382308	0.7505564763617727	0.2889157699769100

0.7494434646382331	0.2505565053617715	0.2889157699769100
0.7494434646382331	0.7505564763617727	0.2889157699769100
0.2494414823483382	0.4988640250630851	0.2889156470911729
0.2494414823483382	0.9988640250630851	0.2889156470911729
0.7494414533483393	0.4988640250630851	0.2889156470911729
0.7494414533483393	0.9988640250630851	0.2889156470911729

Bare- NiCo (25% Co) 111 Facet supercell 2X2X1 - [Etot = -447.05815167 eV]

0.993794164815303

10.0268001556000002	0.0000000000000000	0.0000000000000000
-5.0134000778000001	8.6834636535000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.1868000031000001

Co Ni

20 60

Direct

0.1666650029999985	0.3333350119999992	0.0000000000000000
0.1666650029999985	0.8333350420000016	0.0000000000000000
0.6666650180000033	0.3333350119999992	0.0000000000000000
0.6666650180000033	0.8333350420000016	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0726099979999972
0.0000000000000000	0.5000000000000000	0.0726099979999972
0.5000000000000000	0.0000000000000000	0.0726099979999972
0.5000000000000000	0.5000000000000000	0.0726099979999972
0.3333356960742080	0.1666643179257861	0.1447750049574452
0.3333356960742080	0.6666643329257909	0.1447750049574452
0.8333357260742105	0.1666643179257861	0.1447750049574452
0.8333357260742105	0.6666643329257909	0.1447750049574452
0.1666704434869999	0.3333295865130026	0.2193115505540675
0.1666704434869999	0.8333295565130001	0.2193115505540675
0.6666704434869999	0.3333295865130026	0.2193115505540675
0.6666704434869999	0.8333295565130001	0.2193115505540675
0.0000045859499664	0.4999954100500332	0.2886886571841742
0.0000045859499664	0.9999954100500332	0.2886886571841742
0.5000045899499668	0.4999954100500332	0.2886886571841742
0.5000045899499668	0.9999954100500332	0.2886886571841742
0.1666650029999985	0.0833349970000015	0.0000000000000000
0.1666650029999985	0.5833349819999967	0.0000000000000000
0.6666650180000033	0.0833349970000015	0.0000000000000000
0.6666650180000033	0.5833349819999967	0.0000000000000000
0.4166649880000008	0.0833349970000015	0.0000000000000000

0.4166649880000008	0.5833349819999967	0.0000000000000000
0.9166649579999984	0.0833349970000015	0.0000000000000000
0.9166649579999984	0.5833349819999967	0.0000000000000000
0.4166649880000008	0.3333350119999992	0.0000000000000000
0.4166649880000008	0.8333350420000016	0.0000000000000000
0.9166649579999984	0.3333350119999992	0.0000000000000000
0.9166649579999984	0.8333350420000016	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0726099979999972
0.0000000000000000	0.7500000000000000	0.0726099979999972
0.5000000000000000	0.2500000000000000	0.0726099979999972
0.5000000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.2500000000000000	0.0726099979999972
0.2500000000000000	0.7500000000000000	0.0726099979999972
0.7500000000000000	0.2500000000000000	0.0726099979999972
0.7500000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.0000000000000000	0.0726099979999972
0.2500000000000000	0.5000000000000000	0.0726099979999972
0.7500000000000000	0.0000000000000000	0.0726099979999972
0.7500000000000000	0.5000000000000000	0.0726099979999972
0.3330524162472273	0.4165222175555243	0.1451676484252502
0.3330524162472273	0.9165222175555243	0.1451676484252502
0.8330524162472273	0.4165222175555243	0.1451676484252502
0.8330524162472273	0.9165222175555243	0.1451676484252502
0.0834775628387234	0.4165224151612748	0.1451674547121158
0.0834775628387234	0.9165223851612794	0.1451674547121158
0.5834775558387193	0.4165224151612748	0.1451674547121158
0.5834775558387193	0.9165223851612794	0.1451674547121158
0.0834777524444803	0.1669475837527727	0.1451676484252502
0.0834777524444803	0.6669475837527727	0.1451676484252502
0.5834777824444757	0.1669475837527727	0.1451676484252502
0.5834777824444757	0.6669475837527727	0.1451676484252502
0.1668770510505979	0.0834320915875821	0.2172445623688759
0.1668770510505979	0.5834320765875844	0.2172445623688759

0.6668770360506002	0.0834320915875821	0.2172445623688759
0.6668770360506002	0.5834320765875844	0.2172445623688759
0.4165669488927790	0.0834330371072198	0.2172446776818262
0.4165669488927790	0.5834330511072210	0.2172446776818262
0.9165669488927790	0.0834330371072198	0.2172446776818262
0.9165669488927790	0.5834330511072210	0.2172446776818262
0.4165678944124167	0.3331229639493998	0.2172445623688759
0.4165678944124167	0.8331229639493998	0.2172445623688759
0.9165679234124156	0.3331229639493998	0.2172445623688759
0.9165679234124156	0.8331229639493998	0.2172445623688759
0.0008713944834753	0.2504292352332769	0.2889490873343235
0.0008713944834753	0.7504292642332757	0.2889490873343235
0.5008714014834794	0.2504292352332769	0.2889490873343235
0.5008714014834794	0.7504292642332757	0.2889490873343235
0.2495694075417205	0.2504305774582818	0.2889482824187439
0.2495694075417205	0.7504305484582829	0.2889482824187439
0.7495693925417228	0.2504305774582818	0.2889482824187439
0.7495693925417228	0.7504305484582829	0.2889482824187439
0.2495707647667231	0.4991285985165206	0.2889490873343235
0.2495707647667231	0.9991285985165206	0.2889490873343235
0.7495707357667243	0.4991285985165206	0.2889490873343235
0.7495707357667243	0.9991285985165206	0.2889490873343235

Pure-Ni 111 Facet supercell 2X2X1 - [Etot = -414.05399553 eV]

1.01798110552312

10.0268001556000002	0.0000000000000000	0.0000000000000000
-5.0134000778000001	8.6834636535000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.1868000031000001

Ni

80

Direct

0.1666650029999985	0.3333350119999992	0.0000000000000000
0.1666650029999985	0.8333350420000016	0.0000000000000000

0.6666650180000033	0.3333350119999992	0.0000000000000000
0.6666650180000033	0.8333350420000016	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0726099979999972
0.0000000000000000	0.5000000000000000	0.0726099979999972
0.5000000000000000	0.0000000000000000	0.0726099979999972
0.5000000000000000	0.5000000000000000	0.0726099979999972
0.3333379266307901	0.1666620873692040	0.1419871965719892
0.3333379266307901	0.6666621023692088	0.1419871965719892
0.8333379566307926	0.1666620873692040	0.1419871965719892
0.8333379566307926	0.6666621023692088	0.1419871965719892
0.1666705248782634	0.3333295051217391	0.2116348075142653
0.1666705248782634	0.8333294751217366	0.2116348075142653
0.6666705248782634	0.3333295051217391	0.2116348075142653
0.6666705248782634	0.8333294751217366	0.2116348075142653
0.0000050457843344	0.4999949502156653	0.2801756840107572
0.0000050457843344	0.9999949502156653	0.2801756840107572
0.5000050497843347	0.4999949502156653	0.2801756840107572
0.5000050497843347	0.9999949502156653	0.2801756840107572
0.1666650029999985	0.0833349970000015	0.0000000000000000
0.1666650029999985	0.5833349819999967	0.0000000000000000
0.6666650180000033	0.0833349970000015	0.0000000000000000
0.6666650180000033	0.5833349819999967	0.0000000000000000
0.4166649880000008	0.0833349970000015	0.0000000000000000
0.4166649880000008	0.5833349819999967	0.0000000000000000
0.9166649579999984	0.0833349970000015	0.0000000000000000
0.9166649579999984	0.5833349819999967	0.0000000000000000
0.4166649880000008	0.3333350119999992	0.0000000000000000
0.4166649880000008	0.8333350420000016	0.0000000000000000
0.9166649579999984	0.3333350119999992	0.0000000000000000
0.9166649579999984	0.8333350420000016	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0726099979999972
0.0000000000000000	0.7500000000000000	0.0726099979999972
0.5000000000000000	0.2500000000000000	0.0726099979999972

0.5000000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.2500000000000000	0.0726099979999972
0.2500000000000000	0.7500000000000000	0.0726099979999972
0.7500000000000000	0.2500000000000000	0.0726099979999972
0.7500000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.0000000000000000	0.0726099979999972
0.2500000000000000	0.5000000000000000	0.0726099979999972
0.7500000000000000	0.0000000000000000	0.0726099979999972
0.7500000000000000	0.5000000000000000	0.0726099979999972
0.3333734635052537	0.4166834890118736	0.1419692388587279
0.3333734635052537	0.9166834890118736	0.1419692388587279
0.8333734635052537	0.4166834890118736	0.1419692388587279
0.8333734635052537	0.9166834890118736	0.1419692388587279
0.0833184196422536	0.4166815583577446	0.1419683661446669
0.0833184196422536	0.9166815283577563	0.1419683661446669
0.5833184126422424	0.4166815583577446	0.1419683661446669
0.5833184126422424	0.9166815283577563	0.1419683661446669
0.0833164809881310	0.1666265364947463	0.1419692388587279
0.0833164809881310	0.6666265364947463	0.1419692388587279
0.5833165109881264	0.1666265364947463	0.1419692388587279
0.5833165109881264	0.6666265364947463	0.1419692388587279
0.1666671267871607	0.0833265077298861	0.2116606263748011
0.1666671267871607	0.5833264927298885	0.2116606263748011
0.6666671117871630	0.0833265077298861	0.2116606263748011
0.6666671117871630	0.5833264927298885	0.2116606263748011
0.4166717466262497	0.0833282393737491	0.2116617771692688
0.4166717466262497	0.5833282533737503	0.2116617771692688
0.9166717466262497	0.0833282393737491	0.2116617771692688
0.9166717466262497	0.5833282533737503	0.2116617771692688
0.4166734782701127	0.3333328882128370	0.2116606263748011
0.4166734782701127	0.8333328882128370	0.2116606263748011
0.9166735072701115	0.3333328882128370	0.2116606263748011
0.9166735072701115	0.8333328882128370	0.2116606263748011

0.0000075353253024	0.2499990047850531	0.2801213495404440
0.0000075353253024	0.7499990337850519	0.2801213495404440
0.5000075423253065	0.2499990047850531	0.2801213495404440
0.5000075423253065	0.7499990337850519	0.2801213495404440
0.2500038375296896	0.2499961474703127	0.2801228248185836
0.2500038375296896	0.7499961184703139	0.2801228248185836
0.7500038225296919	0.2499961474703127	0.2801228248185836
0.7500038225296919	0.7499961184703139	0.2801228248185836
0.2500009952149469	0.4999924576746935	0.2801213495404440
0.2500009952149469	0.9999924576746935	0.2801213495404440
0.7500009662149481	0.4999924576746935	0.2801213495404440
0.7500009662149481	0.9999924576746935	0.2801213495404440

Bare- NiCu (25% Cu) 111 Facet supercell 2X2X1 - [Etot = -380.91454400 eV]

0.998485100048875

10.0268001556000002	0.0000000000000000	0.0000000000000000
-5.0134000778000001	8.6834636535000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.1868000031000001

Cu Ni

20 60

Direct

0.1666650029999985	0.3333350119999992	0.0000000000000000
0.1666650029999985	0.8333350420000016	0.0000000000000000
0.6666650180000033	0.3333350119999992	0.0000000000000000
0.6666650180000033	0.8333350420000016	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0726099979999972
0.0000000000000000	0.5000000000000000	0.0726099979999972
0.5000000000000000	0.0000000000000000	0.0726099979999972
0.5000000000000000	0.5000000000000000	0.0726099979999972
0.3333288493490585	0.1666711646509356	0.1456301058409792
0.3333288493490585	0.6666711796509404	0.1456301058409792
0.8333288793490610	0.1666711646509356	0.1456301058409792
0.8333288793490610	0.6666711796509404	0.1456301058409792

0.1666825622939569	0.3333174677060455	0.2171562731733374
0.1666825622939569	0.8333174377060502	0.2171562731733374
0.6666825622939498	0.3333174677060455	0.2171562731733374
0.6666825622939498	0.8333174377060502	0.2171562731733374
0.0000009067924225	0.4999990892075772	0.2929619156089061
0.0000009067924225	0.9999990892075772	0.2929619156089061
0.5000009107924228	0.4999990892075772	0.2929619156089061
0.5000009107924228	0.9999990892075772	0.2929619156089061
0.1666650029999985	0.0833349970000015	0.0000000000000000
0.1666650029999985	0.5833349819999967	0.0000000000000000
0.6666650180000033	0.0833349970000015	0.0000000000000000
0.6666650180000033	0.5833349819999967	0.0000000000000000
0.4166649880000008	0.0833349970000015	0.0000000000000000
0.4166649880000008	0.5833349819999967	0.0000000000000000
0.9166649579999984	0.0833349970000015	0.0000000000000000
0.9166649579999984	0.5833349819999967	0.0000000000000000
0.4166649880000008	0.3333350119999992	0.0000000000000000
0.4166649880000008	0.8333350420000016	0.0000000000000000
0.9166649579999984	0.3333350119999992	0.0000000000000000
0.9166649579999984	0.8333350420000016	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0726099979999972
0.0000000000000000	0.7500000000000000	0.0726099979999972
0.5000000000000000	0.2500000000000000	0.0726099979999972
0.5000000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.2500000000000000	0.0726099979999972
0.2500000000000000	0.7500000000000000	0.0726099979999972
0.7500000000000000	0.2500000000000000	0.0726099979999972
0.7500000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.0000000000000000	0.0726099979999972
0.2500000000000000	0.5000000000000000	0.0726099979999972
0.7500000000000000	0.0000000000000000	0.0726099979999972
0.7500000000000000	0.5000000000000000	0.0726099979999972
0.3336236873540130	0.4168093850592030	0.1451601048952185

0.3336236873540130	0.9168093850592030	0.1451601048952185
0.8336236873540130	0.4168093850592030	0.1451601048952185
0.8336236873540130	0.9168093850592030	0.1451601048952185
0.0831839805429482	0.4168159974570500	0.1451607056646864
0.0831839805429482	0.9168159674570546	0.1451607056646864
0.5831839735429440	0.4168159974570500	0.1451607056646864
0.5831839735429440	0.9168159674570546	0.1451607056646864
0.0831905849408017	0.1663763126459870	0.1451601048952185
0.0831905849408017	0.6663763126459870	0.1451601048952185
0.5831906149407970	0.1663763126459870	0.1451601048952185
0.5831906149407970	0.6663763126459870	0.1451601048952185
0.1656654918832885	0.0828402366764962	0.2184374980008883
0.1656654918832885	0.5828402216764985	0.2184374980008883
0.6656654768832908	0.0828402366764962	0.2184374980008883
0.6656654768832908	0.5828402216764985	0.2184374980008883
0.4171840749882776	0.0828159110117213	0.2184311558397312
0.4171840749882776	0.5828159250117224	0.2184311558397312
0.9171840749882776	0.0828159110117213	0.2184311558397312
0.9171840749882776	0.5828159250117224	0.2184311558397312
0.4171597493235026	0.3343345231167092	0.2184374980008883
0.4171597493235026	0.8343345231167092	0.2184374980008883
0.9171597783235015	0.3343345231167092	0.2184374980008883
0.9171597783235015	0.8343345231167092	0.2184374980008883
0.9995421743006574	0.2497626512101760	0.2890967058856901
0.9995421743006574	0.7497626802101749	0.2890967058856901
0.4995421813006615	0.2497626512101760	0.2890967058856901
0.4995421813006615	0.7497626802101749	0.2890967058856901
0.2502352597840343	0.2497647252159680	0.2891030384579523
0.2502352597840343	0.7497646962159763	0.2891030384579523
0.7502352447840366	0.2497647252159680	0.2891030384579523
0.7502352447840366	0.7497646962159763	0.2891030384579523
0.2502373487898240	0.5004578186993385	0.2890967058856901
0.2502373487898240	0.0004578186993385	0.2890967058856901

0.7502373197898251 0.5004578186993385 0.2890967058856901

0.7502373197898251 0.0004578186993385 0.2890967058856901

Bare- NiZn (25% Zn) 111 Facet supercell 2X2X1 - [Etot = -344.05478626 eV]

1.01038006037737

10.0268001556000002 0.0000000000000000 0.0000000000000000

-5.0134000778000001 8.6834636535000005 0.0000000000000000

0.0000000000000000 0.0000000000000000 28.1868000031000001

Zn Ni

20 60

Direct

0.1666650029999985 0.3333350119999992 0.0000000000000000

0.1666650029999985 0.8333350420000016 0.0000000000000000

0.6666650180000033 0.3333350119999992 0.0000000000000000

0.6666650180000033 0.8333350420000016 0.0000000000000000

0.0000000000000000 0.0000000000000000 0.0726099979999972

0.0000000000000000 0.5000000000000000 0.0726099979999972

0.5000000000000000 0.0000000000000000 0.0726099979999972

0.5000000000000000 0.5000000000000000 0.0726099979999972

0.3333334697853161 0.1666665442146780 0.1451498879461255

0.3333334697853161 0.6666665592146828 0.1451498879461255

0.8333334997853186 0.1666665442146780 0.1451498879461255

0.8333334997853186 0.6666665592146828 0.1451498879461255

0.1666604477393747 0.3333395822606278 0.2163689804857754

0.1666604477393747 0.8333395522606253 0.2163689804857754

0.6666604477393747 0.3333395822606278 0.2163689804857754

0.6666604477393747 0.8333395522606253 0.2163689804857754

0.0000026806048652 0.4999973153951345 0.2940449738820448

0.0000026806048652 0.9999973153951345 0.2940449738820448

0.5000026846048655 0.4999973153951345 0.2940449738820448

0.5000026846048655 0.9999973153951345 0.2940449738820448

0.1666650029999985 0.0833349970000015 0.0000000000000000

0.1666650029999985 0.5833349819999967 0.0000000000000000

0.6666650180000033	0.0833349970000015	0.0000000000000000
0.6666650180000033	0.5833349819999967	0.0000000000000000
0.4166649880000008	0.0833349970000015	0.0000000000000000
0.4166649880000008	0.5833349819999967	0.0000000000000000
0.9166649579999984	0.0833349970000015	0.0000000000000000
0.9166649579999984	0.5833349819999967	0.0000000000000000
0.4166649880000008	0.3333350119999992	0.0000000000000000
0.4166649880000008	0.8333350420000016	0.0000000000000000
0.9166649579999984	0.3333350119999992	0.0000000000000000
0.9166649579999984	0.8333350420000016	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0726099979999972
0.0000000000000000	0.7500000000000000	0.0726099979999972
0.5000000000000000	0.2500000000000000	0.0726099979999972
0.5000000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.2500000000000000	0.0726099979999972
0.2500000000000000	0.7500000000000000	0.0726099979999972
0.7500000000000000	0.2500000000000000	0.0726099979999972
0.7500000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.0000000000000000	0.0726099979999972
0.2500000000000000	0.5000000000000000	0.0726099979999972
0.7500000000000000	0.0000000000000000	0.0726099979999972
0.7500000000000000	0.5000000000000000	0.0726099979999972
0.3335171787203564	0.4167555585831906	0.1449242104336150
0.3335171787203564	0.9167555585831906	0.1449242104336150
0.8335171787203564	0.4167555585831906	0.1449242104336150
0.8335171787203564	0.9167555585831906	0.1449242104336150
0.0832441902125893	0.4167557877874088	0.1449228372510021
0.0832441902125893	0.9167557577874135	0.1449228372510021
0.5832441832125852	0.4167557877874088	0.1449228372510021
0.5832441832125852	0.9167557577874135	0.1449228372510021
0.0832444114168140	0.1664828212796436	0.1449242104336150
0.0832444114168140	0.6664828212796436	0.1449242104336150
0.5832444414168094	0.1664828212796436	0.1449242104336150

0.5832444414168094	0.6664828212796436	0.1449242104336150
0.1647393718566619	0.0823626219034281	0.2175629257916043
0.1647393718566619	0.5823626069034304	0.2175629257916043
0.6647393568566642	0.0823626219034281	0.2175629257916043
0.6647393568566642	0.5823626069034304	0.2175629257916043
0.4176231126622056	0.0823768733377932	0.2175693514331911
0.4176231126622056	0.5823768873377944	0.2175693514331911
0.9176231126622056	0.0823768733377932	0.2175693514331911
0.9176231126622056	0.5823768873377944	0.2175693514331911
0.4176373640965707	0.3352606431433358	0.2175629257916043
0.4176373640965707	0.8352606431433358	0.2175629257916043
0.9176373930965696	0.3352606431433358	0.2175629257916043
0.9176373930965696	0.8352606431433358	0.2175629257916043
0.9991448969658023	0.2495698959031429	0.2876193404641398
0.9991448969658023	0.7495699249031418	0.2876193404641398
0.4991449039658065	0.2495698959031429	0.2876193404641398
0.4991449039658065	0.7495699249031418	0.2876193404641398
0.2504401862785528	0.2495597987214495	0.2876148099604308
0.2504401862785528	0.7495597697214507	0.2876148099604308
0.7504401712785551	0.2495597987214495	0.2876148099604308
0.7504401712785551	0.7495597697214507	0.2876148099604308
0.2504301040968571	0.5008550960341935	0.2876193404641398
0.2504301040968571	0.0008550960341935	0.2876193404641398
0.7504300750968582	0.5008550960341935	0.2876193404641398
0.7504300750968582	0.0008550960341935	0.2876193404641398

NiSc (25% Sc) 111 Facet with Hydrogen supercell 2X2X1 - [Etot = -469.42312969 eV]

1.04735280294076

10.0268001556000002	0.0000000000000000	0.0000000000000000
-5.0134000778000001	8.6834636535000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.1868000031000001

Sc Ni H

20 60 1

Direct

0.1666650029999985	0.3333350119999992	0.0000000000000000
0.1666650029999985	0.8333350420000016	0.0000000000000000
0.6666650180000033	0.3333350119999992	0.0000000000000000
0.6666650180000033	0.8333350420000016	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0726099979999972
0.0000000000000000	0.5000000000000000	0.0726099979999972
0.5000000000000000	0.0000000000000000	0.0726099979999972
0.5000000000000000	0.5000000000000000	0.0726099979999972
0.3332157034126411	0.1667843105873530	0.1461440951587534
0.3332110822797887	0.6664284866183721	0.1461445878024250
0.8335715723816293	0.1667889317202054	0.1461445878024250
0.8333319735473097	0.6666680854526916	0.1458929731354459
0.1666616594958157	0.3333383705041868	0.2168609925525189
0.1663582105674521	0.8331571752089459	0.2163834494898111
0.6668428247910541	0.3336418194325503	0.2163834494898111
0.6668223108235480	0.8331776891764520	0.2163869412283219
0.9992632611655807	0.5007367348344189	0.2953256752275593
0.9992525238378960	0.9985175813765252	0.2953224640372909
0.5014824186234748	0.5007474721621037	0.2953224640372909
0.5000046206424926	0.9999953793575074	0.2958359022196930
0.1666650029999985	0.0833349970000015	0.0000000000000000
0.1666650029999985	0.5833349819999967	0.0000000000000000
0.6666650180000033	0.0833349970000015	0.0000000000000000
0.6666650180000033	0.5833349819999967	0.0000000000000000
0.4166649880000008	0.0833349970000015	0.0000000000000000
0.4166649880000008	0.5833349819999967	0.0000000000000000
0.9166649579999984	0.0833349970000015	0.0000000000000000
0.9166649579999984	0.5833349819999967	0.0000000000000000
0.4166649880000008	0.3333350119999992	0.0000000000000000
0.4166649880000008	0.8333350420000016	0.0000000000000000
0.9166649579999984	0.3333350119999992	0.0000000000000000
0.9166649579999984	0.8333350420000016	0.0000000000000000

0.0000000000000000	0.2500000000000000	0.0726099979999972
0.0000000000000000	0.7500000000000000	0.0726099979999972
0.5000000000000000	0.2500000000000000	0.0726099979999972
0.5000000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.2500000000000000	0.0726099979999972
0.2500000000000000	0.7500000000000000	0.0726099979999972
0.7500000000000000	0.2500000000000000	0.0726099979999972
0.7500000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.0000000000000000	0.0726099979999972
0.2500000000000000	0.5000000000000000	0.0726099979999972
0.7500000000000000	0.0000000000000000	0.0726099979999972
0.7500000000000000	0.5000000000000000	0.0726099979999972
0.3335731167800517	0.4167856172447202	0.1449549724650439
0.3335904246079551	0.9167906986824761	0.1448287089621871
0.8338019211250511	0.4169052231331207	0.1447501326090119
0.8338090393645956	0.9168979729429267	0.1447486525988140
0.0832113216980375	0.4167886563019607	0.1449555171866521
0.0830872481074749	0.9168937109432633	0.1447462682077827
0.5831062300567353	0.4169127298925233	0.1447462682077827
0.5832065522388490	0.9167933887611497	0.1448281647913632
0.0832143527552844	0.1664268832199483	0.1449549724650439
0.0830947468668839	0.6661980788749489	0.1447501326090119
0.5832093013175239	0.1664095753920449	0.1448287089621871
0.5831020270570733	0.6661909606354044	0.1447486525988140
0.1625221739141125	0.0814690697808231	0.2186926973756798
0.1625246375900744	0.5810644904024116	0.2186915904702715
0.6619067309979059	0.0809589410260401	0.2183840931449481
0.6621550277458610	0.5810815554035997	0.2182874286396626
0.4190512814938927	0.0809487045061061	0.2183865368466726
0.4185364872443884	0.5810588511521786	0.2186909177660823
0.9189411488478214	0.0814634987556104	0.2186909177660823
0.9189248189105257	0.5810751810894743	0.2182897425980954
0.4185309162191757	0.3374778410858852	0.2186926973756798

0.4190410449739588	0.8380932690020941	0.2183840931449481
0.9189355095975884	0.3374753774099233	0.2186915904702715
0.9189184445964003	0.8378449722541390	0.2182874286396626
0.9975389592238173	0.2487662644318931	0.2879229200450339
0.9968193480757961	0.7484080085846969	0.2864874287330039
0.4966465313221420	0.2480368506968915	0.2862955124231021
0.4966420882283558	0.7486080934216659	0.2862951460080652
0.2512365512055794	0.2487634337944229	0.2879245067720433
0.2519652969856878	0.7486084951680070	0.2862933279740361
0.7513914458319988	0.2480346880143145	0.2862933279740361
0.7515932367550633	0.7484067042449425	0.2864851606720435
0.2512337355681069	0.5024610337761786	0.2879229200450339
0.2519631493031085	0.0033534686778580	0.2862955124231021
0.7515919914153031	0.5031806449241998	0.2864874287330039
0.7513919065783341	0.0033579117716442	0.2862951460080652
0.1666655946242912	0.3333344353757113	0.3145263549217248

NiTi (25% Ti) 111 Facet with Hydrogen supercell 2X2X1 - [Etot = -503.16328396 eV]

1.01798110552312

10.0268001556000002	0.0000000000000000	0.0000000000000000
-5.0134000778000001	8.6834636535000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.1868000031000001

Ti Ni H

20 60 1

Direct

0.1666650029999985	0.3333350119999992	0.0000000000000000
0.1666650029999985	0.8333350420000016	0.0000000000000000
0.6666650180000033	0.3333350119999992	0.0000000000000000
0.6666650180000033	0.8333350420000016	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0726099979999972
0.0000000000000000	0.5000000000000000	0.0726099979999972
0.5000000000000000	0.0000000000000000	0.0726099979999972
0.5000000000000000	0.5000000000000000	0.0726099979999972

0.3333656322824226	0.1666343817175715	0.1448202170617350
0.3333653933298066	0.6667255880243346	0.1448200060016092
0.8332744709756668	0.1666346206701874	0.1448200060016092
0.8333342231517378	0.6666658358482636	0.1445422406821280
0.1666698357194463	0.3333301942805562	0.2199677355473710
0.1668350683446533	0.8334137056298871	0.2211471430159548
0.6665862943701129	0.3331649616553491	0.2211471430159548
0.6665868604972403	0.8334131395027597	0.2211473948185443
0.9982545186839147	0.5017454773160850	0.2882521574497403
0.9982534110215155	0.9965023452862454	0.2882521140126713
0.5034976547137546	0.5017465849784841	0.2882521140126713
0.5000026959805268	0.9999973040194732	0.2885688338890873
0.1666650029999985	0.0833349970000015	0.0000000000000000
0.1666650029999985	0.5833349819999967	0.0000000000000000
0.6666650180000033	0.0833349970000015	0.0000000000000000
0.6666650180000033	0.5833349819999967	0.0000000000000000
0.4166649880000008	0.0833349970000015	0.0000000000000000
0.4166649880000008	0.5833349819999967	0.0000000000000000
0.9166649579999984	0.0833349970000015	0.0000000000000000
0.9166649579999984	0.5833349819999967	0.0000000000000000
0.4166649880000008	0.3333350119999992	0.0000000000000000
0.4166649880000008	0.8333350420000016	0.0000000000000000
0.9166649579999984	0.3333350119999992	0.0000000000000000
0.9166649579999984	0.8333350420000016	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0726099979999972
0.0000000000000000	0.7500000000000000	0.0726099979999972
0.5000000000000000	0.2500000000000000	0.0726099979999972
0.5000000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.2500000000000000	0.0726099979999972
0.2500000000000000	0.7500000000000000	0.0726099979999972
0.7500000000000000	0.2500000000000000	0.0726099979999972
0.7500000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.0000000000000000	0.0726099979999972

0.2500000000000000	0.5000000000000000	0.0726099979999972
0.7500000000000000	0.0000000000000000	0.0726099979999972
0.7500000000000000	0.5000000000000000	0.0726099979999972
0.3327889104263306	0.4163925509945301	0.1454205648104150
0.3327730640108939	0.9163836305764619	0.1454144147596210
0.8326775485126277	0.4162816655423143	0.1453982482391112
0.8326773782424155	0.9163932211266612	0.1453987964386627
0.0836073108676914	0.4163926671323068	0.1454204321149888
0.0837193067880762	0.9163933258495049	0.1453986384704535
0.5836066151504937	0.4162806712119220	0.1453986384704535
0.5836155802427427	0.9163843607572559	0.1454145530057147
0.0836074190054745	0.1672110895736694	0.1454205648104150
0.0837183044576904	0.6673224514873723	0.1453982482391112
0.5836163694235381	0.1672269359891061	0.1454144147596210
0.5836067788733388	0.6673226217575845	0.1453987964386627
0.1660755578064865	0.0835460073178069	0.2176489739163685
0.1660752130801058	0.5825224308684227	0.2176488211018395
0.6659993428122135	0.0829963708368240	0.2174893917803971
0.6658980797121359	0.5829447332888691	0.2173759134149122
0.4170027884957719	0.0829971975042270	0.2174888732595264
0.4164540201615878	0.5825230589657622	0.2176490853723294
0.9174769410342378	0.0835459658384110	0.2176490853723294
0.9170554163133176	0.5829445836866824	0.2173756974535337
0.4164539786821919	0.3339244571935112	0.2176489739163685
0.4170036151631749	0.8340006571877865	0.2174893917803971
0.9174775691315773	0.3339248019198919	0.2176488211018395
0.9170552667111309	0.8341019202878641	0.2173759134149122
0.0014171611850173	0.2507038830843769	0.2897021760739378
0.0011235471611499	0.7505571438880452	0.2893573803590286
0.5010338763320092	0.2507380738821254	0.2893645347821874
0.5010333257810089	0.7502852264354800	0.2893646137349251
0.2492983961748934	0.2507015888251090	0.2897037309668136
0.2492605675579043	0.7502857222069181	0.2893647906887580

0.7497142187930876	0.2507394174420980	0.2893647906887580
0.7494438557176224	0.7505560852823834	0.2893582105713506
0.2492961169156231	0.4985828318149785	0.2897021760739378
0.2492619261178746	0.9989661236679908	0.2893645347821874
0.7494428561119548	0.4988764458388459	0.2893573803590286
0.7497147735645200	0.9989666742189911	0.2893646137349251
0.1666718491714860	0.3333281808285165	0.3215108865330976

NiV (25% V) 111 Facet with Hydrogen supercell 2X2X1 - [Etot = -504.57052261 eV]

1.00458661266245

10.0268001556000002	0.0000000000000000	0.0000000000000000
-5.0134000778000001	8.6834636535000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.1868000031000001

V Ni H

20 60 1

Direct

0.1666650029999985	0.3333350119999992	0.0000000000000000
0.1666650029999985	0.8333350420000016	0.0000000000000000
0.6666650180000033	0.3333350119999992	0.0000000000000000
0.6666650180000033	0.8333350420000016	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0726099979999972
0.0000000000000000	0.5000000000000000	0.0726099979999972
0.5000000000000000	0.0000000000000000	0.0726099979999972
0.5000000000000000	0.5000000000000000	0.0726099979999972
0.3333301184466464	0.1666698955533477	0.1448981377342875
0.3333286299297669	0.6666646499822164	0.1448955867167356
0.8333354090177849	0.1666713840702272	0.1448955867167356
0.8333345160471524	0.6666655429528490	0.1448340749757193
0.1666658440635800	0.3333341859364225	0.2211965002399126
0.1669212901569139	0.8334639005814708	0.2230238801237263
0.6665360994185292	0.3330787398430886	0.2230238801237263
0.6665378635787391	0.8334621364212609	0.2230134468608895
0.9980017036644355	0.5019982923355641	0.2906139465043793

0.9980044327176785	0.9960084335917685	0.2906121350380459
0.5039915664082315	0.5019955632823212	0.2906121350380459
0.4999976979104233	0.0000023020895767	0.2905799431229283
0.1666650029999985	0.0833349970000015	0.0000000000000000
0.1666650029999985	0.5833349819999967	0.0000000000000000
0.6666650180000033	0.0833349970000015	0.0000000000000000
0.6666650180000033	0.5833349819999967	0.0000000000000000
0.4166649880000008	0.0833349970000015	0.0000000000000000
0.4166649880000008	0.5833349819999967	0.0000000000000000
0.9166649579999984	0.0833349970000015	0.0000000000000000
0.9166649579999984	0.5833349819999967	0.0000000000000000
0.4166649880000008	0.3333350119999992	0.0000000000000000
0.4166649880000008	0.8333350420000016	0.0000000000000000
0.9166649579999984	0.3333350119999992	0.0000000000000000
0.9166649579999984	0.8333350420000016	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0726099979999972
0.0000000000000000	0.7500000000000000	0.0726099979999972
0.5000000000000000	0.2500000000000000	0.0726099979999972
0.5000000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.2500000000000000	0.0726099979999972
0.2500000000000000	0.7500000000000000	0.0726099979999972
0.7500000000000000	0.2500000000000000	0.0726099979999972
0.7500000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.0000000000000000	0.0726099979999972
0.2500000000000000	0.5000000000000000	0.0726099979999972
0.7500000000000000	0.0000000000000000	0.0726099979999972
0.7500000000000000	0.5000000000000000	0.0726099979999972
0.3326775621994358	0.4163370485560520	0.1453100580979623
0.3326621209375844	0.9163355229081276	0.1451933901666536
0.8326964954754601	0.4162431908216035	0.1451611434559936
0.8327039453509713	0.9164650276105633	0.1451597753528162
0.0836584629309414	0.4163415150690568	0.1453103080043832
0.0837584402428320	0.9164589864270667	0.1451618902026865

0.5835409545729320	0.4162415377571662	0.1451618902026865
0.5836617201395882	0.9163382208604105	0.1451919242036297
0.0836629214439526	0.1673224378005642	0.1453100580979623
0.0837567791784011	0.6673035045245399	0.1451611434559936
0.5836644770918724	0.1673378790624156	0.1451933901666536
0.5835349723894367	0.6672960546490287	0.1451597753528162
0.1657434519348300	0.0831848542674720	0.2168699947632575
0.1657371928086988	0.5825528969774396	0.2168727503556696
0.6656944551644628	0.0828463488996150	0.2166215705339809
0.6653636245526471	0.5826941806869996	0.2165570116630704
0.4171534877885605	0.0828464982114383	0.2166233601035614
0.4168165545973679	0.5825701330529398	0.2168681555999186
0.9174298669470602	0.0831834314026310	0.2168681555999186
0.9173198395597879	0.5826801604402121	0.2165595330505852
0.4168151317325268	0.3342565630651677	0.2168699947632575
0.4171536371003839	0.8343055448355372	0.2166215705339809
0.9174471030225604	0.3342628221912989	0.2168727503556696
0.9173058193130004	0.8346363754473529	0.2165570116630704
0.0012332152911370	0.2506063418375746	0.2896517111915884
0.0005985256932348	0.7503008316861397	0.2893820379231187
0.5004177451767617	0.2502870361621419	0.2894327944396480
0.5004549871522315	0.7501541306089763	0.2894305919577889
0.2493925522542924	0.2506074327457100	0.2896552434281787
0.2497119894375430	0.7501471905450998	0.2894308837673307
0.7498527504549060	0.2502879955624593	0.2894308837673307
0.7496864632957951	0.7503134777042106	0.2893790945784005
0.2493936581624254	0.4987667777088589	0.2896517111915884
0.2497129638378581	0.9995822548232383	0.2894327944396480
0.7496991683138603	0.4994014673067610	0.2893820379231187
0.7498458693910237	0.9995450128477685	0.2894305919577889
0.1666659171826765	0.3333341128173259	0.3229928306355134

0.995572721824907

10.026800155600002 0.000000000000000 0.000000000000000

-5.0134000778000001 8.6834636535000005 0.000000000000000

0.000000000000000 0.000000000000000 28.1868000031000001

Cr Ni H

20 60 1

Direct

0.1666650029999985 0.3333350119999992 0.000000000000000

0.1666650029999985 0.8333350420000016 0.000000000000000

0.6666650180000033 0.3333350119999992 0.000000000000000

0.6666650180000033 0.8333350420000016 0.000000000000000

0.000000000000000 0.000000000000000 0.0726099979999972

0.000000000000000 0.500000000000000 0.0726099979999972

0.500000000000000 0.000000000000000 0.0726099979999972

0.500000000000000 0.500000000000000 0.0726099979999972

0.3333043069231607 0.1666957070768333 0.1454685715034145

0.3333028558953472 0.6666028353348565 0.1454605657118506

0.8333972236651448 0.1666971581046468 0.1454605657118506

0.8333358504808714 0.666642085191299 0.1453180658616375

0.1666651767929679 0.3333348532070346 0.2205440015647397

0.1668018368366688 0.8334023422922954 0.2220762215036487

0.6665976577077046 0.3331981931633337 0.2220762215036487

0.6666047659466088 0.8333952340533912 0.2220519471662143

0.9986602887845777 0.5013397072154220 0.2919959677516246

0.9986470746719505 0.9973174889890117 0.2920037396882122

0.5026825110109883 0.5013529213280492 0.2920037396882122

0.5000110330907575 0.9999889669092425 0.2921565986567813

0.1666650029999985 0.0833349970000015 0.000000000000000

0.1666650029999985 0.5833349819999967 0.000000000000000

0.6666650180000033 0.0833349970000015 0.000000000000000

0.6666650180000033 0.5833349819999967 0.000000000000000

0.4166649880000008 0.0833349970000015 0.000000000000000

0.4166649880000008 0.5833349819999967 0.000000000000000

0.9166649579999984	0.0833349970000015	0.0000000000000000
0.9166649579999984	0.5833349819999967	0.0000000000000000
0.4166649880000008	0.3333350119999992	0.0000000000000000
0.4166649880000008	0.8333350420000016	0.0000000000000000
0.9166649579999984	0.3333350119999992	0.0000000000000000
0.9166649579999984	0.8333350420000016	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0726099979999972
0.0000000000000000	0.7500000000000000	0.0726099979999972
0.5000000000000000	0.2500000000000000	0.0726099979999972
0.5000000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.2500000000000000	0.0726099979999972
0.2500000000000000	0.7500000000000000	0.0726099979999972
0.7500000000000000	0.2500000000000000	0.0726099979999972
0.7500000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.0000000000000000	0.0726099979999972
0.2500000000000000	0.5000000000000000	0.0726099979999972
0.7500000000000000	0.0000000000000000	0.0726099979999972
0.7500000000000000	0.5000000000000000	0.0726099979999972
0.3331628195923528	0.4165825767133811	0.1457198222095712
0.3328132233450845	0.9163996760587736	0.1457509139982278
0.8325453426295297	0.4162866652824988	0.1456764528316441
0.8325505527609494	0.9162547005697945	0.1456733851389771
0.0834277118197875	0.4165722661802107	0.1457189886524617
0.0837020056946400	0.9162605384759814	0.1456775984215639
0.5837394025240172	0.4162979723053581	0.1456775984215639
0.5836046218193047	0.9163953191806939	0.1457474009011790
0.0834173932866236	0.1668371804076472	0.1457198222095712
0.0837133047175058	0.6674546573704703	0.1456764528316441
0.5836003239412264	0.1671867766549155	0.1457509139982278
0.5837452994302055	0.6674494472390506	0.1456733851389771
0.1668112117157463	0.0832938527073424	0.2181138366019226
0.1668136963960691	0.5835205227939966	0.2181033871296449
0.6665823376732689	0.0832839435758643	0.2178215510274839

0.6666401954014702	0.5833179446497638	0.2175735783990476
0.4167102265821683	0.0832897594178306	0.2178310083349970
0.4167159265102001	0.5835165385646235	0.2181050806162688
0.9164834614353765	0.0832840594897988	0.2181050806162688
0.9166785920620200	0.5833214079379800	0.2175719964834713
0.4167061332926565	0.3331888032842514	0.2181138366019226
0.4167160424241345	0.8334176623267311	0.2178215510274839
0.9164794772060034	0.3331863186039286	0.2181033871296449
0.9166820553502362	0.8333598045985298	0.2175735783990476
0.0014219758281371	0.2507040197395582	0.2913555304404341
0.0017401541398385	0.7508767575766555	0.2905149960084188
0.5015813175689914	0.2507564451446029	0.2907113585173136
0.5015884495826697	0.7508275961233295	0.2906983170611568
0.2492814082761399	0.2507185767238624	0.2913601554536598
0.2492654866057649	0.7508247152742911	0.2907039158631974
0.7491752257257147	0.2507344983942374	0.2907039158631974
0.7491168524454253	0.7508830885545805	0.2905077774978224
0.2492959802604418	0.4985780171718588	0.2913555304404341
0.2492435548553971	0.9984186824310086	0.2907113585173136
0.7491232424233445	0.4982598388601573	0.2905149960084188
0.7491724038766705	0.9984115504173303	0.2906983170611568
0.1666694615119368	0.3333305684880656	0.3252121545763558

NiMn (25% Mn) 111 Facet with Hydrogen supercell 2X2X1 - [Etot = -498.31615918 eV]

1.0000000000000000

9.9196901320999995	0.0000000000000000	0.0000000000000000
-4.9598426818999997	8.5906995225999996	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.8856849669999995

Mn	Ni	H
20	60	1

Direct

0.1666650029999985	0.3333350119999992	0.0000000000000000
0.1666650029999985	0.8333350420000016	0.0000000000000000

0.6666650180000033	0.3333350119999992	0.0000000000000000
0.6666650180000033	0.8333350420000016	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0726099979999972
0.0000000000000000	0.5000000000000000	0.0726099979999972
0.5000000000000000	0.0000000000000000	0.0726099979999972
0.5000000000000000	0.5000000000000000	0.0726099979999972
0.3332152805190205	0.1666249272505027	0.1474970528066493
0.3332075461619084	0.6665128102487330	0.1475087046767953
0.8333139861045638	0.1666217293897461	0.1475029852596705
0.8332412555039497	0.6665829898579645	0.1474620154961599
0.1665330588684029	0.3332195536757041	0.2215247626687429
0.1662850880851821	0.8330813174706009	0.2213153974296063
0.6666506151812399	0.3334355325707250	0.2213354563734455
0.6666529457420438	0.8330829318883701	0.2213237539929906
0.5010638596955275	0.5004495229202206	0.2986612130846282
0.4998245165996309	0.9998371284264138	0.2989912409073767
0.9992109468608348	0.5004522983942294	0.2986546629069693
0.9992149309950094	0.9986160877571493	0.2986664251206719
0.1666650029999985	0.0833349970000015	0.0000000000000000
0.1666650029999985	0.5833349819999967	0.0000000000000000
0.6666650180000033	0.0833349970000015	0.0000000000000000
0.6666650180000033	0.5833349819999967	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0726099979999972
0.0000000000000000	0.7500000000000000	0.0726099979999972
0.5000000000000000	0.2500000000000000	0.0726099979999972
0.5000000000000000	0.7500000000000000	0.0726099979999972
0.4166649880000008	0.0833349970000015	0.0000000000000000
0.4166649880000008	0.5833349819999967	0.0000000000000000
0.9166649579999984	0.0833349970000015	0.0000000000000000
0.9166649579999984	0.5833349819999967	0.0000000000000000
0.2500000000000000	0.2500000000000000	0.0726099979999972
0.2500000000000000	0.7500000000000000	0.0726099979999972
0.7500000000000000	0.2500000000000000	0.0726099979999972

0.7500000000000000	0.7500000000000000	0.0726099979999972
0.4166649880000008	0.3333350119999992	0.0000000000000000
0.4166649880000008	0.8333350420000016	0.0000000000000000
0.9166649579999984	0.3333350119999992	0.0000000000000000
0.9166649579999984	0.8333350420000016	0.0000000000000000
0.2500000000000000	0.0000000000000000	0.0726099979999972
0.2500000000000000	0.5000000000000000	0.0726099979999972
0.7500000000000000	0.0000000000000000	0.0726099979999972
0.7500000000000000	0.5000000000000000	0.0726099979999972
0.3332981174893632	0.4166203261066741	0.1471506872131059
0.3333312295363058	0.9166253790002870	0.1470864759523351
0.8333114404160753	0.4165796646240167	0.1470855622914726
0.8333213107684188	0.9166654599763859	0.1470849393475220
0.1658157498661907	0.0829549203203115	0.2218214088676191
0.1658111842960253	0.5827466644036434	0.2218330857335360
0.6653992437291265	0.0826403477761346	0.2216695327908837
0.6655260459919674	0.5826946745918562	0.2216634767946317
0.4996322461642535	0.2493898815412905	0.2943530018927021
0.4996437768301831	0.7500972492315796	0.2943503539451555
0.9998256534778847	0.2498563364977144	0.2957126215906456
0.9997824560060522	0.7498179489096373	0.2945142400713010
0.0832282337087236	0.4166204821292396	0.1471521690955555
0.0832435061018018	0.9166543197274777	0.1470813051335469
0.5831872267769285	0.4165839174493797	0.1470866379492506
0.5832084624170051	0.9166314382794027	0.1470885999994707
0.4170946781893434	0.0826493004383622	0.2216648130135823
0.4167899865261617	0.5827445258718669	0.2218357633980617
0.9169900638545485	0.0829513769403505	0.2218313070680509
0.9170110412900527	0.5826983284781164	0.2216518788302864
0.2498376046750508	0.2498533839477730	0.2957032635391030
0.2502674365566833	0.7501045154156500	0.2943467532020065
0.7495865953234926	0.2493994155319825	0.2943543708836671
0.7498561440633082	0.7498196924561213	0.2945237671374556

0.0832269368857510	0.1665504276571497	0.1471503843089152
0.0832477503599520	0.6665081346528936	0.1470821691353379
0.5832204496928028	0.1665193386221588	0.1470903721353523
0.5831717110221319	0.6665154844621100	0.1470852794561708
0.4167935999467431	0.3339130292015966	0.2218231423273807
0.4170948570168136	0.8343264081234949	0.2216688721660560
0.9169769269966039	0.3339184438276703	0.2218247151727724
0.9170195632705003	0.8341927077647071	0.2216577323958830
0.2502594666885045	0.0000368125885046	0.2943360639044386
0.2498501938526374	0.4998824719268100	0.2957220345250562
0.7495908811284835	0.0000446835412191	0.2943462673916102
0.7498652239567818	0.4998950763080998	0.2945250404038973
0.1664830330437539	0.3331463125528700	0.3291019479052295

NiFe (25% Fe) 111 Facet with Hydrogen supercell 2X2X1 - [Etot = -483.63851074 eV]

1.0000000000000000

10.0268001556000002	0.0000000000000000	0.0000000000000000
-5.0134000778000001	8.6834636535000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.1868000031000001

Fe Ni H

20 60 1

Direct

0.1666650029999985	0.3333350119999992	0.0000000000000000
0.1666650029999985	0.8333350420000016	0.0000000000000000
0.6666650180000033	0.3333350119999992	0.0000000000000000
0.6666650180000033	0.8333350420000016	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0726099979999972
0.0000000000000000	0.5000000000000000	0.0726099979999972
0.5000000000000000	0.0000000000000000	0.0726099979999972
0.5000000000000000	0.5000000000000000	0.0726099979999972
0.3332864487836318	0.1667135652163552	0.1447407954409172
0.3332863200037366	0.6665683516545968	0.1447388140892087
0.8334317073454045	0.1667136939962575	0.1447388140892087

0.8333348157035800	0.6666652432964213	0.1445708350706454
0.1666698080254676	0.3333302219745349	0.2186093740334840
0.1666331018730034	0.8333112403534031	0.2192801760214209
0.6666887596465969	0.3333669281269991	0.2192801760214209
0.6666893367888136	0.8333106632111864	0.2192738538399936
0.9988574387126548	0.5011425572873449	0.2883904590212438
0.9988527222929520	0.9976988106921496	0.2883886008130929
0.5023011893078504	0.5011472737070477	0.2883886008130929
0.5000082613860002	0.9999917386139998	0.2885596595686835
0.1666650029999985	0.0833349970000015	0.0000000000000000
0.1666650029999985	0.5833349819999967	0.0000000000000000
0.6666650180000033	0.0833349970000015	0.0000000000000000
0.6666650180000033	0.5833349819999967	0.0000000000000000
0.4166649880000008	0.0833349970000015	0.0000000000000000
0.4166649880000008	0.5833349819999967	0.0000000000000000
0.9166649579999984	0.0833349970000015	0.0000000000000000
0.9166649579999984	0.5833349819999967	0.0000000000000000
0.4166649880000008	0.3333350119999992	0.0000000000000000
0.4166649880000008	0.8333350420000016	0.0000000000000000
0.9166649579999984	0.3333350119999992	0.0000000000000000
0.9166649579999984	0.8333350420000016	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0726099979999972
0.0000000000000000	0.7500000000000000	0.0726099979999972
0.5000000000000000	0.2500000000000000	0.0726099979999972
0.5000000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.2500000000000000	0.0726099979999972
0.2500000000000000	0.7500000000000000	0.0726099979999972
0.7500000000000000	0.2500000000000000	0.0726099979999972
0.7500000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.0000000000000000	0.0726099979999972
0.2500000000000000	0.5000000000000000	0.0726099979999972
0.7500000000000000	0.0000000000000000	0.0726099979999972
0.7500000000000000	0.5000000000000000	0.0726099979999972

0.3330940551442296	0.4165453983449154	0.1451619252346248
0.3330350339102424	0.9165150226703602	0.1451416801023626
0.8329675908063763	0.4165264386715748	0.1451184455136385
0.8329694685162323	0.9164362560097032	0.1451151147447618
0.0834573998302872	0.4165425781697110	0.1451644202864060
0.0834736822845841	0.9164346002995387	0.1451170904642183
0.5835653407004600	0.4165262957154141	0.1451170904642183
0.5834845221220561	0.9165154188779425	0.1451394025013428
0.0834545716550892	0.1669059448557704	0.1451619252346248
0.0834735313284298	0.6670324091936237	0.1451184455136385
0.5834849773296398	0.1669649660897576	0.1451416801023626
0.5835637439902968	0.6670305314837677	0.1451151147447618
0.1670406591114570	0.0836571307091774	0.2172678979155194
0.1670375889402038	0.5833707698189627	0.2172644959062353
0.6670860917710826	0.0835349189626342	0.2172659981264289
0.6668934561213291	0.5834447742436737	0.2171900051023457
0.4164607756266392	0.0835392103733597	0.2172687194071869
0.4163466445973896	0.5833756934098417	0.2172625613281696
0.9166243065901583	0.0836533414026093	0.2172625613281696
0.9165591584848443	0.5834408415151557	0.2171912402572715
0.4163428552908215	0.3329593558885406	0.2172678979155194
0.4164650670373646	0.8329139082289174	0.2172659981264289
0.9166292301810373	0.3329624260597939	0.2172644959062353
0.9165552257563263	0.8331065438786709	0.2171900051023457
0.0008858945131109	0.2504329110219032	0.2896219568735603
0.0011495172518039	0.7505691576909470	0.2888645089054194
0.5010825211934673	0.2504199385465000	0.2888194131155757
0.5010878089298600	0.7506496579410111	0.2888176969973344
0.2495654974452748	0.2504344875547275	0.2896221121050289
0.2495832189911056	0.7506495515644644	0.2888199597999375
0.7493503894355413	0.2504167660088967	0.2888199597999375
0.7494277807947398	0.7505721602052660	0.2888628845088661
0.2495670889780897	0.4991140984868849	0.2896219568735603

0.2495800614535000	0.9989174788065327	0.2888194131155757
0.7494308423090530	0.4988504757481920	0.2888645089054194
0.7493503420589889	0.9989121910701400	0.2888176969973344
0.1666725584862760	0.3333274715137264	0.3226365107435143

NiCo (25% Co) 111 Facet with Hydrogen supercell 2X2X1 - [Etot = -450.92529772 eV]

0.993794164815303

10.0268001556000002	0.0000000000000000	0.0000000000000000
-5.0134000778000001	8.6834636535000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.1868000031000001

Co Ni H

20 60 1

Direct

0.1666650029999985	0.3333350119999992	0.0000000000000000
0.1666650029999985	0.8333350420000016	0.0000000000000000
0.6666650180000033	0.3333350119999992	0.0000000000000000
0.6666650180000033	0.8333350420000016	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0726099979999972
0.0000000000000000	0.5000000000000000	0.0726099979999972
0.5000000000000000	0.0000000000000000	0.0726099979999972
0.5000000000000000	0.5000000000000000	0.0726099979999972
0.3333115464162120	0.1666884675837821	0.1448063774476154
0.3333120560670864	0.6666169870011061	0.1448055002542006
0.8333830719988953	0.1666879579329077	0.1448055002542006
0.8333368026015435	0.6666632563984578	0.1447225110932280
0.1666712069710741	0.3333288230289284	0.2187410534966290
0.1666256356508455	0.8333083986986125	0.2192288648150225
0.6666916013013875	0.3333743943491569	0.2192288648150225
0.6666925795041934	0.8333074204958066	0.2192290668675199
0.9989016449818209	0.5010983510181788	0.2885658982458139
0.9988983357927310	0.9977877118672467	0.2885550037033582
0.5022122881327533	0.5011016602072687	0.2885550037033582
0.5000042712214139	0.9999957287785861	0.2887727888223495

0.1666650029999985	0.0833349970000015	0.0000000000000000
0.1666650029999985	0.5833349819999967	0.0000000000000000
0.6666650180000033	0.0833349970000015	0.0000000000000000
0.6666650180000033	0.5833349819999967	0.0000000000000000
0.4166649880000008	0.0833349970000015	0.0000000000000000
0.4166649880000008	0.5833349819999967	0.0000000000000000
0.9166649579999984	0.0833349970000015	0.0000000000000000
0.9166649579999984	0.5833349819999967	0.0000000000000000
0.4166649880000008	0.3333350119999992	0.0000000000000000
0.4166649880000008	0.8333350420000016	0.0000000000000000
0.9166649579999984	0.3333350119999992	0.0000000000000000
0.9166649579999984	0.8333350420000016	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0726099979999972
0.0000000000000000	0.7500000000000000	0.0726099979999972
0.5000000000000000	0.2500000000000000	0.0726099979999972
0.5000000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.2500000000000000	0.0726099979999972
0.2500000000000000	0.7500000000000000	0.0726099979999972
0.7500000000000000	0.2500000000000000	0.0726099979999972
0.7500000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.0000000000000000	0.0726099979999972
0.2500000000000000	0.5000000000000000	0.0726099979999972
0.7500000000000000	0.0000000000000000	0.0726099979999972
0.7500000000000000	0.5000000000000000	0.0726099979999972
0.3330922747296299	0.4165435212254209	0.1452145309818320
0.3330914069868811	0.9165425767741766	0.1451066199353903
0.8330089015528230	0.4165698926017143	0.1450486446093819
0.8330126722352134	0.9164327490106672	0.1450489687484833
0.0834572581237296	0.4165427198762686	0.1452131951888092
0.0834284900581892	0.9164336474636841	0.1450492897256623
0.5835662935363146	0.4165714879418090	0.1450492897256623
0.5834572317584303	0.9165427092415683	0.1451078551227525
0.0834564487745837	0.1669077252703701	0.1452145309818320

0.0834300773982903	0.6669910984471770	0.1450486446093819
0.5834574232258234	0.1669085930131189	0.1451066199353903
0.5835672509893328	0.6669873277647866	0.1450489687484833
0.1670122114426107	0.0836470542652634	0.2172869122777286
0.1669996784385219	0.5833458090207415	0.2172858901192782
0.6669254206733015	0.0834597861742381	0.2172244016201077
0.6666432510903633	0.5833148574746048	0.2172255328866513
0.4165432652405627	0.0834567207594361	0.2172239342490769
0.4163516937061971	0.5833495464785159	0.2172861325763620
0.9166504535214841	0.0836482922938018	0.2172861325763620
0.9166902695169057	0.5833097304830943	0.2172267878798451
0.4163529317347354	0.3329878035573870	0.2172869122777286
0.4165401998257607	0.8330745793266985	0.2172244016201077
0.9166541909792585	0.3330003365614758	0.2172858901192782
0.9166851425253952	0.8333567489096367	0.2172255328866513
0.0006625042214878	0.2503328508106151	0.2899234785878306
0.0009943795936493	0.7504834353336491	0.2888547153609053
0.5008255055983710	0.2502892974332411	0.2887927417645813
0.5008153723475104	0.7505186037107308	0.2887911985466616
0.2496727691263629	0.2503272158736394	0.2899200883998461
0.2497053249650349	0.7505098403953028	0.2887926077038969
0.7494901006047030	0.2502946600349674	0.2887926077038969
0.7495076124547708	0.7504923285452350	0.2888542547801052
0.2496671491893849	0.4993374887785080	0.2899234785878306
0.2497107025667589	0.9991744944016290	0.2887927417645813
0.7495165646663509	0.4990056134063465	0.2888547153609053
0.7494813962892692	0.9991846276524896	0.2887911985466616
0.1666678644409814	0.3333321655590211	0.3235403276261124

Pure-Ni 111 Facet with Hydrogen supercell 2X2X1 - [Etot = -417.97240235 eV]

1.01798110552312

10.0268001556000002	0.0000000000000000	0.0000000000000000
-5.0134000778000001	8.6834636535000005	0.0000000000000000

0.0000000000000000 0.0000000000000000 28.1868000031000001

Ni H

80 1

Direct

0.1666650029999985 0.3333350119999992 0.0000000000000000
0.1666650029999985 0.8333350420000016 0.0000000000000000
0.6666650180000033 0.3333350119999992 0.0000000000000000
0.6666650180000033 0.8333350420000016 0.0000000000000000
0.0000000000000000 0.0000000000000000 0.0726099979999972
0.0000000000000000 0.5000000000000000 0.0726099979999972
0.5000000000000000 0.0000000000000000 0.0726099979999972
0.5000000000000000 0.5000000000000000 0.0726099979999972
0.3332639878454131 0.1667360261545809 0.1419733819454123
0.3332706696180807 0.6665296013936697 0.1419744409170178
0.8334704576063316 0.1667293443819133 0.1419744409170178
0.8333352476911884 0.6666648113088129 0.1420391838918675
0.1666749455429297 0.3333250844570728 0.2112713596132210
0.1666415572883935 0.8333133988722281 0.2116682136789336
0.6666866011277719 0.3333584727116090 0.2116682136789336
0.6666835407618379 0.8333164592381621 0.2116645909751327
0.9987853894056045 0.5012146065943952 0.2800487530449516
0.9987960408857575 0.9975643051865006 0.2800385165218344
0.5024356948134994 0.5012039551142422 0.2800385165218344
0.5000044546927569 0.9999955453072431 0.2801793779852133
0.1666650029999985 0.0833349970000015 0.0000000000000000
0.1666650029999985 0.5833349819999967 0.0000000000000000
0.6666650180000033 0.0833349970000015 0.0000000000000000
0.6666650180000033 0.5833349819999967 0.0000000000000000
0.4166649880000008 0.0833349970000015 0.0000000000000000
0.4166649880000008 0.5833349819999967 0.0000000000000000
0.9166649579999984 0.0833349970000015 0.0000000000000000
0.9166649579999984 0.5833349819999967 0.0000000000000000
0.4166649880000008 0.3333350119999992 0.0000000000000000

0.4166649880000008	0.8333350420000016	0.0000000000000000
0.9166649579999984	0.3333350119999992	0.0000000000000000
0.9166649579999984	0.8333350420000016	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0726099979999972
0.0000000000000000	0.7500000000000000	0.0726099979999972
0.5000000000000000	0.2500000000000000	0.0726099979999972
0.5000000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.2500000000000000	0.0726099979999972
0.2500000000000000	0.7500000000000000	0.0726099979999972
0.7500000000000000	0.2500000000000000	0.0726099979999972
0.7500000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.0000000000000000	0.0726099979999972
0.2500000000000000	0.5000000000000000	0.0726099979999972
0.7500000000000000	0.0000000000000000	0.0726099979999972
0.7500000000000000	0.5000000000000000	0.0726099979999972
0.3335179425858001	0.4167614614678925	0.1419614435188734
0.3333074053447618	0.9166497482758516	0.1419647087841227
0.8331695178680434	0.4165893927489321	0.1419509688911162
0.8331546259635871	0.9165661858985743	0.1419444932317120
0.0832410144976947	0.4167589635023035	0.1419635136221657
0.0834066775429605	0.9165622395397151	0.1419485458255494
0.5834377014602836	0.4165933004570377	0.1419485458255494
0.5833448898023832	0.9166550511976155	0.1419607776237015
0.0832385085321121	0.1664820574141999	0.1419614435188734
0.0834105772510725	0.6668304821319566	0.1419509688911162
0.5833502517241484	0.1666925946552382	0.1419647087841227
0.5834338141014257	0.6668453740364129	0.1419444932317120
0.1669281098317796	0.0838161489953393	0.2117150597377346
0.1669378948729019	0.5831003425046362	0.2117200847517822
0.6668093095939369	0.0833935234222025	0.2116236541844572
0.6664859574217559	0.5832455635703937	0.2116284353925124
0.4166032875295045	0.0833966984704944	0.2116241326880299
0.4161897539370827	0.5831029576088227	0.2117144139364058

0.9168970423911773	0.0838102320629162	0.2117144139364058
0.9167604372167162	0.5832395627832838	0.2116326659841050
0.4161838370046596	0.3330719051682181	0.2117150597377346
0.4166064625777963	0.8331906904060631	0.2116236541844572
0.9168996574953638	0.3330621201270958	0.2117200847517822
0.9167544364296063	0.8335140425782441	0.2116284353925124
0.9998282429788716	0.2498975461831847	0.2812232031397386
0.0001535457765556	0.7500753330413232	0.2801641635868251
0.4997571732709361	0.2497113999541867	0.2800879386925246
0.4997697983778124	0.7500327160476701	0.2800877273041138
0.2500979833648884	0.2499020016351139	0.2812236781313260
0.2502802647042870	0.7500396605716517	0.2800914657031228
0.7499602804283541	0.2497197202957153	0.2800914657031228
0.7499308460383958	0.7500690949616100	0.2801622436918052
0.2501024538168153	0.5001717500211242	0.2812232031397386
0.2502886000458133	0.0002428267290639	0.2800879386925246
0.7499246669586768	0.4998464472234403	0.2801641635868251
0.7499672839523299	0.0002302016221876	0.2800877273041138
0.1666730935151648	0.3333269364848377	0.3114365579502447

NiCu (25% Cu) 111 Facet with Hydrogen supercell 2X2X1 - [Etot = -384.89628749 eV]

0.998485100048875

10.0268001556000002	0.0000000000000000	0.0000000000000000
-5.0134000778000001	8.6834636535000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.1868000031000001

Cu Ni H

20 60 1

Direct

0.1666650029999985	0.3333350119999992	0.0000000000000000
0.1666650029999985	0.8333350420000016	0.0000000000000000
0.6666650180000033	0.3333350119999992	0.0000000000000000
0.6666650180000033	0.8333350420000016	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0726099979999972

0.0000000000000000	0.5000000000000000	0.0726099979999972
0.5000000000000000	0.0000000000000000	0.0726099979999972
0.5000000000000000	0.5000000000000000	0.0726099979999972
0.3333105765030737	0.1666894374969203	0.1456140221127100
0.3333231344815459	0.6666189152926165	0.1456090335055578
0.8333811437073848	0.1666768795184481	0.1456090335055578
0.8333308162382522	0.6666692427617491	0.1457040555273252
0.1666593572402846	0.3333406727597179	0.2174824367266055
0.1665724311383983	0.8332609310511145	0.2171561364583354
0.6667390689488855	0.3334275988616042	0.2171561364583354
0.6667163916429359	0.8332836083570641	0.2171640607083205
0.9994652900400283	0.5005347059599714	0.2927948960501894
0.9994697926158480	0.9989337915095433	0.2927931707191505
0.5010662084904567	0.5005302033841517	0.2927931707191505
0.5000077818701882	0.9999922181298118	0.2928920389614618
0.1666650029999985	0.0833349970000015	0.0000000000000000
0.1666650029999985	0.5833349819999967	0.0000000000000000
0.6666650180000033	0.0833349970000015	0.0000000000000000
0.6666650180000033	0.5833349819999967	0.0000000000000000
0.4166649880000008	0.0833349970000015	0.0000000000000000
0.4166649880000008	0.5833349819999967	0.0000000000000000
0.9166649579999984	0.0833349970000015	0.0000000000000000
0.9166649579999984	0.5833349819999967	0.0000000000000000
0.4166649880000008	0.3333350119999992	0.0000000000000000
0.4166649880000008	0.8333350420000016	0.0000000000000000
0.9166649579999984	0.3333350119999992	0.0000000000000000
0.9166649579999984	0.8333350420000016	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0726099979999972
0.0000000000000000	0.7500000000000000	0.0726099979999972
0.5000000000000000	0.2500000000000000	0.0726099979999972
0.5000000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.2500000000000000	0.0726099979999972
0.2500000000000000	0.7500000000000000	0.0726099979999972

0.7500000000000000	0.2500000000000000	0.0726099979999972
0.7500000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.0000000000000000	0.0726099979999972
0.2500000000000000	0.5000000000000000	0.0726099979999972
0.7500000000000000	0.0000000000000000	0.0726099979999972
0.7500000000000000	0.5000000000000000	0.0726099979999972
0.3336299803663181	0.4168075703957399	0.1453030526238379
0.3336277313407408	0.9168083828906930	0.1451454683873479
0.8335507504304687	0.4167801179657502	0.1451665390131183
0.8335358053024677	0.9167560400938228	0.1451642136069538
0.0831949933844101	0.4168049846155881	0.1453090505600230
0.0832160054467579	0.9167637867353875	0.1451627983097765
0.5832361542646112	0.4167839725532403	0.1451627983097765
0.5831967566072009	0.9168031843927977	0.1451475134953881
0.0831923996042647	0.1663700196336819	0.1453030526238379
0.0832198520342544	0.6664492495695313	0.1451665390131183
0.5831916171093070	0.1663722686592592	0.1451454683873479
0.5832439599061772	0.6664641946975323	0.1451642136069538
0.1658474663464986	0.0829870866989282	0.2184086438597888
0.1658433350039559	0.5828462814723352	0.2184048545338868
0.6656737629700373	0.0828423368906996	0.2182969842190232
0.6655476176741644	0.5827605169523054	0.2184260890547591
0.4171760910860698	0.0828238949139291	0.2182959397558761
0.4169957515375060	0.5828396722498752	0.2184099964446773
0.9171603277501248	0.0830042344624928	0.2184099964446773
0.9172404738882776	0.5827595261117224	0.2184188924452855
0.4170128993010707	0.3341525486534991	0.2184086438597888
0.4171576491092992	0.8343262370299627	0.2182969842190232
0.9171537185276648	0.3341566799960418	0.2184048545338868
0.9172394830476946	0.8344523823258356	0.2184260890547591
0.9983079737992426	0.2491442377544146	0.2903753895728300
0.9997321571174425	0.7498585883848463	0.2891586400653736
0.4993538645963298	0.2494295701898182	0.2889463208112204

0.4993431758980762	0.7499088520806509	0.2889530064421564
0.2508644631395427	0.2491355218604596	0.2903701404162575
0.2505714306498703	0.7499128513158340	0.2889508480605016
0.7500870896841718	0.2494285543501320	0.2889508480605016
0.7501405507288581	0.7498593902711477	0.2891620768015670
0.2508557622455854	0.5016920192007532	0.2903753895728300
0.2505704298101818	0.0006461354036702	0.2889463208112204
0.7501414116151537	0.5002678358825534	0.2891586400653736
0.7500911479193491	0.0006568241019238	0.2889530064421564
0.1666768238361058	0.3333232061638967	0.3213602494994845

NiZn (25% Zn) 111 Facet with Hydrogen supercell 2X2X1 - [Etot = -348.72763126 eV]

1.01038006037737

10.0268001556000002	0.0000000000000000	0.0000000000000000
-5.0134000778000001	8.6834636535000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.1868000031000001

Zn Ni H

20 60 1

Direct

0.1666650029999985	0.3333350119999992	0.0000000000000000
0.1666650029999985	0.8333350420000016	0.0000000000000000
0.6666650180000033	0.3333350119999992	0.0000000000000000
0.6666650180000033	0.8333350420000016	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0726099979999972
0.0000000000000000	0.5000000000000000	0.0726099979999972
0.5000000000000000	0.0000000000000000	0.0726099979999972
0.5000000000000000	0.5000000000000000	0.0726099979999972
0.3332348911438601	0.1667651228561340	0.1454027874876189
0.3332362967914406	0.6664653902690745	0.1454036857226129
0.8335346687309269	0.1667637172085534	0.1454036857226129
0.8333348627560824	0.6666651962439190	0.1454378125422053
0.1666693874681684	0.3333306425318341	0.2171878407534962
0.1664946304815587	0.8332430455072100	0.2161576862551726

0.6667569544927900	0.3335053995184438	0.2161576862551726
0.6667554092989647	0.8332445907010353	0.2161581955298928
0.9998594532101137	0.5001405427898860	0.2938205966171950
0.9998607478266379	0.9997094493442802	0.2938192771689856
0.5002905506557198	0.5001392481733618	0.2938192771689856
0.5000039209114249	0.9999960790885751	0.2940961605235088
0.1666650029999985	0.0833349970000015	0.0000000000000000
0.1666650029999985	0.5833349819999967	0.0000000000000000
0.6666650180000033	0.0833349970000015	0.0000000000000000
0.6666650180000033	0.5833349819999967	0.0000000000000000
0.4166649880000008	0.0833349970000015	0.0000000000000000
0.4166649880000008	0.5833349819999967	0.0000000000000000
0.9166649579999984	0.0833349970000015	0.0000000000000000
0.9166649579999984	0.5833349819999967	0.0000000000000000
0.4166649880000008	0.3333350119999992	0.0000000000000000
0.4166649880000008	0.8333350420000016	0.0000000000000000
0.9166649579999984	0.3333350119999992	0.0000000000000000
0.9166649579999984	0.8333350420000016	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0726099979999972
0.0000000000000000	0.7500000000000000	0.0726099979999972
0.5000000000000000	0.2500000000000000	0.0726099979999972
0.5000000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.2500000000000000	0.0726099979999972
0.2500000000000000	0.7500000000000000	0.0726099979999972
0.7500000000000000	0.2500000000000000	0.0726099979999972
0.7500000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.0000000000000000	0.0726099979999972
0.2500000000000000	0.5000000000000000	0.0726099979999972
0.7500000000000000	0.0000000000000000	0.0726099979999972
0.7500000000000000	0.5000000000000000	0.0726099979999972
0.3333142957139543	0.4166563364331637	0.1449259920229053
0.3335228695596655	0.9167620497845022	0.1446508104879385
0.8336529900553060	0.4166664574406482	0.1446717213438831

0.8336486059224555	0.9169826676868809	0.1446720441718128
0.0833469623301966	0.4166530156698016	0.1449270615798284
0.0833325779898999	0.9169803456319343	0.1446720797828860
0.5830195953680644	0.4166674000100983	0.1446720797828860
0.5832361885389830	0.9167637524610157	0.1446507441551006
0.0833436335668409	0.1666857042860457	0.1449259920229053
0.0833335125593564	0.6663470099446940	0.1446717213438831
0.5832379502154978	0.1664771304403345	0.1446508104879385
0.5830173323131191	0.6663513940775445	0.1446720441718128
0.1647755166197129	0.0824346835306713	0.2177282504470384
0.1647745200126636	0.5823310584927128	0.2177300170448007
0.6645262180191267	0.0822598624366009	0.2174698086131457
0.6642084946874718	0.5821011140974122	0.2175444215417670
0.4177399026930146	0.0822600833069842	0.2174675664506225
0.4175661615379482	0.5823332102031031	0.2177295054585642
0.9176667897968969	0.0824338244620506	0.2177295054585642
0.9178975974500503	0.5821024025499497	0.2175438934050788
0.4175653024693275	0.3352244983802848	0.2177282504470384
0.4177401235633980	0.8354737819808733	0.2174698086131457
0.9176689415072872	0.3352254949873341	0.2177300170448007
0.9178988859025878	0.8357915053125282	0.2175444215417670
0.9985394121035895	0.2492651170926834	0.2894874899805089
0.9993809778024101	0.7496835673924451	0.2875113658056634
0.4987742913200677	0.2488251786509821	0.2872255752951958
0.4987727351882256	0.7499345727795301	0.2872272015814517
0.2507356976764754	0.2492642873235269	0.2894870141697439
0.2511763378019083	0.7499380154731696	0.2872273034085708
0.7500619255268361	0.2488236471980940	0.2872273034085708
0.7503158054047034	0.7496841355953023	0.2875125764940947
0.2507348829073166	0.5014605808964063	0.2894874899805089
0.2511748213490179	0.0012257086799323	0.2872255752951958
0.7503164326075549	0.5006190151975858	0.2875113658056634
0.7500654272204699	0.0012272648117744	0.2872272015814517

0.1666696102703824 0.3333304197296201 0.3196824235584614

Bare- NiSc (25% Sc) 200 Facet supercell 2X2X1 - [Etot = -236.96351133 eV]

1.04735280294076

7.0844001770000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.0844001770000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.0844993591000005

Sc Ni

12 28

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.1310425452973263
0.0000000000000000	0.5000000000000000	0.1310425452973263
0.5000000000000000	0.0000000000000000	0.1310425452973263
0.5000000000000000	0.5000000000000000	0.1310425452973263
0.0000000000000000	0.0000000000000000	0.2641528516798530
0.0000000000000000	0.5000000000000000	0.2641528516798530
0.5000000000000000	0.0000000000000000	0.2641528516798530
0.5000000000000000	0.5000000000000000	0.2641528516798530
0.2500000000000000	0.2500000000000000	0.0000000000000000
0.2500000000000000	0.7500000000000000	0.0000000000000000
0.7500000000000000	0.2500000000000000	0.0000000000000000
0.7500000000000000	0.7500000000000000	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0653899980000006
0.0000000000000000	0.7500000000000000	0.0653899980000006
0.5000000000000000	0.2500000000000000	0.0653899980000006
0.5000000000000000	0.7500000000000000	0.0653899980000006
0.2500000000000000	0.0000000000000000	0.0653899980000006
0.2500000000000000	0.5000000000000000	0.0653899980000006

0.7500000000000000	0.0000000000000000	0.0653899980000006
0.7500000000000000	0.5000000000000000	0.0653899980000006
0.2500000000000000	0.2500000000000000	0.1307262018750777
0.2500000000000000	0.7500000000000000	0.1307262018750777
0.7500000000000000	0.2500000000000000	0.1307262018750777
0.7500000000000000	0.7500000000000000	0.1307262018750777
0.0000000000000000	0.2500000000000000	0.1970729602766639
0.0000000000000000	0.7500000000000000	0.1970729602766639
0.5000000000000000	0.2500000000000000	0.1970729602766639
0.5000000000000000	0.7500000000000000	0.1970729602766639
0.2500000000000000	0.0000000000000000	0.1970729602766639
0.2500000000000000	0.5000000000000000	0.1970729602766639
0.7500000000000000	0.0000000000000000	0.1970729602766639
0.7500000000000000	0.5000000000000000	0.1970729602766639
0.2500000000000000	0.2500000000000000	0.2517333951720957
0.2500000000000000	0.7500000000000000	0.2517333951720957
0.7500000000000000	0.2500000000000000	0.2517333951720957
0.7500000000000000	0.7500000000000000	0.2517333951720957

Bare- NiTi (25% Ti) 200 Facet supercell 2X2X1 - [Etot = -251.89040363 eV]

1.01798110552312

7.0844001770000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.0844001770000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.0844993591000005

Ti Ni

12 28

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.1315154384329844
0.0000000000000000	0.5000000000000000	0.1315154384329844

0.5000000000000000	0.0000000000000000	0.1315154384329844
0.5000000000000000	0.5000000000000000	0.1315154384329844
0.0000000000000000	0.0000000000000000	0.2652791379492072
0.0000000000000000	0.5000000000000000	0.2652791379492072
0.5000000000000000	0.0000000000000000	0.2652791379492072
0.5000000000000000	0.5000000000000000	0.2652791379492072
0.2500000000000000	0.2500000000000000	0.0000000000000000
0.2500000000000000	0.7500000000000000	0.0000000000000000
0.7500000000000000	0.2500000000000000	0.0000000000000000
0.7500000000000000	0.7500000000000000	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0653899980000006
0.0000000000000000	0.7500000000000000	0.0653899980000006
0.5000000000000000	0.2500000000000000	0.0653899980000006
0.5000000000000000	0.7500000000000000	0.0653899980000006
0.2500000000000000	0.0000000000000000	0.0653899980000006
0.2500000000000000	0.5000000000000000	0.0653899980000006
0.7500000000000000	0.0000000000000000	0.0653899980000006
0.7500000000000000	0.5000000000000000	0.0653899980000006
0.2500000000000000	0.2500000000000000	0.1308958383395691
0.2500000000000000	0.7500000000000000	0.1308958383395691
0.7500000000000000	0.2500000000000000	0.1308958383395691
0.7500000000000000	0.7500000000000000	0.1308958383395691
0.0000000000000000	0.2500000000000000	0.1965421368997227
0.0000000000000000	0.7500000000000000	0.1965421368997227
0.5000000000000000	0.2500000000000000	0.1965421368997227
0.5000000000000000	0.7500000000000000	0.1965421368997227
0.2500000000000000	0.0000000000000000	0.1965421368997227
0.2500000000000000	0.5000000000000000	0.1965421368997227
0.7500000000000000	0.0000000000000000	0.1965421368997227
0.7500000000000000	0.5000000000000000	0.1965421368997227
0.2500000000000000	0.2500000000000000	0.2572113090435622
0.2500000000000000	0.7500000000000000	0.2572113090435622
0.7500000000000000	0.2500000000000000	0.2572113090435622

0.7500000000000000 0.7500000000000000 0.2572113090435622

Bare- NiV (25% V) 200 Facet supercell 2X2X1 - [Etot = -251.00618601 eV]

1.00458661266245

7.0844001770000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.0844001770000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.0844993591000005

V Ni

12 28

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.1307616103900031
0.0000000000000000	0.5000000000000000	0.1307616103900031
0.5000000000000000	0.0000000000000000	0.1307616103900031
0.5000000000000000	0.5000000000000000	0.1307616103900031
0.0000000000000000	0.0000000000000000	0.2646446537211702
0.0000000000000000	0.5000000000000000	0.2646446537211702
0.5000000000000000	0.0000000000000000	0.2646446537211702
0.5000000000000000	0.5000000000000000	0.2646446537211702
0.2500000000000000	0.2500000000000000	0.0000000000000000
0.2500000000000000	0.7500000000000000	0.0000000000000000
0.7500000000000000	0.2500000000000000	0.0000000000000000
0.7500000000000000	0.7500000000000000	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0653899980000006
0.0000000000000000	0.7500000000000000	0.0653899980000006
0.5000000000000000	0.2500000000000000	0.0653899980000006
0.5000000000000000	0.7500000000000000	0.0653899980000006
0.2500000000000000	0.0000000000000000	0.0653899980000006
0.2500000000000000	0.5000000000000000	0.0653899980000006
0.7500000000000000	0.0000000000000000	0.0653899980000006

0.7500000000000000	0.5000000000000000	0.0653899980000006
0.2500000000000000	0.2500000000000000	0.1306105587269855
0.2500000000000000	0.7500000000000000	0.1306105587269855
0.7500000000000000	0.2500000000000000	0.1306105587269855
0.7500000000000000	0.7500000000000000	0.1306105587269855
0.0000000000000000	0.2500000000000000	0.1956455907635402
0.0000000000000000	0.7500000000000000	0.1956455907635402
0.5000000000000000	0.2500000000000000	0.1956455907635402
0.5000000000000000	0.7500000000000000	0.1956455907635402
0.2500000000000000	0.0000000000000000	0.1956455907635402
0.2500000000000000	0.5000000000000000	0.1956455907635402
0.7500000000000000	0.0000000000000000	0.1956455907635402
0.7500000000000000	0.5000000000000000	0.1956455907635402
0.2500000000000000	0.2500000000000000	0.2574233840485647
0.2500000000000000	0.7500000000000000	0.2574233840485647
0.7500000000000000	0.2500000000000000	0.2574233840485647
0.7500000000000000	0.7500000000000000	0.2574233840485647

Bare- NiCr (25% Cr) 200 Facet supercell 2X2X1 - [Etot = -251.45606664 eV]

0.995572721824907

7.084400177000000	0.000000000000000	0.000000000000000
0.000000000000000	7.084400177000000	0.000000000000000
0.000000000000000	0.000000000000000	27.084499359100005

Cr Ni

12 28

Direct

0.000000000000000	0.000000000000000	0.000000000000000
0.000000000000000	0.500000000000000	0.000000000000000
0.500000000000000	0.000000000000000	0.000000000000000
0.500000000000000	0.500000000000000	0.000000000000000
0.000000000000000	0.000000000000000	0.1316542368568605
0.000000000000000	0.500000000000000	0.1316542368568605
0.500000000000000	0.000000000000000	0.1316542368568605

0.5000000000000000	0.5000000000000000	0.1316542368568605
0.0000000000000000	0.0000000000000000	0.2665245603646156
0.0000000000000000	0.5000000000000000	0.2665245603646156
0.5000000000000000	0.0000000000000000	0.2665245603646156
0.5000000000000000	0.5000000000000000	0.2665245603646156
0.2500000000000000	0.2500000000000000	0.0000000000000000
0.2500000000000000	0.7500000000000000	0.0000000000000000
0.7500000000000000	0.2500000000000000	0.0000000000000000
0.7500000000000000	0.7500000000000000	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0653899980000006
0.0000000000000000	0.7500000000000000	0.0653899980000006
0.5000000000000000	0.2500000000000000	0.0653899980000006
0.5000000000000000	0.7500000000000000	0.0653899980000006
0.2500000000000000	0.0000000000000000	0.0653899980000006
0.2500000000000000	0.5000000000000000	0.0653899980000006
0.7500000000000000	0.0000000000000000	0.0653899980000006
0.7500000000000000	0.5000000000000000	0.0653899980000006
0.2500000000000000	0.2500000000000000	0.1313944603006831
0.2500000000000000	0.7500000000000000	0.1313944603006831
0.7500000000000000	0.2500000000000000	0.1313944603006831
0.7500000000000000	0.7500000000000000	0.1313944603006831
0.0000000000000000	0.2500000000000000	0.1972560321995260
0.0000000000000000	0.7500000000000000	0.1972560321995260
0.5000000000000000	0.2500000000000000	0.1972560321995260
0.5000000000000000	0.7500000000000000	0.1972560321995260
0.2500000000000000	0.0000000000000000	0.1972560321995260
0.2500000000000000	0.5000000000000000	0.1972560321995260
0.7500000000000000	0.0000000000000000	0.1972560321995260
0.7500000000000000	0.5000000000000000	0.1972560321995260
0.2500000000000000	0.2500000000000000	0.2601018645656197
0.2500000000000000	0.7500000000000000	0.2601018645656197
0.7500000000000000	0.2500000000000000	0.2601018645656197
0.7500000000000000	0.7500000000000000	0.2601018645656197

Bare- NiMn (25% Mn) 200 Facet supercell 2X2X1 - [Etot = -251.85591824 eV]

0.989317187668226

7.084400177000000	0.000000000000000	0.000000000000000
0.000000000000000	7.084400177000000	0.000000000000000
0.000000000000000	0.000000000000000	27.084499359100005

Mn Ni

12 28

Direct

0.000000000000000	0.000000000000000	0.000000000000000
0.000000000000000	0.500000000000000	0.000000000000000
0.500000000000000	0.000000000000000	0.000000000000000
0.500000000000000	0.500000000000000	0.000000000000000
0.000000000000000	0.000000000000000	0.1337698263595968
0.000000000000000	0.500000000000000	0.1337698263595968
0.500000000000000	0.000000000000000	0.1337698263595968
0.500000000000000	0.500000000000000	0.1337698263595968
0.000000000000000	0.000000000000000	0.2715000394439571
0.000000000000000	0.500000000000000	0.2715000394439571
0.500000000000000	0.000000000000000	0.2715000394439571
0.500000000000000	0.500000000000000	0.2715000394439571
0.250000000000000	0.250000000000000	0.000000000000000
0.250000000000000	0.750000000000000	0.000000000000000
0.750000000000000	0.250000000000000	0.000000000000000
0.750000000000000	0.750000000000000	0.000000000000000
0.000000000000000	0.250000000000000	0.0653899980000006
0.000000000000000	0.750000000000000	0.0653899980000006
0.500000000000000	0.250000000000000	0.0653899980000006
0.500000000000000	0.750000000000000	0.0653899980000006
0.250000000000000	0.000000000000000	0.0653899980000006
0.250000000000000	0.500000000000000	0.0653899980000006
0.750000000000000	0.000000000000000	0.0653899980000006
0.750000000000000	0.500000000000000	0.0653899980000006

0.2500000000000000	0.2500000000000000	0.1334414099143828
0.2500000000000000	0.7500000000000000	0.1334414099143828
0.7500000000000000	0.2500000000000000	0.1334414099143828
0.7500000000000000	0.7500000000000000	0.1334414099143828
0.0000000000000000	0.2500000000000000	0.2015209686675448
0.0000000000000000	0.7500000000000000	0.2015209686675448
0.5000000000000000	0.2500000000000000	0.2015209686675448
0.5000000000000000	0.7500000000000000	0.2015209686675448
0.2500000000000000	0.0000000000000000	0.2015209686675448
0.2500000000000000	0.5000000000000000	0.2015209686675448
0.7500000000000000	0.0000000000000000	0.2015209686675448
0.7500000000000000	0.5000000000000000	0.2015209686675448
0.2500000000000000	0.2500000000000000	0.2656869777385040
0.2500000000000000	0.7500000000000000	0.2656869777385040
0.7500000000000000	0.2500000000000000	0.2656869777385040
0.7500000000000000	0.7500000000000000	0.2656869777385040

Bare- NiFe (25% Fe) 200 Facet supercell 2X2X1 - [Etot = -241.93424633 eV]

1.0000000000000000

7.0844001770000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.0844001770000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.0844993591000005

Fe Ni

12 28

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.1308150637505392
0.0000000000000000	0.5000000000000000	0.1308150637505392
0.5000000000000000	0.0000000000000000	0.1308150637505392
0.5000000000000000	0.5000000000000000	0.1308150637505392

0.0000000000000000	0.0000000000000000	0.2615715394668001
0.0000000000000000	0.5000000000000000	0.2615715394668001
0.5000000000000000	0.0000000000000000	0.2615715394668001
0.5000000000000000	0.5000000000000000	0.2615715394668001
0.2500000000000000	0.2500000000000000	0.0000000000000000
0.2500000000000000	0.7500000000000000	0.0000000000000000
0.7500000000000000	0.2500000000000000	0.0000000000000000
0.7500000000000000	0.7500000000000000	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0653899980000006
0.0000000000000000	0.7500000000000000	0.0653899980000006
0.5000000000000000	0.2500000000000000	0.0653899980000006
0.5000000000000000	0.7500000000000000	0.0653899980000006
0.2500000000000000	0.0000000000000000	0.0653899980000006
0.2500000000000000	0.5000000000000000	0.0653899980000006
0.7500000000000000	0.0000000000000000	0.0653899980000006
0.7500000000000000	0.5000000000000000	0.0653899980000006
0.2500000000000000	0.2500000000000000	0.1308036703203186
0.2500000000000000	0.7500000000000000	0.1308036703203186
0.7500000000000000	0.2500000000000000	0.1308036703203186
0.7500000000000000	0.7500000000000000	0.1308036703203186
0.0000000000000000	0.2500000000000000	0.1964348914370930
0.0000000000000000	0.7500000000000000	0.1964348914370930
0.5000000000000000	0.2500000000000000	0.1964348914370930
0.5000000000000000	0.7500000000000000	0.1964348914370930
0.2500000000000000	0.0000000000000000	0.1964348914370930
0.2500000000000000	0.5000000000000000	0.1964348914370930
0.7500000000000000	0.0000000000000000	0.1964348914370930
0.7500000000000000	0.5000000000000000	0.1964348914370930
0.2500000000000000	0.2500000000000000	0.2591798791499969
0.2500000000000000	0.7500000000000000	0.2591798791499969
0.7500000000000000	0.2500000000000000	0.2591798791499969
0.7500000000000000	0.7500000000000000	0.2591798791499969

Bare- NiCo (25% Co) 200 Facet supercell 2X2X1 - [Etot = -222.09981359 eV]

0.993794164815303

7.0844001770000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.0844001770000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.0844993591000005

Co Ni

12 28

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.1308311864820837
0.0000000000000000	0.5000000000000000	0.1308311864820837
0.5000000000000000	0.0000000000000000	0.1308311864820837
0.5000000000000000	0.5000000000000000	0.1308311864820837
0.0000000000000000	0.0000000000000000	0.2607322158043175
0.0000000000000000	0.5000000000000000	0.2607322158043175
0.5000000000000000	0.0000000000000000	0.2607322158043175
0.5000000000000000	0.5000000000000000	0.2607322158043175
0.2500000000000000	0.2500000000000000	0.0000000000000000
0.2500000000000000	0.7500000000000000	0.0000000000000000
0.7500000000000000	0.2500000000000000	0.0000000000000000
0.7500000000000000	0.7500000000000000	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0653899980000006
0.0000000000000000	0.7500000000000000	0.0653899980000006
0.5000000000000000	0.2500000000000000	0.0653899980000006
0.5000000000000000	0.7500000000000000	0.0653899980000006
0.2500000000000000	0.0000000000000000	0.0653899980000006
0.2500000000000000	0.5000000000000000	0.0653899980000006
0.7500000000000000	0.0000000000000000	0.0653899980000006
0.7500000000000000	0.5000000000000000	0.0653899980000006
0.2500000000000000	0.2500000000000000	0.1309176206376250

0.2500000000000000	0.7500000000000000	0.1309176206376250
0.7500000000000000	0.2500000000000000	0.1309176206376250
0.7500000000000000	0.7500000000000000	0.1309176206376250
0.0000000000000000	0.2500000000000000	0.1966978463506166
0.0000000000000000	0.7500000000000000	0.1966978463506166
0.5000000000000000	0.2500000000000000	0.1966978463506166
0.5000000000000000	0.7500000000000000	0.1966978463506166
0.2500000000000000	0.0000000000000000	0.1966978463506166
0.2500000000000000	0.5000000000000000	0.1966978463506166
0.7500000000000000	0.0000000000000000	0.1966978463506166
0.7500000000000000	0.5000000000000000	0.1966978463506166
0.2500000000000000	0.2500000000000000	0.2595134611992549
0.2500000000000000	0.7500000000000000	0.2595134611992549
0.7500000000000000	0.2500000000000000	0.2595134611992549
0.7500000000000000	0.7500000000000000	0.2595134611992549

Pure-Ni 200 Facet supercell 2X2X1 - [Etot = -203.61032669 eV]

1.01798110552312

7.0844001770000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.0844001770000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.0844993591000005

Ni

40

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.1273484974330827
0.0000000000000000	0.5000000000000000	0.1273484974330827
0.5000000000000000	0.0000000000000000	0.1273484974330827
0.5000000000000000	0.5000000000000000	0.1273484974330827
0.0000000000000000	0.0000000000000000	0.2492718720670695

0.0000000000000000	0.5000000000000000	0.2492718720670695
0.5000000000000000	0.0000000000000000	0.2492718720670695
0.5000000000000000	0.5000000000000000	0.2492718720670695
0.2500000000000000	0.2500000000000000	0.0000000000000000
0.2500000000000000	0.7500000000000000	0.0000000000000000
0.7500000000000000	0.2500000000000000	0.0000000000000000
0.7500000000000000	0.7500000000000000	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0653899980000006
0.0000000000000000	0.7500000000000000	0.0653899980000006
0.5000000000000000	0.2500000000000000	0.0653899980000006
0.5000000000000000	0.7500000000000000	0.0653899980000006
0.2500000000000000	0.0000000000000000	0.0653899980000006
0.2500000000000000	0.5000000000000000	0.0653899980000006
0.7500000000000000	0.0000000000000000	0.0653899980000006
0.7500000000000000	0.5000000000000000	0.0653899980000006
0.2500000000000000	0.2500000000000000	0.1273364080441439
0.2500000000000000	0.7500000000000000	0.1273364080441439
0.7500000000000000	0.2500000000000000	0.1273364080441439
0.7500000000000000	0.7500000000000000	0.1273364080441439
0.0000000000000000	0.2500000000000000	0.1899727533166100
0.0000000000000000	0.7500000000000000	0.1899727533166100
0.5000000000000000	0.2500000000000000	0.1899727533166100
0.5000000000000000	0.7500000000000000	0.1899727533166100
0.2500000000000000	0.0000000000000000	0.1899727533166100
0.2500000000000000	0.5000000000000000	0.1899727533166100
0.7500000000000000	0.0000000000000000	0.1899727533166100
0.7500000000000000	0.5000000000000000	0.1899727533166100
0.2500000000000000	0.2500000000000000	0.2492695932662272
0.2500000000000000	0.7500000000000000	0.2492695932662272
0.7500000000000000	0.2500000000000000	0.2492695932662272
0.7500000000000000	0.7500000000000000	0.2492695932662272

Bare- NiCu (25% Cu) 200 Facet supercell 2X2X1 - [Etot = -184.69603141 eV]

0.998485100048875

7.0844001770000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.0844001770000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.0844993591000005

Cu Ni

12 28

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.1313946536162192
0.0000000000000000	0.5000000000000000	0.1313946536162192
0.5000000000000000	0.0000000000000000	0.1313946536162192
0.5000000000000000	0.5000000000000000	0.1313946536162192
0.0000000000000000	0.0000000000000000	0.2634817293910956
0.0000000000000000	0.5000000000000000	0.2634817293910956
0.5000000000000000	0.0000000000000000	0.2634817293910956
0.5000000000000000	0.5000000000000000	0.2634817293910956
0.2500000000000000	0.2500000000000000	0.0000000000000000
0.2500000000000000	0.7500000000000000	0.0000000000000000
0.7500000000000000	0.2500000000000000	0.0000000000000000
0.7500000000000000	0.7500000000000000	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0653899980000006
0.0000000000000000	0.7500000000000000	0.0653899980000006
0.5000000000000000	0.2500000000000000	0.0653899980000006
0.5000000000000000	0.7500000000000000	0.0653899980000006
0.2500000000000000	0.0000000000000000	0.0653899980000006
0.2500000000000000	0.5000000000000000	0.0653899980000006
0.7500000000000000	0.0000000000000000	0.0653899980000006
0.7500000000000000	0.5000000000000000	0.0653899980000006
0.2500000000000000	0.2500000000000000	0.1311315066231558
0.2500000000000000	0.7500000000000000	0.1311315066231558

0.7500000000000000	0.2500000000000000	0.1311315066231558
0.7500000000000000	0.7500000000000000	0.1311315066231558
0.0000000000000000	0.2500000000000000	0.1975016266732936
0.0000000000000000	0.7500000000000000	0.1975016266732936
0.5000000000000000	0.2500000000000000	0.1975016266732936
0.5000000000000000	0.7500000000000000	0.1975016266732936
0.2500000000000000	0.0000000000000000	0.1975016266732936
0.2500000000000000	0.5000000000000000	0.1975016266732936
0.7500000000000000	0.0000000000000000	0.1975016266732936
0.7500000000000000	0.5000000000000000	0.1975016266732936
0.2500000000000000	0.2500000000000000	0.2590786018433775
0.2500000000000000	0.7500000000000000	0.2590786018433775
0.7500000000000000	0.2500000000000000	0.2590786018433775
0.7500000000000000	0.7500000000000000	0.2590786018433775

Bare- NiZn (25% Zn) 200 Facet supercell 2X2X1 - [Etot = -164.37259736 eV]

1.01038006037737

7.0844001770000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.0844001770000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.0844993591000005

Zn Ni

12 28

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.1309191281788173
0.0000000000000000	0.5000000000000000	0.1309191281788173
0.5000000000000000	0.0000000000000000	0.1309191281788173
0.5000000000000000	0.5000000000000000	0.1309191281788173
0.0000000000000000	0.0000000000000000	0.2638061277048536
0.0000000000000000	0.5000000000000000	0.2638061277048536

0.5000000000000000	0.0000000000000000	0.2638061277048536
0.5000000000000000	0.5000000000000000	0.2638061277048536
0.2500000000000000	0.2500000000000000	0.0000000000000000
0.2500000000000000	0.7500000000000000	0.0000000000000000
0.7500000000000000	0.2500000000000000	0.0000000000000000
0.7500000000000000	0.7500000000000000	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0653899980000006
0.0000000000000000	0.7500000000000000	0.0653899980000006
0.5000000000000000	0.2500000000000000	0.0653899980000006
0.5000000000000000	0.7500000000000000	0.0653899980000006
0.2500000000000000	0.0000000000000000	0.0653899980000006
0.2500000000000000	0.5000000000000000	0.0653899980000006
0.7500000000000000	0.0000000000000000	0.0653899980000006
0.7500000000000000	0.5000000000000000	0.0653899980000006
0.2500000000000000	0.2500000000000000	0.1308154385594236
0.2500000000000000	0.7500000000000000	0.1308154385594236
0.7500000000000000	0.2500000000000000	0.1308154385594236
0.7500000000000000	0.7500000000000000	0.1308154385594236
0.0000000000000000	0.2500000000000000	0.1964718969898058
0.0000000000000000	0.7500000000000000	0.1964718969898058
0.5000000000000000	0.2500000000000000	0.1964718969898058
0.5000000000000000	0.7500000000000000	0.1964718969898058
0.2500000000000000	0.0000000000000000	0.1964718969898058
0.2500000000000000	0.5000000000000000	0.1964718969898058
0.7500000000000000	0.0000000000000000	0.1964718969898058
0.7500000000000000	0.5000000000000000	0.1964718969898058
0.2500000000000000	0.2500000000000000	0.2571356678845973
0.2500000000000000	0.7500000000000000	0.2571356678845973
0.7500000000000000	0.2500000000000000	0.2571356678845973
0.7500000000000000	0.7500000000000000	0.2571356678845973

NiSc (25% Sc) 200 Facet with Hydrogen supercell 2X2X1 - [Etot = -240.78858450 eV]

1.04735280294076

7.0844001770000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.0844001770000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.0844993591000005

Sc	Ni	H
12	28	1

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0000000000000000
0.0016091787463424	0.0000000000000000	0.1313379994056305
0.0003376704753961	0.5000000000000000	0.1306523607905135
0.4983908212536576	0.0000000000000000	0.1313379994056305
0.4996623295246039	0.5000000000000000	0.1306523607905135
0.9998088645627732	0.0000000000000000	0.2651101251143402
0.9850692932660365	0.5000000000000000	0.2627544774729529
0.5001911354372268	0.0000000000000000	0.2651101251143402
0.5149307067339635	0.5000000000000000	0.2627544774729529
0.2500000000000000	0.2500000000000000	0.0000000000000000
0.2500000000000000	0.7500000000000000	0.0000000000000000
0.7500000000000000	0.2500000000000000	0.0000000000000000
0.7500000000000000	0.7500000000000000	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0653899980000006
0.0000000000000000	0.7500000000000000	0.0653899980000006
0.5000000000000000	0.2500000000000000	0.0653899980000006
0.5000000000000000	0.7500000000000000	0.0653899980000006
0.2500000000000000	0.0000000000000000	0.0653899980000006
0.2500000000000000	0.5000000000000000	0.0653899980000006
0.7500000000000000	0.0000000000000000	0.0653899980000006
0.7500000000000000	0.5000000000000000	0.0653899980000006
0.2500000000000000	0.2488108924304200	0.1310670968474668

0.2500000000000000	0.7511891075695800	0.1310670968474668
0.7500000000000000	0.2497644293727248	0.1308376001053659
0.7500000000000000	0.7502355706272752	0.1308376001053659
0.0051308219809627	0.2479422922009675	0.1973433028359750
0.0051308219809627	0.7520577077990325	0.1973433028359750
0.4948691780190373	0.2479422922009675	0.1973433028359750
0.4948691780190373	0.7520577077990325	0.1973433028359750
0.2500000000000000	0.0000000000000000	0.2019067938619656
0.2500000000000000	0.5000000000000000	0.1950251988459044
0.7500000000000000	0.0000000000000000	0.1962600347438723
0.7500000000000000	0.5000000000000000	0.1952727140360793
0.2500000000000000	0.2671492698165849	0.2563177523350220
0.2500000000000000	0.7328507301834151	0.2563177523350220
0.7500000000000000	0.2457166756196898	0.2501497701870363
0.7500000000000000	0.7542833243803031	0.2501497701870363
0.2500000000000000	0.5000000000000000	0.2864900394577319

NiTi (25% Ti) 200 Facet with Hydrogen supercell 2X2X1 - [Etot = -255.84437464 eV]

1.01798110552312

7.0844001770000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.0844001770000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.0844993591000005

Ti Ni H

12 28 1

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0000000000000000
0.0001441113916343	0.0000000000000000	0.1315998410575432
0.0008823657244861	0.5000000000000000	0.1313323039741050
0.4998558886083657	0.0000000000000000	0.1315998410575432
0.4991176342755139	0.5000000000000000	0.1313323039741050

0.9971802769557385	0.0000000000000000	0.2653735189097475
0.9900400970156014	0.5000000000000000	0.2658017118630767
0.5028197230442615	0.0000000000000000	0.2653735189097475
0.5099599029843986	0.5000000000000000	0.2658017118630767
0.2500000000000000	0.2500000000000000	0.0000000000000000
0.2500000000000000	0.7500000000000000	0.0000000000000000
0.7500000000000000	0.2500000000000000	0.0000000000000000
0.7500000000000000	0.7500000000000000	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0653899980000006
0.0000000000000000	0.7500000000000000	0.0653899980000006
0.5000000000000000	0.2500000000000000	0.0653899980000006
0.5000000000000000	0.7500000000000000	0.0653899980000006
0.2500000000000000	0.0000000000000000	0.0653899980000006
0.2500000000000000	0.5000000000000000	0.0653899980000006
0.7500000000000000	0.0000000000000000	0.0653899980000006
0.7500000000000000	0.5000000000000000	0.0653899980000006
0.2500000000000000	0.2474992812884338	0.1308455381700355
0.2500000000000000	0.7525007187115662	0.1308455381700355
0.7500000000000000	0.2494531016306212	0.1307552263231457
0.7500000000000000	0.7505468983693788	0.1307552263231457
0.0012580143739314	0.2500503922262283	0.1965967146531398
0.0012580143739314	0.7499496077737717	0.1965967146531398
0.4987419856260686	0.2500503922262283	0.1965967146531398
0.4987419856260686	0.7499496077737717	0.1965967146531398
0.2500000000000000	0.0000000000000000	0.1993689385340573
0.2500000000000000	0.5000000000000000	0.1946565508451386
0.7500000000000000	0.0000000000000000	0.1964335518941951
0.7500000000000000	0.5000000000000000	0.1957218101378544
0.2500000000000000	0.2584151963453110	0.2584037982308161
0.2500000000000000	0.7415848036546890	0.2584037982308161
0.7500000000000000	0.2487832182609111	0.2567471768319862
0.7500000000000000	0.7512167817390889	0.2567471768319862
0.2500000000000000	0.5000000000000000	0.2931192133187110

NiV (25% V) 200 Facet with Hydrogen supercell 2X2X1 - [Etot = -254.93709013 eV]

1.00458661266245

7.0844001770000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.0844001770000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.0844993591000005

V Ni H

12 28 1

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0000000000000000
0.9998490527311013	0.0000000000000000	0.1311381563295657
0.0010829175454232	0.5000000000000000	0.1303879127343038
0.5001509472688987	0.0000000000000000	0.1311381563295657
0.4989170824545768	0.5000000000000000	0.1303879127343038
0.9988293703108050	0.0000000000000000	0.2665860399788850
0.9882027800577708	0.5000000000000000	0.2632843509380009
0.5011706296891950	0.0000000000000000	0.2665860399788850
0.5117972199422292	0.5000000000000000	0.2632843509380009
0.2500000000000000	0.2500000000000000	0.0000000000000000
0.2500000000000000	0.7500000000000000	0.0000000000000000
0.7500000000000000	0.2500000000000000	0.0000000000000000
0.7500000000000000	0.7500000000000000	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0653899980000006
0.0000000000000000	0.7500000000000000	0.0653899980000006
0.5000000000000000	0.2500000000000000	0.0653899980000006
0.5000000000000000	0.7500000000000000	0.0653899980000006
0.2500000000000000	0.0000000000000000	0.0653899980000006
0.2500000000000000	0.5000000000000000	0.0653899980000006
0.7500000000000000	0.0000000000000000	0.0653899980000006
0.7500000000000000	0.5000000000000000	0.0653899980000006

0.2500000000000000	0.2474090423402372	0.1307115094433896
0.2500000000000000	0.7525909576597628	0.1307115094433896
0.7500000000000000	0.2500667740410061	0.1304624519540939
0.7500000000000000	0.7499332259589939	0.1304624519540939
0.0009335191450757	0.2511263336308193	0.1958412419630592
0.0009335191450757	0.7488736663691806	0.1958412419630592
0.4990664808549243	0.2511263336308193	0.1958412419630592
0.4990664808549243	0.7488736663691806	0.1958412419630592
0.2500000000000000	0.0000000000000000	0.1981240886681312
0.2500000000000000	0.5000000000000000	0.1935824112348378
0.7500000000000000	0.0000000000000000	0.1956842971509593
0.7500000000000000	0.5000000000000000	0.1947357799873966
0.2500000000000000	0.2646884412482983	0.2590210888074200
0.2500000000000000	0.7353115587517017	0.2590210888074200
0.7500000000000000	0.2540605269208074	0.2571960151590738
0.7500000000000000	0.7459394730791926	0.2571960151590738
0.2500000000000000	0.5000000000000000	0.2903472485069310

NiCr (25% Cr) 200 Facet with Hydrogen supercell 2X2X1 - [Etot = -255.31348045 eV]

0.995572721824907

7.0844001770000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.0844001770000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.0844993591000005

Cr	Ni	H
12	28	1

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0000000000000000
0.0001715766318071	0.0000000000000000	0.1319319470664766
0.0003421871412357	0.5000000000000000	0.1314664112261568
0.4998284233681929	0.0000000000000000	0.1319319470664766

0.4996578128587643	0.5000000000000000	0.1314664112261568
0.0040976499224783	0.0000000000000000	0.2672723424733974
0.9901252587747251	0.5000000000000000	0.2654401605829335
0.4959023500775217	0.0000000000000000	0.2672723424733974
0.5098747412252749	0.5000000000000000	0.2654401605829335
0.2500000000000000	0.2500000000000000	0.0000000000000000
0.2500000000000000	0.7500000000000000	0.0000000000000000
0.7500000000000000	0.2500000000000000	0.0000000000000000
0.7500000000000000	0.7500000000000000	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0653899980000006
0.0000000000000000	0.7500000000000000	0.0653899980000006
0.5000000000000000	0.2500000000000000	0.0653899980000006
0.5000000000000000	0.7500000000000000	0.0653899980000006
0.2500000000000000	0.0000000000000000	0.0653899980000006
0.2500000000000000	0.5000000000000000	0.0653899980000006
0.7500000000000000	0.0000000000000000	0.0653899980000006
0.7500000000000000	0.5000000000000000	0.0653899980000006
0.2500000000000000	0.2476631737280712	0.1315409169063386
0.2500000000000000	0.7523368262719288	0.1315409169063386
0.7500000000000000	0.2497411181067548	0.1313397641835223
0.7500000000000000	0.7502588818932452	0.1313397641835223
0.0008899822320032	0.2492856612810996	0.1973705234001102
0.0008899822320032	0.7507143387189004	0.1973705234001102
0.4991100177679968	0.2492856612810996	0.1973705234001102
0.4991100177679968	0.7507143387189004	0.1973705234001102
0.2500000000000000	0.0000000000000000	0.1996168834360788
0.2500000000000000	0.5000000000000000	0.1956202563177953
0.7500000000000000	0.0000000000000000	0.1972810748742901
0.7500000000000000	0.5000000000000000	0.1967321367462418
0.2500000000000000	0.2645518765444379	0.2625883911049698
0.2500000000000000	0.7354481234555621	0.2625883911049698
0.7500000000000000	0.2473382491084593	0.2600929459650203
0.7500000000000000	0.7526617508915407	0.2600929459650203

0.2500000000000000 0.5000000000000000 0.2922267405418069

NiMn (25% Mn) 200 Facet with Hydrogen supercell 2X2X1 - [Etot = -255.78286619 eV]

0.989317187668226

7.0844001770000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 7.0844001770000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 27.0844993591000005

Mn Ni H

12 28 1

Direct

0.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 0.5000000000000000 0.0000000000000000

0.5000000000000000 0.0000000000000000 0.0000000000000000

0.5000000000000000 0.5000000000000000 0.0000000000000000

0.0003409153738971 0.0000000000000000 0.1337964123432585

0.9994439969619222 0.5000000000000000 0.1335391377075368

0.4996590846261029 0.0000000000000000 0.1337964123432585

0.5005560030380778 0.5000000000000000 0.1335391377075368

0.0083993978765236 0.0000000000000000 0.2720131993878638

0.9862346758431286 0.5000000000000000 0.2710238020555806

0.4916006021234764 0.0000000000000000 0.2720131993878638

0.5137653241568714 0.5000000000000000 0.2710238020555806

0.2500000000000000 0.2500000000000000 0.0000000000000000

0.2500000000000000 0.7500000000000000 0.0000000000000000

0.7500000000000000 0.2500000000000000 0.0000000000000000

0.7500000000000000 0.7500000000000000 0.0000000000000000

0.0000000000000000 0.2500000000000000 0.0653899980000006

0.0000000000000000 0.7500000000000000 0.0653899980000006

0.5000000000000000 0.2500000000000000 0.0653899980000006

0.5000000000000000 0.7500000000000000 0.0653899980000006

0.2500000000000000 0.0000000000000000 0.0653899980000006

0.2500000000000000 0.5000000000000000 0.0653899980000006

0.7500000000000000 0.0000000000000000 0.0653899980000006

0.7500000000000000	0.5000000000000000	0.0653899980000006
0.2500000000000000	0.2489485287123685	0.1337286942735147
0.2500000000000000	0.7510514712876315	0.1337286942735147
0.7500000000000000	0.2499848175941182	0.1335413867027384
0.7500000000000000	0.7500151824058818	0.1335413867027384
0.0005248659334285	0.2494489225407719	0.2017030444059955
0.0005248659334285	0.7505510774592281	0.2017030444059955
0.4994751340665715	0.2494489225407719	0.2017030444059955
0.4994751340665715	0.7505510774592281	0.2017030444059955
0.2500000000000000	0.0000000000000000	0.2035668392344689
0.2500000000000000	0.5000000000000000	0.1997137574379835
0.7500000000000000	0.0000000000000000	0.2012708590508296
0.7500000000000000	0.5000000000000000	0.2016822831234535
0.2500000000000000	0.2660658602982693	0.2677252757176518
0.2500000000000000	0.7339341397017307	0.2677252757176518
0.7500000000000000	0.2416072234767626	0.2659172790091233
0.7500000000000000	0.7583927765232374	0.2659172790091233
0.2500000000000000	0.5000000000000000	0.2963711632285566

NiFe (25% Fe) 200 Facet with Hydrogen supercell 2X2X1 - [Etot = -245.73437388 eV]

1.0000000000000000

7.0844001770000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.0844001770000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.0844993591000005

Fe	Ni	H
12	28	1

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0000000000000000
0.9999690309503677	0.0000000000000000	0.1308514166296888
0.0004326928950249	0.5000000000000000	0.1307273921679695

0.5000309690496323	0.0000000000000000	0.1308514166296888
0.4995673071049751	0.5000000000000000	0.1307273921679695
0.0008615474166618	0.0000000000000000	0.2618950269538090
0.9921868605316320	0.5000000000000000	0.2620425289280135
0.4991384525833382	0.0000000000000000	0.2618950269538090
0.5078131394683680	0.5000000000000000	0.2620425289280135
0.2500000000000000	0.2500000000000000	0.0000000000000000
0.2500000000000000	0.7500000000000000	0.0000000000000000
0.7500000000000000	0.2500000000000000	0.0000000000000000
0.7500000000000000	0.7500000000000000	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0653899980000006
0.0000000000000000	0.7500000000000000	0.0653899980000006
0.5000000000000000	0.2500000000000000	0.0653899980000006
0.5000000000000000	0.7500000000000000	0.0653899980000006
0.2500000000000000	0.0000000000000000	0.0653899980000006
0.2500000000000000	0.5000000000000000	0.0653899980000006
0.7500000000000000	0.0000000000000000	0.0653899980000006
0.7500000000000000	0.5000000000000000	0.0653899980000006
0.2500000000000000	0.2480157250294255	0.1310126058480563
0.2500000000000000	0.7519842749705745	0.1310126058480563
0.7500000000000000	0.2502799401483102	0.1307496903515997
0.7500000000000000	0.7497200598516898	0.1307496903515997
0.0000992817120462	0.2495258346915818	0.1963645940657202
0.0000992817120462	0.7504741653084182	0.1963645940657202
0.4999007182879538	0.2495258346915818	0.1963645940657202
0.4999007182879538	0.7504741653084182	0.1963645940657202
0.2500000000000000	0.0000000000000000	0.1985086963111868
0.2500000000000000	0.5000000000000000	0.1947249800598669
0.7500000000000000	0.0000000000000000	0.1963884492786576
0.7500000000000000	0.5000000000000000	0.1963946454593142
0.2500000000000000	0.2592372883917662	0.2600950967125399
0.2500000000000000	0.7407627116082338	0.2600950967125399
0.7500000000000000	0.2474386332559959	0.2588080259965295

0.7500000000000000 0.7525613667440041 0.2588080259965295
 0.2500000000000000 0.5000000000000000 0.2860701421870431

NiCo (25% Co) 200 Facet with Hydrogen supercell 2X2X1 - [Etot = -225.89147144 eV]

0.993794164815303

7.0844001770000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 7.0844001770000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 27.0844993591000005

Co Ni H
 12 28 1

Direct

0.0000000000000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 0.5000000000000000 0.0000000000000000
 0.5000000000000000 0.0000000000000000 0.0000000000000000
 0.5000000000000000 0.5000000000000000 0.0000000000000000
 0.0003154867293418 0.0000000000000000 0.1308047203716285
 0.9997346727725898 0.5000000000000000 0.1308213465021026
 0.4996845132706582 0.0000000000000000 0.1308047203716285
 0.5002653272274102 0.5000000000000000 0.1308213465021026
 0.9996570629432853 0.0000000000000000 0.2607399767535412
 0.9967211359774808 0.5000000000000000 0.2610104871906813
 0.5003429370567147 0.0000000000000000 0.2607399767535412
 0.5032788640225192 0.5000000000000000 0.2610104871906813
 0.2500000000000000 0.2500000000000000 0.0000000000000000
 0.2500000000000000 0.7500000000000000 0.0000000000000000
 0.7500000000000000 0.2500000000000000 0.0000000000000000
 0.7500000000000000 0.7500000000000000 0.0000000000000000
 0.0000000000000000 0.2500000000000000 0.0653899980000006
 0.0000000000000000 0.7500000000000000 0.0653899980000006
 0.5000000000000000 0.2500000000000000 0.0653899980000006
 0.5000000000000000 0.7500000000000000 0.0653899980000006
 0.2500000000000000 0.0000000000000000 0.0653899980000006
 0.2500000000000000 0.5000000000000000 0.0653899980000006

0.7500000000000000	0.0000000000000000	0.0653899980000006
0.7500000000000000	0.5000000000000000	0.0653899980000006
0.2500000000000000	0.2489738538063762	0.1310511167932304
0.2500000000000000	0.7510261461936238	0.1310511167932304
0.7500000000000000	0.2501345160264563	0.1308437257185417
0.7500000000000000	0.7498654839735437	0.1308437257185417
0.9996417240616040	0.2492145784539588	0.1965189195360253
0.9996417240616040	0.7507854215460412	0.1965189195360253
0.5003582759383960	0.2492145784539588	0.1965189195360253
0.5003582759383960	0.7507854215460412	0.1965189195360253
0.2500000000000000	0.0000000000000000	0.1978788255492461
0.2500000000000000	0.5000000000000000	0.1952976516344620
0.7500000000000000	0.0000000000000000	0.1966066065040764
0.7500000000000000	0.5000000000000000	0.1966796562962330
0.2500000000000000	0.2550137526022596	0.2602528810655826
0.2500000000000000	0.7449862473977404	0.2602528810655826
0.7500000000000000	0.2491077141595710	0.2593415682170885
0.7500000000000000	0.7508922858404290	0.2593415682170885
0.2500000000000000	0.5000000000000000	0.2840314618722743

Pure-Ni 200 Facet with Hydrogen supercell 2X2X1 - [Etot = -207.47182141 eV]

1.01798110552312

7.0844001770000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.0844001770000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.0844993591000005

Ni H

40 1

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0000000000000000
0.0001994065359412	0.0000000000000000	0.1273332544966976

0.9994370797590264	0.5000000000000000	0.1273857577031023
0.4998005934640588	0.0000000000000000	0.1273332544966976
0.5005629202409736	0.5000000000000000	0.1273857577031023
0.9998312736033839	0.0000000000000000	0.2493631321842500
0.0020913230695001	0.5000000000000000	0.2498006864773501
0.5001687263966161	0.0000000000000000	0.2493631321842500
0.4979086769304999	0.5000000000000000	0.2498006864773501
0.2500000000000000	0.2500000000000000	0.0000000000000000
0.2500000000000000	0.7500000000000000	0.0000000000000000
0.7500000000000000	0.2500000000000000	0.0000000000000000
0.7500000000000000	0.7500000000000000	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0653899980000006
0.0000000000000000	0.7500000000000000	0.0653899980000006
0.5000000000000000	0.2500000000000000	0.0653899980000006
0.5000000000000000	0.7500000000000000	0.0653899980000006
0.2500000000000000	0.0000000000000000	0.0653899980000006
0.2500000000000000	0.5000000000000000	0.0653899980000006
0.7500000000000000	0.0000000000000000	0.0653899980000006
0.7500000000000000	0.5000000000000000	0.0653899980000006
0.2500000000000000	0.2495048766612271	0.1273475614240382
0.2500000000000000	0.7504951233387729	0.1273475614240382
0.7500000000000000	0.2500989833022587	0.1273515230800513
0.7500000000000000	0.7499010166977413	0.1273515230800513
0.9992200599083461	0.2490409550187138	0.1898180742216340
0.9992200599083461	0.7509590449812862	0.1898180742216340
0.5007799400916539	0.2490409550187138	0.1898180742216340
0.5007799400916539	0.7509590449812862	0.1898180742216340
0.2500000000000000	0.0000000000000000	0.1905202706700635
0.2500000000000000	0.5000000000000000	0.1886656489633651
0.7500000000000000	0.0000000000000000	0.1900858123873022
0.7500000000000000	0.5000000000000000	0.1905004123256191
0.2500000000000000	0.2520656948862765	0.2498723702779202
0.2500000000000000	0.7479343051137235	0.2498723702779202

0.7500000000000000 0.2498045618730771 0.2492453276029210
 0.7500000000000000 0.7501954381269229 0.2492453276029210
 0.2500000000000000 0.5000000000000000 0.2681206669428775

NiCu (25% Cu) 200 Facet with Hydrogen supercell 2X2X1 - [Etot = -188.52871626 eV]

0.998485100048875

7.0844001770000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 7.0844001770000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 27.0844993591000005

Cu Ni H
 12 28 1

Direct

0.0000000000000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 0.5000000000000000 0.0000000000000000
 0.5000000000000000 0.0000000000000000 0.0000000000000000
 0.5000000000000000 0.5000000000000000 0.0000000000000000
 0.0005930756671333 0.0000000000000000 0.1314505581818395
 0.9992541526533358 0.5000000000000000 0.1313235553635366
 0.4994069243328667 0.0000000000000000 0.1314505581818395
 0.5007458473466642 0.5000000000000000 0.1313235553635366
 0.0062199352298435 0.0000000000000000 0.2634557076304134
 0.9922859775202042 0.5000000000000000 0.2643065408250109
 0.4937800647701565 0.0000000000000000 0.2634557076304134
 0.5077140224797958 0.5000000000000000 0.2643065408250109
 0.2500000000000000 0.2500000000000000 0.0000000000000000
 0.2500000000000000 0.7500000000000000 0.0000000000000000
 0.7500000000000000 0.2500000000000000 0.0000000000000000
 0.7500000000000000 0.7500000000000000 0.0000000000000000
 0.0000000000000000 0.2500000000000000 0.0653899980000006
 0.0000000000000000 0.7500000000000000 0.0653899980000006
 0.5000000000000000 0.2500000000000000 0.0653899980000006
 0.5000000000000000 0.7500000000000000 0.0653899980000006
 0.2500000000000000 0.0000000000000000 0.0653899980000006

```

0.2500000000000000 0.5000000000000000 0.0653899980000006
0.7500000000000000 0.0000000000000000 0.0653899980000006
0.7500000000000000 0.5000000000000000 0.0653899980000006
0.2500000000000000 0.2492973518341728 0.1311515350055430
0.2500000000000000 0.7507026481658272 0.1311515350055430
0.7500000000000000 0.2499413824171626 0.1311237174759299
0.7500000000000000 0.7500586175828374 0.1311237174759299
0.9993329607583306 0.2495738317086875 0.1973269312481705
0.9993329607583306 0.7504261682913125 0.1973269312481705
0.5006670392416694 0.2495738317086875 0.1973269312481705
0.5006670392416694 0.7504261682913125 0.1973269312481705
0.2500000000000000 0.0000000000000000 0.1983277118368960
0.2500000000000000 0.5000000000000000 0.1957781774549403
0.7500000000000000 0.0000000000000000 0.1972442701336732
0.7500000000000000 0.5000000000000000 0.1979200541390895
0.2500000000000000 0.2611865678164520 0.2600524423727890
0.2500000000000000 0.7388134321835480 0.2600524423727890
0.7500000000000000 0.2437443452131944 0.2589155549142887
0.7500000000000000 0.7562556547868056 0.2589155549142887
0.2500000000000000 0.5000000000000000 0.2828061749508493
    
```

NiZn (25% Zn) 200 Facet with Hydrogen supercell 2X2X1 - [Etot = -167.95033235 eV]

1.01038006037737

```

7.0844001770000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 7.0844001770000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 27.0844993591000005
    
```

```

Zn Ni H
12 28 1
    
```

Direct

```

0.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 0.5000000000000000 0.0000000000000000
0.5000000000000000 0.0000000000000000 0.0000000000000000
0.5000000000000000 0.5000000000000000 0.0000000000000000
    
```

0.0008317956540225	0.0000000000000000	0.1311716620071408
0.9988435035833021	0.5000000000000000	0.1306818115800823
0.4991682043459775	0.0000000000000000	0.1311716620071408
0.5011564964166979	0.5000000000000000	0.1306818115800823
0.0084788439591463	0.0000000000000000	0.2639284386616509
0.9814738819760080	0.5000000000000000	0.2642212404198077
0.4915211560408537	0.0000000000000000	0.2639284386616509
0.5185261180239920	0.5000000000000000	0.2642212404198077
0.2500000000000000	0.2500000000000000	0.0000000000000000
0.2500000000000000	0.7500000000000000	0.0000000000000000
0.7500000000000000	0.2500000000000000	0.0000000000000000
0.7500000000000000	0.7500000000000000	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0653899980000006
0.0000000000000000	0.7500000000000000	0.0653899980000006
0.5000000000000000	0.2500000000000000	0.0653899980000006
0.5000000000000000	0.7500000000000000	0.0653899980000006
0.2500000000000000	0.0000000000000000	0.0653899980000006
0.2500000000000000	0.5000000000000000	0.0653899980000006
0.7500000000000000	0.0000000000000000	0.0653899980000006
0.7500000000000000	0.5000000000000000	0.0653899980000006
0.2500000000000000	0.2482663742630820	0.1311060433408500
0.2500000000000000	0.7517336257369180	0.1311060433408500
0.7500000000000000	0.2497164683084776	0.1308855321619120
0.7500000000000000	0.7502835316915224	0.1308855321619120
0.0012671545617380	0.2499289586186038	0.1967063124089847
0.0012671545617380	0.7500710413813962	0.1967063124089847
0.4987328454382620	0.2499289586186038	0.1967063124089847
0.4987328454382620	0.7500710413813962	0.1967063124089847
0.2500000000000000	0.0000000000000000	0.1987774276113328
0.2500000000000000	0.5000000000000000	0.1937358354766161
0.7500000000000000	0.0000000000000000	0.1958664644789891
0.7500000000000000	0.5000000000000000	0.1963385359678682
0.2500000000000000	0.2741800188824186	0.2598735426082328

0.2500000000000000	0.7258199811175885	0.2598735426082328
0.7500000000000000	0.2399339803571792	0.2572786757811869
0.7500000000000000	0.7600660196428208	0.2572786757811869
0.2500000000000000	0.5000000000000000	0.2851581929793667

Bare- NiSc (25% Sc) 220 Facet supercell 2X2X1 - [Etot = -328.56112666 eV]

1.04735280294076

7.0900001526000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.0268001556000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.5200996398999997

Sc Ni

16 40

Direct

0.0000000000000000	0.2500000000000000	0.0000000000000000
0.0000000000000000	0.7500000000000000	0.0000000000000000
0.5000000000000000	0.2500000000000000	0.0000000000000000
0.5000000000000000	0.7500000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0910900009999978
0.0000000000000000	0.5000000000000000	0.0910900009999978
0.5000000000000000	0.0000000000000000	0.0910900009999978
0.5000000000000000	0.5000000000000000	0.0910900009999978
0.0000000000000000	0.2500000000000000	0.1802765203686718
0.0000000000000000	0.7500000000000000	0.1802765203686718
0.5000000000000000	0.2500000000000000	0.1802765203686718
0.5000000000000000	0.7500000000000000	0.1802765203686718
0.0000000000000000	0.0000000000000000	0.2729065180152475
0.0000000000000000	0.5000000000000000	0.2729065180152475
0.5000000000000000	0.0000000000000000	0.2729065180152475
0.5000000000000000	0.5000000000000000	0.2729065180152475
0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0000000000000000

0.5000000000000000	0.5000000000000000	0.0000000000000000
0.2500000000000000	0.1250000000000000	0.0455400009999991
0.2500000000000000	0.6250000000000000	0.0455400009999991
0.7500000000000000	0.1250000000000000	0.0455400009999991
0.7500000000000000	0.6250000000000000	0.0455400009999991
0.2500000000000000	0.3750000000000000	0.0455400009999991
0.2500000000000000	0.8750000000000000	0.0455400009999991
0.7500000000000000	0.3750000000000000	0.0455400009999991
0.7500000000000000	0.8750000000000000	0.0455400009999991
0.0000000000000000	0.2500000000000000	0.0889434874281392
0.0000000000000000	0.7500000000000000	0.0889434874281392
0.5000000000000000	0.2500000000000000	0.0889434874281392
0.5000000000000000	0.7500000000000000	0.0889434874281392
0.2500000000000000	0.3759440965842202	0.1365211495551222
0.2500000000000000	0.8759440665842249	0.1365211495551222
0.7500000000000000	0.3759440965842202	0.1365211495551222
0.7500000000000000	0.8759440665842249	0.1365211495551222
0.2500000000000000	0.1240559184157775	0.1365211495551222
0.2500000000000000	0.6240559334157751	0.1365211495551222
0.7500000000000000	0.1240559184157775	0.1365211495551222
0.7500000000000000	0.6240559334157751	0.1365211495551222
0.0000000000000000	0.0000000000000000	0.1839895729184775
0.0000000000000000	0.5000000000000000	0.1839895729184775
0.5000000000000000	0.0000000000000000	0.1839895729184775
0.5000000000000000	0.5000000000000000	0.1839895729184775
0.2500000000000000	0.1234679085232244	0.2294222682762310
0.2500000000000000	0.6234679015232274	0.2294222682762310
0.7500000000000000	0.1234679085232244	0.2294222682762310
0.7500000000000000	0.6234679015232274	0.2294222682762310
0.2500000000000000	0.3765320984767726	0.2294222682762310
0.2500000000000000	0.8765320984767726	0.2294222682762310
0.7500000000000000	0.3765320984767726	0.2294222682762310
0.7500000000000000	0.8765320984767726	0.2294222682762310

0.0000000000000000	0.2500000000000000	0.2661383550878469
0.0000000000000000	0.7500000000000000	0.2661383550878469
0.5000000000000000	0.2500000000000000	0.2661383550878469
0.5000000000000000	0.7500000000000000	0.2661383550878469

Bare- NiTi (25% Ti) 220 Facet supercell 2X2X1 - [Etot = -348.99973858 eV]

1.01798110552312

7.090000152600000	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.026800155600002	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.520099639899997

Ti Ni

16 40

Direct

0.0000000000000000	0.2500000000000000	0.0000000000000000
0.0000000000000000	0.7500000000000000	0.0000000000000000
0.5000000000000000	0.2500000000000000	0.0000000000000000
0.5000000000000000	0.7500000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0910900009999978
0.0000000000000000	0.5000000000000000	0.0910900009999978
0.5000000000000000	0.0000000000000000	0.0910900009999978
0.5000000000000000	0.5000000000000000	0.0910900009999978
0.0000000000000000	0.2500000000000000	0.1831708284496614
0.0000000000000000	0.7500000000000000	0.1831708284496614
0.5000000000000000	0.2500000000000000	0.1831708284496614
0.5000000000000000	0.7500000000000000	0.1831708284496614
0.0000000000000000	0.0000000000000000	0.2697017755456841
0.0000000000000000	0.5000000000000000	0.2697017755456841
0.5000000000000000	0.0000000000000000	0.2697017755456841
0.5000000000000000	0.5000000000000000	0.2697017755456841
0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0000000000000000

0.2500000000000000	0.1250000000000000	0.0455400009999991
0.2500000000000000	0.6250000000000000	0.0455400009999991
0.7500000000000000	0.1250000000000000	0.0455400009999991
0.7500000000000000	0.6250000000000000	0.0455400009999991
0.2500000000000000	0.3750000000000000	0.0455400009999991
0.2500000000000000	0.8750000000000000	0.0455400009999991
0.7500000000000000	0.3750000000000000	0.0455400009999991
0.7500000000000000	0.8750000000000000	0.0455400009999991
0.0000000000000000	0.2500000000000000	0.0903792668438257
0.0000000000000000	0.7500000000000000	0.0903792668438257
0.5000000000000000	0.2500000000000000	0.0903792668438257
0.5000000000000000	0.7500000000000000	0.0903792668438257
0.2500000000000000	0.3748598846929170	0.1374993947505772
0.2500000000000000	0.8748598546929216	0.1374993947505772
0.7500000000000000	0.3748598846929170	0.1374993947505772
0.7500000000000000	0.8748598546929216	0.1374993947505772
0.2500000000000000	0.1251401303070807	0.1374993947505772
0.2500000000000000	0.6251401453070784	0.1374993947505772
0.7500000000000000	0.1251401303070807	0.1374993947505772
0.7500000000000000	0.6251401453070784	0.1374993947505772
0.0000000000000000	0.0000000000000000	0.1837526080311775
0.0000000000000000	0.5000000000000000	0.1837526080311775
0.5000000000000000	0.0000000000000000	0.1837526080311775
0.5000000000000000	0.5000000000000000	0.1837526080311775
0.2500000000000000	0.1228231505927511	0.2307470259288493
0.2500000000000000	0.6228231435927540	0.2307470259288493
0.7500000000000000	0.1228231505927511	0.2307470259288493
0.7500000000000000	0.6228231435927540	0.2307470259288493
0.2500000000000000	0.3771768564072460	0.2307470259288493
0.2500000000000000	0.8771768564072460	0.2307470259288493
0.7500000000000000	0.3771768564072460	0.2307470259288493
0.7500000000000000	0.8771768564072460	0.2307470259288493
0.0000000000000000	0.2500000000000000	0.2685556921147807

0.0000000000000000	0.7500000000000000	0.2685556921147807
0.5000000000000000	0.2500000000000000	0.2685556921147807
0.5000000000000000	0.7500000000000000	0.2685556921147807

Bare- NiV (25% V) 220 Facet supercell 2X2X1 - [Etot = -349.55862889 eV]

1.00458661266245

7.090000152600000	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.026800155600002	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.520099639899997

V Ni

16 40

Direct

0.0000000000000000	0.2500000000000000	0.0000000000000000
0.0000000000000000	0.7500000000000000	0.0000000000000000
0.5000000000000000	0.2500000000000000	0.0000000000000000
0.5000000000000000	0.7500000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0910900009999978
0.0000000000000000	0.5000000000000000	0.0910900009999978
0.5000000000000000	0.0000000000000000	0.0910900009999978
0.5000000000000000	0.5000000000000000	0.0910900009999978
0.0000000000000000	0.2500000000000000	0.1849628740434994
0.0000000000000000	0.7500000000000000	0.1849628740434994
0.5000000000000000	0.2500000000000000	0.1849628740434994
0.5000000000000000	0.7500000000000000	0.1849628740434994
0.0000000000000000	0.0000000000000000	0.2737009002776603
0.0000000000000000	0.5000000000000000	0.2737009002776603
0.5000000000000000	0.0000000000000000	0.2737009002776603
0.5000000000000000	0.5000000000000000	0.2737009002776603
0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0000000000000000
0.2500000000000000	0.1250000000000000	0.0455400009999991

0.2500000000000000	0.6250000000000000	0.0455400009999991
0.7500000000000000	0.1250000000000000	0.0455400009999991
0.7500000000000000	0.6250000000000000	0.0455400009999991
0.2500000000000000	0.3750000000000000	0.0455400009999991
0.2500000000000000	0.8750000000000000	0.0455400009999991
0.7500000000000000	0.3750000000000000	0.0455400009999991
0.7500000000000000	0.8750000000000000	0.0455400009999991
0.0000000000000000	0.2500000000000000	0.0917572987542030
0.0000000000000000	0.7500000000000000	0.0917572987542030
0.5000000000000000	0.2500000000000000	0.0917572987542030
0.5000000000000000	0.7500000000000000	0.0917572987542030
0.2500000000000000	0.3747574008595507	0.1369035818241642
0.2500000000000000	0.8747573708595553	0.1369035818241642
0.7500000000000000	0.3747574008595507	0.1369035818241642
0.7500000000000000	0.8747573708595553	0.1369035818241642
0.2500000000000000	0.1252426141404470	0.1369035818241642
0.2500000000000000	0.6252426291404447	0.1369035818241642
0.7500000000000000	0.1252426141404470	0.1369035818241642
0.7500000000000000	0.6252426291404447	0.1369035818241642
0.0000000000000000	0.0000000000000000	0.1818867909250130
0.0000000000000000	0.5000000000000000	0.1818867909250130
0.5000000000000000	0.0000000000000000	0.1818867909250130
0.5000000000000000	0.5000000000000000	0.1818867909250130
0.2500000000000000	0.1228362047361884	0.2281365363762262
0.2500000000000000	0.6228361977361914	0.2281365363762262
0.7500000000000000	0.1228362047361884	0.2281365363762262
0.7500000000000000	0.6228361977361914	0.2281365363762262
0.2500000000000000	0.3771638022638086	0.2281365363762262
0.2500000000000000	0.8771638022638086	0.2281365363762262
0.7500000000000000	0.3771638022638086	0.2281365363762262
0.7500000000000000	0.8771638022638086	0.2281365363762262
0.0000000000000000	0.2500000000000000	0.2692632341875623
0.0000000000000000	0.7500000000000000	0.2692632341875623

0.5000000000000000 0.2500000000000000 0.2692632341875623

0.5000000000000000 0.7500000000000000 0.2692632341875623

Bare- NiCr (25% Cr) 220 Facet supercell 2X2X1 - [Etot = -349.74533449 eV]

0.995572721824907

7.090000152600000 0.0000000000000000 0.0000000000000000

0.0000000000000000 10.0268001556000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 27.5200996398999997

Cr Ni

16 40

Direct

0.0000000000000000 0.2500000000000000 0.0000000000000000

0.0000000000000000 0.7500000000000000 0.0000000000000000

0.5000000000000000 0.2500000000000000 0.0000000000000000

0.5000000000000000 0.7500000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 0.0910900009999978

0.0000000000000000 0.5000000000000000 0.0910900009999978

0.5000000000000000 0.0000000000000000 0.0910900009999978

0.5000000000000000 0.5000000000000000 0.0910900009999978

0.0000000000000000 0.2500000000000000 0.1846507157262849

0.0000000000000000 0.7500000000000000 0.1846507157262849

0.5000000000000000 0.2500000000000000 0.1846507157262849

0.5000000000000000 0.7500000000000000 0.1846507157262849

0.0000000000000000 0.0000000000000000 0.2758805127395618

0.0000000000000000 0.5000000000000000 0.2758805127395618

0.5000000000000000 0.0000000000000000 0.2758805127395618

0.5000000000000000 0.5000000000000000 0.2758805127395618

0.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 0.5000000000000000 0.0000000000000000

0.5000000000000000 0.0000000000000000 0.0000000000000000

0.5000000000000000 0.5000000000000000 0.0000000000000000

0.2500000000000000 0.1250000000000000 0.0455400009999991

0.2500000000000000 0.6250000000000000 0.0455400009999991

0.7500000000000000	0.1250000000000000	0.0455400009999991
0.7500000000000000	0.6250000000000000	0.0455400009999991
0.2500000000000000	0.3750000000000000	0.0455400009999991
0.2500000000000000	0.8750000000000000	0.0455400009999991
0.7500000000000000	0.3750000000000000	0.0455400009999991
0.7500000000000000	0.8750000000000000	0.0455400009999991
0.0000000000000000	0.2500000000000000	0.0929699409127238
0.0000000000000000	0.7500000000000000	0.0929699409127238
0.5000000000000000	0.2500000000000000	0.0929699409127238
0.5000000000000000	0.7500000000000000	0.0929699409127238
0.2500000000000000	0.3747388764608175	0.1376758883179932
0.2500000000000000	0.8747388464608221	0.1376758883179932
0.7500000000000000	0.3747388764608175	0.1376758883179932
0.7500000000000000	0.8747388464608221	0.1376758883179932
0.2500000000000000	0.1252611385391802	0.1376758883179932
0.2500000000000000	0.6252611535391779	0.1376758883179932
0.7500000000000000	0.1252611385391802	0.1376758883179932
0.7500000000000000	0.6252611535391779	0.1376758883179932
0.0000000000000000	0.0000000000000000	0.1822185402360219
0.0000000000000000	0.5000000000000000	0.1822185402360219
0.5000000000000000	0.0000000000000000	0.1822185402360219
0.5000000000000000	0.5000000000000000	0.1822185402360219
0.2500000000000000	0.1241268930125798	0.2296760538993894
0.2500000000000000	0.6241268860125828	0.2296760538993894
0.7500000000000000	0.1241268930125798	0.2296760538993894
0.7500000000000000	0.6241268860125828	0.2296760538993894
0.2500000000000000	0.3758731139874172	0.2296760538993894
0.2500000000000000	0.8758731139874172	0.2296760538993894
0.7500000000000000	0.3758731139874172	0.2296760538993894
0.7500000000000000	0.8758731139874172	0.2296760538993894
0.0000000000000000	0.2500000000000000	0.2705993016191357
0.0000000000000000	0.7500000000000000	0.2705993016191357
0.5000000000000000	0.2500000000000000	0.2705993016191357

0.5000000000000000 0.7500000000000000 0.2705993016191357

Bare- NiMn (25% Mn) 220 Facet supercell 2X2X1 - [Etot = -349.44429759 eV]

0.989317187668226

7.0900001526000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 10.0268001556000002 0.0000000000000000
0.0000000000000000 0.0000000000000000 27.5200996398999997

Mn Ni

16 40

Direct

0.0000000000000000 0.2500000000000000 0.0000000000000000
0.0000000000000000 0.7500000000000000 0.0000000000000000
0.5000000000000000 0.2500000000000000 0.0000000000000000
0.5000000000000000 0.7500000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 0.09109000099999978
0.0000000000000000 0.5000000000000000 0.09109000099999978
0.5000000000000000 0.0000000000000000 0.09109000099999978
0.5000000000000000 0.5000000000000000 0.09109000099999978
0.0000000000000000 0.2500000000000000 0.1859781551164943
0.0000000000000000 0.7500000000000000 0.1859781551164943
0.5000000000000000 0.2500000000000000 0.1859781551164943
0.5000000000000000 0.7500000000000000 0.1859781551164943
0.0000000000000000 0.0000000000000000 0.2807063341992091
0.0000000000000000 0.5000000000000000 0.2807063341992091
0.5000000000000000 0.0000000000000000 0.2807063341992091
0.5000000000000000 0.5000000000000000 0.2807063341992091
0.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 0.5000000000000000 0.0000000000000000
0.5000000000000000 0.0000000000000000 0.0000000000000000
0.5000000000000000 0.5000000000000000 0.0000000000000000
0.2500000000000000 0.1250000000000000 0.04554000099999991
0.2500000000000000 0.6250000000000000 0.04554000099999991
0.7500000000000000 0.1250000000000000 0.04554000099999991

0.7500000000000000	0.6250000000000000	0.04554000099999991
0.2500000000000000	0.3750000000000000	0.04554000099999991
0.2500000000000000	0.8750000000000000	0.04554000099999991
0.7500000000000000	0.3750000000000000	0.04554000099999991
0.7500000000000000	0.8750000000000000	0.04554000099999991
0.0000000000000000	0.2500000000000000	0.0928607146838800
0.0000000000000000	0.7500000000000000	0.0928607146838800
0.5000000000000000	0.2500000000000000	0.0928607146838800
0.5000000000000000	0.7500000000000000	0.0928607146838800
0.2500000000000000	0.3754265022537311	0.1393946604531209
0.2500000000000000	0.8754264722537357	0.1393946604531209
0.7500000000000000	0.3754265022537311	0.1393946604531209
0.7500000000000000	0.8754264722537357	0.1393946604531209
0.2500000000000000	0.1245735127462666	0.1393946604531209
0.2500000000000000	0.6245735277462643	0.1393946604531209
0.7500000000000000	0.1245735127462666	0.1393946604531209
0.7500000000000000	0.6245735277462643	0.1393946604531209
0.0000000000000000	0.0000000000000000	0.1862512040510751
0.0000000000000000	0.5000000000000000	0.1862512040510751
0.5000000000000000	0.0000000000000000	0.1862512040510751
0.5000000000000000	0.5000000000000000	0.1862512040510751
0.2500000000000000	0.1245836585341351	0.2340410573981444
0.2500000000000000	0.6245836515341381	0.2340410573981444
0.7500000000000000	0.1245836585341351	0.2340410573981444
0.7500000000000000	0.6245836515341381	0.2340410573981444
0.2500000000000000	0.3754163484658619	0.2340410573981444
0.2500000000000000	0.8754163484658619	0.2340410573981444
0.7500000000000000	0.3754163484658619	0.2340410573981444
0.7500000000000000	0.8754163484658619	0.2340410573981444
0.0000000000000000	0.2500000000000000	0.2757333051301529
0.0000000000000000	0.7500000000000000	0.2757333051301529
0.5000000000000000	0.2500000000000000	0.2757333051301529
0.5000000000000000	0.7500000000000000	0.2757333051301529

Bare- NiFe (25% Fe) 220 Facet supercell 2X2X1 - [Etot = -335.64641028 eV]

1.0000000000000000

7.0900001526000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 10.0268001556000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 27.5200996398999997

Fe Ni

16 40

Direct

0.0000000000000000 0.2500000000000000 0.0000000000000000

0.0000000000000000 0.7500000000000000 0.0000000000000000

0.5000000000000000 0.2500000000000000 0.0000000000000000

0.5000000000000000 0.7500000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 0.09109000099999978

0.0000000000000000 0.5000000000000000 0.09109000099999978

0.5000000000000000 0.0000000000000000 0.09109000099999978

0.5000000000000000 0.5000000000000000 0.09109000099999978

0.0000000000000000 0.2500000000000000 0.1824138568842955

0.0000000000000000 0.7500000000000000 0.1824138568842955

0.5000000000000000 0.2500000000000000 0.1824138568842955

0.5000000000000000 0.7500000000000000 0.1824138568842955

0.0000000000000000 0.0000000000000000 0.2698632462982999

0.0000000000000000 0.5000000000000000 0.2698632462982999

0.5000000000000000 0.0000000000000000 0.2698632462982999

0.5000000000000000 0.5000000000000000 0.2698632462982999

0.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 0.5000000000000000 0.0000000000000000

0.5000000000000000 0.0000000000000000 0.0000000000000000

0.5000000000000000 0.5000000000000000 0.0000000000000000

0.2500000000000000 0.1250000000000000 0.04554000099999991

0.2500000000000000 0.6250000000000000 0.04554000099999991

0.7500000000000000 0.1250000000000000 0.04554000099999991

0.7500000000000000 0.6250000000000000 0.04554000099999991

0.2500000000000000	0.3750000000000000	0.0455400009999991
0.2500000000000000	0.8750000000000000	0.0455400009999991
0.7500000000000000	0.3750000000000000	0.0455400009999991
0.7500000000000000	0.8750000000000000	0.0455400009999991
0.0000000000000000	0.2500000000000000	0.0900604966333205
0.0000000000000000	0.7500000000000000	0.0900604966333205
0.5000000000000000	0.2500000000000000	0.0900604966333205
0.5000000000000000	0.7500000000000000	0.0900604966333205
0.2500000000000000	0.3749205152567185	0.1370439497211677
0.2500000000000000	0.8749204852567232	0.1370439497211677
0.7500000000000000	0.3749205152567185	0.1370439497211677
0.7500000000000000	0.8749204852567232	0.1370439497211677
0.2500000000000000	0.1250794997432791	0.1370439497211677
0.2500000000000000	0.6250795147432768	0.1370439497211677
0.7500000000000000	0.1250794997432791	0.1370439497211677
0.7500000000000000	0.6250795147432768	0.1370439497211677
0.0000000000000000	0.0000000000000000	0.1827781493552365
0.0000000000000000	0.5000000000000000	0.1827781493552365
0.5000000000000000	0.0000000000000000	0.1827781493552365
0.5000000000000000	0.5000000000000000	0.1827781493552365
0.2500000000000000	0.1243699440501658	0.2301477034749340
0.2500000000000000	0.6243699370501687	0.2301477034749340
0.7500000000000000	0.1243699440501658	0.2301477034749340
0.7500000000000000	0.6243699370501687	0.2301477034749340
0.2500000000000000	0.3756300629498313	0.2301477034749340
0.2500000000000000	0.8756300629498313	0.2301477034749340
0.7500000000000000	0.3756300629498313	0.2301477034749340
0.7500000000000000	0.8756300629498313	0.2301477034749340
0.0000000000000000	0.2500000000000000	0.2695190767121503
0.0000000000000000	0.7500000000000000	0.2695190767121503
0.5000000000000000	0.2500000000000000	0.2695190767121503
0.5000000000000000	0.7500000000000000	0.2695190767121503

Bare- NiCo (25% Co) 220 Facet supercell 2X2X1 - [Etot = -309.08023845 eV]

0.993794164815303

7.090000152600000	0.000000000000000	0.000000000000000
0.000000000000000	10.026800155600002	0.000000000000000
0.000000000000000	0.000000000000000	27.520099639899997

Fe Ni

16 40

Direct

0.000000000000000	0.250000000000000	0.000000000000000
0.000000000000000	0.750000000000000	0.000000000000000
0.500000000000000	0.250000000000000	0.000000000000000
0.500000000000000	0.750000000000000	0.000000000000000
0.000000000000000	0.000000000000000	0.0910900009999978
0.000000000000000	0.500000000000000	0.0910900009999978
0.500000000000000	0.000000000000000	0.0910900009999978
0.500000000000000	0.500000000000000	0.0910900009999978
0.000000000000000	0.250000000000000	0.1822139803999505
0.000000000000000	0.750000000000000	0.1822139803999505
0.500000000000000	0.250000000000000	0.1822139803999505
0.500000000000000	0.750000000000000	0.1822139803999505
0.000000000000000	0.000000000000000	0.2691468443507219
0.000000000000000	0.500000000000000	0.2691468443507219
0.500000000000000	0.000000000000000	0.2691468443507219
0.500000000000000	0.500000000000000	0.2691468443507219
0.000000000000000	0.000000000000000	0.000000000000000
0.000000000000000	0.500000000000000	0.000000000000000
0.500000000000000	0.000000000000000	0.000000000000000
0.500000000000000	0.500000000000000	0.000000000000000
0.250000000000000	0.125000000000000	0.0455400009999991
0.250000000000000	0.625000000000000	0.0455400009999991
0.750000000000000	0.125000000000000	0.0455400009999991
0.750000000000000	0.625000000000000	0.0455400009999991
0.250000000000000	0.375000000000000	0.0455400009999991

0.2500000000000000	0.8750000000000000	0.0455400009999991
0.7500000000000000	0.3750000000000000	0.0455400009999991
0.7500000000000000	0.8750000000000000	0.0455400009999991
0.0000000000000000	0.2500000000000000	0.0904041628694259
0.0000000000000000	0.7500000000000000	0.0904041628694259
0.5000000000000000	0.2500000000000000	0.0904041628694259
0.5000000000000000	0.7500000000000000	0.0904041628694259
0.2500000000000000	0.3745531558462147	0.1367785304228875
0.2500000000000000	0.8745531258462194	0.1367785304228875
0.7500000000000000	0.3745531558462147	0.1367785304228875
0.7500000000000000	0.8745531258462194	0.1367785304228875
0.2500000000000000	0.1254468591537830	0.1367785304228875
0.2500000000000000	0.6254468741537806	0.1367785304228875
0.7500000000000000	0.1254468591537830	0.1367785304228875
0.7500000000000000	0.6254468741537806	0.1367785304228875
0.0000000000000000	0.0000000000000000	0.1816015195879288
0.0000000000000000	0.5000000000000000	0.1816015195879288
0.5000000000000000	0.0000000000000000	0.1816015195879288
0.5000000000000000	0.5000000000000000	0.1816015195879288
0.2500000000000000	0.1243176538489976	0.2296437448500939
0.2500000000000000	0.6243176468490006	0.2296437448500939
0.7500000000000000	0.1243176538489976	0.2296437448500939
0.7500000000000000	0.6243176468490006	0.2296437448500939
0.2500000000000000	0.3756823531509994	0.2296437448500939
0.2500000000000000	0.8756823531509994	0.2296437448500939
0.7500000000000000	0.3756823531509994	0.2296437448500939
0.7500000000000000	0.8756823531509994	0.2296437448500939
0.0000000000000000	0.2500000000000000	0.2691872348322235
0.0000000000000000	0.7500000000000000	0.2691872348322235
0.5000000000000000	0.2500000000000000	0.2691872348322235
0.5000000000000000	0.7500000000000000	0.2691872348322235

Pure-Ni 220 Facet supercell 2X2X1 - [Etot = -283.84110616 eV]

1.01798110552312

7.090000152600000	0.000000000000000	0.000000000000000
0.000000000000000	10.026800155600002	0.000000000000000
0.000000000000000	0.000000000000000	27.520099639899997

Ni

56

Direct

0.000000000000000	0.250000000000000	0.000000000000000
0.000000000000000	0.750000000000000	0.000000000000000
0.500000000000000	0.250000000000000	0.000000000000000
0.500000000000000	0.750000000000000	0.000000000000000
0.000000000000000	0.000000000000000	0.0910900009999978
0.000000000000000	0.500000000000000	0.0910900009999978
0.500000000000000	0.000000000000000	0.0910900009999978
0.500000000000000	0.500000000000000	0.0910900009999978
0.000000000000000	0.250000000000000	0.1753785761349178
0.000000000000000	0.750000000000000	0.1753785761349178
0.500000000000000	0.250000000000000	0.1753785761349178
0.500000000000000	0.750000000000000	0.1753785761349178
0.000000000000000	0.000000000000000	0.2601367025777961
0.000000000000000	0.500000000000000	0.2601367025777961
0.500000000000000	0.000000000000000	0.2601367025777961
0.500000000000000	0.500000000000000	0.2601367025777961
0.000000000000000	0.000000000000000	0.000000000000000
0.000000000000000	0.500000000000000	0.000000000000000
0.500000000000000	0.000000000000000	0.000000000000000
0.500000000000000	0.500000000000000	0.000000000000000
0.250000000000000	0.125000000000000	0.0455400009999991
0.250000000000000	0.625000000000000	0.0455400009999991
0.750000000000000	0.125000000000000	0.0455400009999991
0.750000000000000	0.625000000000000	0.0455400009999991
0.250000000000000	0.375000000000000	0.0455400009999991
0.250000000000000	0.875000000000000	0.0455400009999991

0.7500000000000000	0.3750000000000000	0.0455400009999991
0.7500000000000000	0.8750000000000000	0.0455400009999991
0.0000000000000000	0.2500000000000000	0.0877372377675272
0.0000000000000000	0.7500000000000000	0.0877372377675272
0.5000000000000000	0.2500000000000000	0.0877372377675272
0.5000000000000000	0.7500000000000000	0.0877372377675272
0.2500000000000000	0.3746298380697368	0.1330617520166797
0.2500000000000000	0.8746298080697414	0.1330617520166797
0.7500000000000000	0.3746298380697368	0.1330617520166797
0.7500000000000000	0.8746298080697414	0.1330617520166797
0.2500000000000000	0.1253701769302609	0.1330617520166797
0.2500000000000000	0.6253701919302586	0.1330617520166797
0.7500000000000000	0.1253701769302609	0.1330617520166797
0.7500000000000000	0.6253701919302586	0.1330617520166797
0.0000000000000000	0.0000000000000000	0.1765021534114410
0.0000000000000000	0.5000000000000000	0.1765021534114410
0.5000000000000000	0.0000000000000000	0.1765021534114410
0.5000000000000000	0.5000000000000000	0.1765021534114410
0.2500000000000000	0.1250227029215694	0.2219691965114237
0.2500000000000000	0.6250226959215723	0.2219691965114237
0.7500000000000000	0.1250227029215694	0.2219691965114237
0.7500000000000000	0.6250226959215723	0.2219691965114237
0.2500000000000000	0.3749773040784277	0.2219691965114237
0.2500000000000000	0.8749773040784277	0.2219691965114237
0.7500000000000000	0.3749773040784277	0.2219691965114237
0.7500000000000000	0.8749773040784277	0.2219691965114237
0.0000000000000000	0.2500000000000000	0.2594914765372778
0.0000000000000000	0.7500000000000000	0.2594914765372778
0.5000000000000000	0.2500000000000000	0.2594914765372778
0.5000000000000000	0.7500000000000000	0.2594914765372778

Bare- NiCu (25% Cu) 220 Facet supercell 2X2X1 - [Etot = -258.56599398 eV]

0.998485100048875

7.090000152600000	0.000000000000000	0.000000000000000
0.000000000000000	10.026800155600002	0.000000000000000
0.000000000000000	0.000000000000000	27.520099639899997

Cu Ni

16 40

Direct

0.000000000000000	0.250000000000000	0.000000000000000
0.000000000000000	0.750000000000000	0.000000000000000
0.500000000000000	0.250000000000000	0.000000000000000
0.500000000000000	0.750000000000000	0.000000000000000
0.000000000000000	0.000000000000000	0.0910900009999978
0.000000000000000	0.500000000000000	0.0910900009999978
0.500000000000000	0.000000000000000	0.0910900009999978
0.500000000000000	0.500000000000000	0.0910900009999978
0.000000000000000	0.250000000000000	0.1812836558276629
0.000000000000000	0.750000000000000	0.1812836558276629
0.500000000000000	0.250000000000000	0.1812836558276629
0.500000000000000	0.750000000000000	0.1812836558276629
0.000000000000000	0.000000000000000	0.2730371062792400
0.000000000000000	0.500000000000000	0.2730371062792400
0.500000000000000	0.000000000000000	0.2730371062792400
0.500000000000000	0.500000000000000	0.2730371062792400
0.000000000000000	0.000000000000000	0.000000000000000
0.000000000000000	0.500000000000000	0.000000000000000
0.500000000000000	0.000000000000000	0.000000000000000
0.500000000000000	0.500000000000000	0.000000000000000
0.250000000000000	0.125000000000000	0.0455400009999991
0.250000000000000	0.625000000000000	0.0455400009999991
0.750000000000000	0.125000000000000	0.0455400009999991
0.750000000000000	0.625000000000000	0.0455400009999991
0.250000000000000	0.375000000000000	0.0455400009999991
0.250000000000000	0.875000000000000	0.0455400009999991
0.750000000000000	0.375000000000000	0.0455400009999991

0.7500000000000000	0.8750000000000000	0.04554000099999991
0.0000000000000000	0.2500000000000000	0.0906492756339929
0.0000000000000000	0.7500000000000000	0.0906492756339929
0.5000000000000000	0.2500000000000000	0.0906492756339929
0.5000000000000000	0.7500000000000000	0.0906492756339929
0.2500000000000000	0.3753284903196530	0.1367710371465023
0.2500000000000000	0.8753284603196576	0.1367710371465023
0.7500000000000000	0.3753284903196530	0.1367710371465023
0.7500000000000000	0.8753284603196576	0.1367710371465023
0.2500000000000000	0.1246715246803447	0.1367710371465023
0.2500000000000000	0.6246715396803424	0.1367710371465023
0.7500000000000000	0.1246715246803447	0.1367710371465023
0.7500000000000000	0.6246715396803424	0.1367710371465023
0.0000000000000000	0.0000000000000000	0.1826151505366127
0.0000000000000000	0.5000000000000000	0.1826151505366127
0.5000000000000000	0.0000000000000000	0.1826151505366127
0.5000000000000000	0.5000000000000000	0.1826151505366127
0.2500000000000000	0.1255736346664804	0.2287916037133471
0.2500000000000000	0.6255736276664834	0.2287916037133471
0.7500000000000000	0.1255736346664804	0.2287916037133471
0.7500000000000000	0.6255736276664834	0.2287916037133471
0.2500000000000000	0.3744263723335166	0.2287916037133471
0.2500000000000000	0.8744263723335166	0.2287916037133471
0.7500000000000000	0.3744263723335166	0.2287916037133471
0.7500000000000000	0.8744263723335166	0.2287916037133471
0.0000000000000000	0.2500000000000000	0.2696953807352216
0.0000000000000000	0.7500000000000000	0.2696953807352216
0.5000000000000000	0.2500000000000000	0.2696953807352216
0.5000000000000000	0.7500000000000000	0.2696953807352216

Bare- NiZn (25% Zn) 220 Facet supercell 2X2X1 - [Etot = -230.77875689 eV]

1.01038006037737

7.0900001526000000	0.0000000000000000	0.0000000000000000
--------------------	--------------------	--------------------

0.0000000000000000 10.0268001556000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 27.5200996398999997

Zn Ni

16 40

Direct

0.0000000000000000 0.2500000000000000 0.0000000000000000

0.0000000000000000 0.7500000000000000 0.0000000000000000

0.5000000000000000 0.2500000000000000 0.0000000000000000

0.5000000000000000 0.7500000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 0.09109000099999978

0.0000000000000000 0.5000000000000000 0.09109000099999978

0.5000000000000000 0.0000000000000000 0.09109000099999978

0.5000000000000000 0.5000000000000000 0.09109000099999978

0.0000000000000000 0.2500000000000000 0.1808294241720105

0.0000000000000000 0.7500000000000000 0.1808294241720105

0.5000000000000000 0.2500000000000000 0.1808294241720105

0.5000000000000000 0.7500000000000000 0.1808294241720105

0.0000000000000000 0.0000000000000000 0.2736022190675911

0.0000000000000000 0.5000000000000000 0.2736022190675911

0.5000000000000000 0.0000000000000000 0.2736022190675911

0.5000000000000000 0.5000000000000000 0.2736022190675911

0.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 0.5000000000000000 0.0000000000000000

0.5000000000000000 0.0000000000000000 0.0000000000000000

0.5000000000000000 0.5000000000000000 0.0000000000000000

0.2500000000000000 0.1250000000000000 0.04554000099999991

0.2500000000000000 0.6250000000000000 0.04554000099999991

0.7500000000000000 0.1250000000000000 0.04554000099999991

0.7500000000000000 0.6250000000000000 0.04554000099999991

0.2500000000000000 0.3750000000000000 0.04554000099999991

0.2500000000000000 0.8750000000000000 0.04554000099999991

0.7500000000000000 0.3750000000000000 0.04554000099999991

0.7500000000000000 0.8750000000000000 0.04554000099999991

0.0000000000000000	0.2500000000000000	0.0908944302055374
0.0000000000000000	0.7500000000000000	0.0908944302055374
0.5000000000000000	0.2500000000000000	0.0908944302055374
0.5000000000000000	0.7500000000000000	0.0908944302055374
0.2500000000000000	0.3754391005850408	0.1365678346375319
0.2500000000000000	0.8754390705850454	0.1365678346375319
0.7500000000000000	0.3754391005850408	0.1365678346375319
0.7500000000000000	0.8754390705850454	0.1365678346375319
0.2500000000000000	0.1245609144149569	0.1365678346375319
0.2500000000000000	0.6245609294149546	0.1365678346375319
0.7500000000000000	0.1245609144149569	0.1365678346375319
0.7500000000000000	0.6245609294149546	0.1365678346375319
0.0000000000000000	0.0000000000000000	0.1821934700678227
0.0000000000000000	0.5000000000000000	0.1821934700678227
0.5000000000000000	0.0000000000000000	0.1821934700678227
0.5000000000000000	0.5000000000000000	0.1821934700678227
0.2500000000000000	0.1242644364486480	0.2283746263393809
0.2500000000000000	0.6242644294486510	0.2283746263393809
0.7500000000000000	0.1242644364486480	0.2283746263393809
0.7500000000000000	0.6242644294486510	0.2283746263393809
0.2500000000000000	0.3757355705513490	0.2283746263393809
0.2500000000000000	0.8757355705513490	0.2283746263393809
0.7500000000000000	0.3757355705513490	0.2283746263393809
0.7500000000000000	0.8757355705513490	0.2283746263393809
0.0000000000000000	0.2500000000000000	0.2687224200509561
0.0000000000000000	0.7500000000000000	0.2687224200509561
0.5000000000000000	0.2500000000000000	0.2687224200509561
0.5000000000000000	0.7500000000000000	0.2687224200509561

NiSc (25% Sc) 220 Facet with Hydrogen supercell 2X2X1 - [Etot = -332.62902497 eV]

1.04735280294076

7.090000152600000	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.0268001556000002	0.0000000000000000

0.0000000000000000 0.0000000000000000 27.5200996398999997

Sc Ni H

16 40 1

Direct

0.0000000000000000 0.2500000000000000 0.0000000000000000

0.0000000000000000 0.7500000000000000 0.0000000000000000

0.5000000000000000 0.2500000000000000 0.0000000000000000

0.5000000000000000 0.7500000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 0.09109000099999978

0.0000000000000000 0.5000000000000000 0.09109000099999978

0.5000000000000000 0.0000000000000000 0.09109000099999978

0.5000000000000000 0.5000000000000000 0.09109000099999978

0.9986855312968643 0.2501600212666943 0.1801442266706701

0.0008007812609208 0.7501665202296124 0.1801664459620014

0.5013144687031357 0.2501600212666943 0.1801442266706701

0.4991992187390792 0.7501665202296124 0.1801664459620014

0.9970941467093013 0.9983643988987794 0.2729800998638865

0.9971335723470034 0.5022619133891624 0.2729691062451565

0.5029058532906987 0.9983643988987794 0.2729800998638865

0.5028664276529966 0.5022619133891624 0.2729691062451565

0.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 0.5000000000000000 0.0000000000000000

0.5000000000000000 0.0000000000000000 0.0000000000000000

0.5000000000000000 0.5000000000000000 0.0000000000000000

0.2500000000000000 0.1250000000000000 0.04554000099999991

0.2500000000000000 0.6250000000000000 0.04554000099999991

0.7500000000000000 0.1250000000000000 0.04554000099999991

0.7500000000000000 0.6250000000000000 0.04554000099999991

0.2500000000000000 0.3750000000000000 0.04554000099999991

0.2500000000000000 0.8750000000000000 0.04554000099999991

0.7500000000000000 0.3750000000000000 0.04554000099999991

0.7500000000000000 0.8750000000000000 0.04554000099999991

0.0002007494946454 0.2500059559462784 0.0889642846576990

0.9998896892322193	0.7500159210075950	0.0888684900409871
0.4997992505053546	0.2500059559462784	0.0889642846576990
0.5001103107677807	0.7500159210075950	0.0888684900409871
0.2500000000000000	0.3759598733961624	0.1367946320147553
0.2500000000000000	0.8758423494745529	0.1362399574779545
0.7500000000000000	0.3762918465052607	0.1364426974620372
0.7500000000000000	0.8758029301971462	0.1364487578254767
0.2500000000000000	0.1243369831626921	0.1367849279595887
0.2500000000000000	0.6244666893099975	0.1361884582357291
0.7500000000000000	0.1237820486061452	0.1364732102209345
0.7500000000000000	0.6242539672159637	0.1364796011749903
0.0006646831218546	0.0004377826423294	0.1840889605136127
0.0007022744216911	0.4999112503835335	0.1840870268760071
0.4993353168781454	0.0004377826423294	0.1840889605136127
0.4992977255783089	0.4999112503835335	0.1840870268760071
0.2500000000000000	0.1220112300377494	0.2298624655508661
0.2500000000000000	0.6236274348847530	0.2296845718739604
0.7500000000000000	0.1237414994925956	0.2296562008518350
0.7500000000000000	0.6239484825229269	0.2290703382828170
0.2500000000000000	0.3785008417558373	0.2298667129760119
0.2500000000000000	0.8768991474934182	0.2296892549899709
0.7500000000000000	0.3768211055748552	0.2296280515451059
0.7500000000000000	0.8766013003298738	0.2290517072702087
0.9985460833491402	0.2503258324013586	0.2662085329802082
0.9991050700257986	0.7503317681748527	0.2660438833173941
0.5014539166508598	0.2503258324013586	0.2662085329802082
0.5008949299742014	0.7503317681748527	0.2660438833173941
0.2500000000000000	0.2501260196077126	0.2686474194003239

NiTi (25% Ti) 220 Facet with Hydrogen supercell 2X2X1 - [Etot = -352.34576879 eV]

1.01798110552312

7.0900001526000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.0268001556000002	0.0000000000000000

0.0000000000000000 0.0000000000000000 27.5200996398999997

Ti Ni H

16 40 1

Direct

0.0000000000000000 0.2500000000000000 0.0000000000000000
0.0000000000000000 0.7500000000000000 0.0000000000000000
0.5000000000000000 0.2500000000000000 0.0000000000000000
0.5000000000000000 0.7500000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 0.09109000099999978
0.0000000000000000 0.5000000000000000 0.09109000099999978
0.5000000000000000 0.0000000000000000 0.09109000099999978
0.5000000000000000 0.5000000000000000 0.09109000099999978
0.9984608453768615 0.2496959727977526 0.1822788418800130
0.0017367470487883 0.7497042243644927 0.1829760748240545
0.5015391546231385 0.2496959727977526 0.1822788418800130
0.4982632529512117 0.7497042243644927 0.1829760748240545
0.9951681029065611 0.9963438241376750 0.2703619442186707
0.9951828999582517 0.5026752510702792 0.2703897759826432
0.5048318970934389 0.9963438241376750 0.2703619442186707
0.5048171000417483 0.5026752510702792 0.2703897759826432
0.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 0.5000000000000000 0.0000000000000000
0.5000000000000000 0.0000000000000000 0.0000000000000000
0.5000000000000000 0.5000000000000000 0.0000000000000000
0.2500000000000000 0.1250000000000000 0.04554000099999991
0.2500000000000000 0.6250000000000000 0.04554000099999991
0.7500000000000000 0.1250000000000000 0.04554000099999991
0.7500000000000000 0.6250000000000000 0.04554000099999991
0.2500000000000000 0.3750000000000000 0.04554000099999991
0.2500000000000000 0.8750000000000000 0.04554000099999991
0.7500000000000000 0.3750000000000000 0.04554000099999991
0.7500000000000000 0.8750000000000000 0.04554000099999991
0.0000146443915554 0.2499597558410755 0.0903597108774719

0.0000034504425415	0.7499006989071972	0.0903829178281015
0.4999853556084446	0.2499597558410755	0.0903597108774719
0.4999965495574585	0.7499006989071972	0.0903829178281015
0.2500000000000000	0.3744090045769752	0.1376535706475792
0.2500000000000000	0.8749219929306449	0.1374704398440514
0.7500000000000000	0.3748914414762581	0.1374167005929081
0.7500000000000000	0.8746763150332484	0.1374696182130677
0.2500000000000000	0.1251596744194856	0.1376585688339418
0.2500000000000000	0.6246584326044271	0.1374879563636711
0.7500000000000000	0.1246904037325294	0.1374288309121354
0.7500000000000000	0.6248588027056527	0.1374998106085101
0.0010367112421719	0.0001018045012557	0.1837195454139575
0.0011007380462615	0.4993095899016780	0.1837732095070450
0.4989632887578281	0.0001018045012557	0.1837195454139575
0.4988992619537385	0.4993095899016780	0.1837732095070450
0.2500000000000000	0.1211690555610758	0.2310452907930696
0.2500000000000000	0.6221682939151307	0.2311325050384809
0.7500000000000000	0.1226649923844079	0.2303372332042102
0.7500000000000000	0.6224643862031556	0.2298942675280600
0.2500000000000000	0.3779300668049643	0.2310731284202987
0.2500000000000000	0.8770848011700920	0.2310648220415104
0.7500000000000000	0.3765439789382867	0.2303273056781237
0.7500000000000000	0.8767911070349896	0.2297975873458782
0.9981901386031495	0.2495198934163128	0.2685993515096854
0.9985116903100462	0.7496306231704395	0.2685617611542526
0.5018098613968505	0.2495198934163128	0.2685993515096854
0.5014883096899538	0.7496306231704395	0.2685617611542526
0.2500000000000000	0.2496935546795882	0.2743030814293022

NiV (25% V) 220 Facet with Hydrogen supercell 2X2X1 - [Etot = -353.16533057 eV]

1.00458661266245

7.0900001526000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.0268001556000002	0.0000000000000000

0.0000000000000000 0.0000000000000000 27.5200996398999997

V Ni H

16 40 1

Direct

0.0000000000000000 0.2500000000000000 0.0000000000000000
0.0000000000000000 0.7500000000000000 0.0000000000000000
0.5000000000000000 0.2500000000000000 0.0000000000000000
0.5000000000000000 0.7500000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 0.09109000099999978
0.0000000000000000 0.5000000000000000 0.09109000099999978
0.5000000000000000 0.0000000000000000 0.09109000099999978
0.5000000000000000 0.5000000000000000 0.09109000099999978
0.9983061093111445 0.2502693948227517 0.1837560105794580
0.0019499291798439 0.7503011777717532 0.1845929673490758
0.5016938906888555 0.2502693948227517 0.1837560105794580
0.4980500708201561 0.7503011777717532 0.1845929673490758
0.9930543522449256 0.9972175202491016 0.2740976176105505
0.9930939775948460 0.5036991100498085 0.2740455343335881
0.5069456477550744 0.9972175202491016 0.2740976176105505
0.5069060224051540 0.5036991100498085 0.2740455343335881
0.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 0.5000000000000000 0.0000000000000000
0.5000000000000000 0.0000000000000000 0.0000000000000000
0.5000000000000000 0.5000000000000000 0.0000000000000000
0.2500000000000000 0.1250000000000000 0.04554000099999991
0.2500000000000000 0.6250000000000000 0.04554000099999991
0.7500000000000000 0.1250000000000000 0.04554000099999991
0.7500000000000000 0.6250000000000000 0.04554000099999991
0.2500000000000000 0.3750000000000000 0.04554000099999991
0.2500000000000000 0.8750000000000000 0.04554000099999991
0.7500000000000000 0.3750000000000000 0.04554000099999991
0.7500000000000000 0.8750000000000000 0.04554000099999991
0.0002468123829473 0.2500916439172514 0.0918084557892058

0.0000930479388686	0.7500765411881218	0.0917352062788837
0.4997531876170527	0.2500916439172514	0.0918084557892058
0.4999069520611314	0.7500765411881218	0.0917352062788837
0.2500000000000000	0.3745481362469505	0.1373100273740846
0.2500000000000000	0.8752174037572971	0.1368910505721885
0.7500000000000000	0.3750086171120586	0.1368346268850260
0.7500000000000000	0.8750740324990005	0.1367476479748504
0.2500000000000000	0.1258058114237599	0.1373367070323539
0.2500000000000000	0.6251245712703550	0.1368721945375455
0.7500000000000000	0.1253775236879804	0.1368395914016105
0.7500000000000000	0.6252770750498655	0.1367127267122257
0.0010163411959425	0.0007411675360132	0.1820183579457293
0.0010239891637980	0.4998306755108288	0.1819729601449893
0.4989836588040575	0.0007411675360132	0.1820183579457293
0.4989760108362020	0.4998306755108288	0.1819729601449893
0.2500000000000000	0.1227759219339504	0.2292913040481324
0.2500000000000000	0.6230196160894295	0.2285838199559578
0.7500000000000000	0.1233000156613997	0.2275517803640952
0.7500000000000000	0.6236377773283692	0.2271392313960803
0.2500000000000000	0.3779374901588994	0.2292151080432063
0.2500000000000000	0.8777806474801508	0.2286206436379246
0.7500000000000000	0.3774708873544057	0.2275623466767556
0.7500000000000000	0.8771747209954199	0.2271863356792565
0.9961251175086048	0.2504558537988686	0.2692095174989504
0.9981028834968626	0.7504733662543899	0.2691536514371791
0.5038748824913952	0.2504558537988686	0.2692095174989504
0.5018971165031374	0.7504733662543899	0.2691536514371791
0.2500000000000000	0.2511843272659746	0.2744812001720334

NiCr (25% Cr) 220 Facet with Hydrogen supercell 2X2X1 - [Etot = -353.54792671 eV]

0.995572721824907

7.090000152600000	0.000000000000000	0.000000000000000
0.000000000000000	10.026800155600002	0.000000000000000

0.0000000000000000 0.0000000000000000 27.5200996398999997

Cr Ni H

16 40 1

Direct

0.0000000000000000 0.2500000000000000 0.0000000000000000

0.0000000000000000 0.7500000000000000 0.0000000000000000

0.5000000000000000 0.2500000000000000 0.0000000000000000

0.5000000000000000 0.7500000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 0.09109000099999978

0.0000000000000000 0.5000000000000000 0.09109000099999978

0.5000000000000000 0.0000000000000000 0.09109000099999978

0.5000000000000000 0.5000000000000000 0.09109000099999978

0.9982664619312445 0.2493912146836834 0.1839413454004344

0.0011542918227434 0.7494612031944783 0.1844608397280965

0.5017335380687555 0.2493912146836834 0.1839413454004344

0.4988457081772566 0.7494612031944783 0.1844608397280965

0.9950192580179049 0.9968888395413771 0.2761374198315565

0.9950475264693779 0.5013287010093137 0.2760722468080701

0.5049807419820951 0.9968888395413771 0.2761374198315565

0.5049524735306221 0.5013287010093137 0.2760722468080701

0.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 0.5000000000000000 0.0000000000000000

0.5000000000000000 0.0000000000000000 0.0000000000000000

0.5000000000000000 0.5000000000000000 0.0000000000000000

0.2500000000000000 0.1250000000000000 0.04554000099999991

0.2500000000000000 0.6250000000000000 0.04554000099999991

0.7500000000000000 0.1250000000000000 0.04554000099999991

0.7500000000000000 0.6250000000000000 0.04554000099999991

0.2500000000000000 0.3750000000000000 0.04554000099999991

0.2500000000000000 0.8750000000000000 0.04554000099999991

0.7500000000000000 0.3750000000000000 0.04554000099999991

0.7500000000000000 0.8750000000000000 0.04554000099999991

0.0004196207285361 0.2498531985385739 0.0928933144800936

0.0001055792149955	0.7499024578859164	0.0929169054446888
0.4995803792714639	0.2498531985385739	0.0928933144800936
0.4998944207850045	0.7499024578859164	0.0929169054446888
0.2500000000000000	0.3742812628784904	0.1380345077712306
0.2500000000000000	0.8743902043302754	0.1376105719368468
0.7500000000000000	0.3747278400777816	0.1374879188702351
0.7500000000000000	0.8743212054558924	0.1375463588035757
0.2500000000000000	0.1249716959183402	0.1380651190102000
0.2500000000000000	0.6249166155796146	0.1375878478468593
0.7500000000000000	0.1245271877535004	0.1375063646505481
0.7500000000000000	0.6249771882603596	0.1375301122089567
0.0008447424477112	0.9993754801344821	0.1823527529577973
0.0008361841576345	0.4994811602172078	0.1823123356091330
0.4991552575522888	0.9993754801344821	0.1823527529577973
0.4991638158423655	0.4994811602172078	0.1823123356091330
0.2500000000000000	0.1227123394039964	0.2308184495235039
0.2500000000000000	0.6232555126376056	0.2298875358503238
0.7500000000000000	0.1230383190567750	0.2292444184161582
0.7500000000000000	0.6239843348500784	0.2288824774252944
0.2500000000000000	0.3757461727213709	0.2307205401983481
0.2500000000000000	0.8752235687677796	0.2299148946876670
0.7500000000000000	0.3754507006385737	0.2291962921979902
0.7500000000000000	0.8745502878939178	0.2289320494826512
0.9953625230499910	0.2491635775053211	0.2710406637225731
0.9991164805156316	0.7491279351161921	0.2704941199513016
0.5046374769500090	0.2491635775053211	0.2710406637225731
0.5008835194843684	0.7491279351161921	0.2704941199513016
0.2500000000000000	0.2497393901085374	0.2766024808598360

NiMn (25% Mn) 220 Facet with Hydrogen supercell 2X2X1 -[Etot = -353.29975965 eV]

0.989317187668226

7.090000152600000	0.000000000000000	0.000000000000000
0.000000000000000	10.026800155600002	0.000000000000000

0.0000000000000000 0.0000000000000000 27.5200996398999997

Mn Ni H

16 40 1

Direct

0.0000000000000000 0.2500000000000000 0.0000000000000000
0.0000000000000000 0.7500000000000000 0.0000000000000000
0.5000000000000000 0.2500000000000000 0.0000000000000000
0.5000000000000000 0.7500000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 0.09109000099999978
0.0000000000000000 0.5000000000000000 0.09109000099999978
0.5000000000000000 0.0000000000000000 0.09109000099999978
0.5000000000000000 0.5000000000000000 0.09109000099999978
0.9997769281276305 0.2488858757320571 0.1856288704301505
0.0012979032857316 0.7488948761406320 0.1858954142318012
0.5002230718723695 0.2488858757320571 0.1856288704301505
0.4987020967142684 0.7488948761406320 0.1858954142318012
0.9949986881772119 0.9971111075541685 0.2806665072463943
0.9946184987879718 0.4996648890288782 0.2806811774802966
0.5050013118227881 0.9971111075541685 0.2806665072463943
0.5053815012120282 0.4996648890288782 0.2806811774802966
0.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 0.5000000000000000 0.0000000000000000
0.5000000000000000 0.0000000000000000 0.0000000000000000
0.5000000000000000 0.5000000000000000 0.0000000000000000
0.2500000000000000 0.1250000000000000 0.04554000099999991
0.2500000000000000 0.6250000000000000 0.04554000099999991
0.7500000000000000 0.1250000000000000 0.04554000099999991
0.7500000000000000 0.6250000000000000 0.04554000099999991
0.2500000000000000 0.3750000000000000 0.04554000099999991
0.2500000000000000 0.8750000000000000 0.04554000099999991
0.7500000000000000 0.3750000000000000 0.04554000099999991
0.7500000000000000 0.8750000000000000 0.04554000099999991
0.0001586975240713 0.2498301313801932 0.0927435603549327

0.9999241205486697	0.7498288037800336	0.0928128268193404
0.4998413024759287	0.2498301313801932	0.0927435603549327
0.5000758794513303	0.7498288037800336	0.0928128268193404
0.2500000000000000	0.3747142941186112	0.1395914594284520
0.2500000000000000	0.8747215552997076	0.1392991838266937
0.7500000000000000	0.3749618108833346	0.1391946370579262
0.7500000000000000	0.8746566936684772	0.1393810188260289
0.2500000000000000	0.1239945899270936	0.1396003306908469
0.2500000000000000	0.6239948635697488	0.1393228217722964
0.7500000000000000	0.1237253048108613	0.1392285126629531
0.7500000000000000	0.6240506107571164	0.1393898926883068
0.0012006340343689	0.9988570477526579	0.1861827374346703
0.0012532024572707	0.4989253191990315	0.1861905529797951
0.4987993659656311	0.9988570477526579	0.1861827374346703
0.4987467975427293	0.4989253191990315	0.1861905529797951
0.2500000000000000	0.1222663324388193	0.2351735801421384
0.2500000000000000	0.6231123296937042	0.2346002906890874
0.7500000000000000	0.1227856653031978	0.2331272218565275
0.7500000000000000	0.6238113261481146	0.2333527752184565
0.2500000000000000	0.3748255751297052	0.2352178925750721
0.2500000000000000	0.8740117827755896	0.2345079679552811
0.7500000000000000	0.3743083847366222	0.2330534116640166
0.7500000000000000	0.8734420234607185	0.2333918695270825
0.9940443025904813	0.2484095806748456	0.2759704936710179
0.9985789965340359	0.7483850732989268	0.2757207290220265
0.5059556974095187	0.2484095806748456	0.2759704936710179
0.5014210034659641	0.7483850732989268	0.2757207290220265
0.2500000000000000	0.2480354850354445	0.2809595041827038

NiFe (25% Fe) 220 Facet with Hydrogen supercell 2X2X1 - [Etot = -339.39908880 eV]

1.0000000000000000

7.0900001526000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.0268001556000002	0.0000000000000000

0.0000000000000000 0.0000000000000000 27.5200996398999997

Fe Ni H

16 40 1

Direct

0.0000000000000000 0.2500000000000000 0.0000000000000000
0.0000000000000000 0.7500000000000000 0.0000000000000000
0.5000000000000000 0.2500000000000000 0.0000000000000000
0.5000000000000000 0.7500000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 0.09109000099999978
0.0000000000000000 0.5000000000000000 0.09109000099999978
0.5000000000000000 0.0000000000000000 0.09109000099999978
0.5000000000000000 0.5000000000000000 0.09109000099999978
0.9995134435069417 0.2498461807133054 0.1819322619557795
0.0012387694882747 0.7498410496805406 0.1821590678111562
0.5004865564930583 0.2498461807133054 0.1819322619557795
0.4987612305117253 0.7498410496805406 0.1821590678111562
0.9957124359950313 0.9975813102300606 0.2699112301345110
0.9957296907276501 0.5019160224694232 0.2698865948804752
0.5042875640049687 0.9975813102300606 0.2699112301345110
0.5042703092723499 0.5019160224694232 0.2698865948804752
0.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 0.5000000000000000 0.0000000000000000
0.5000000000000000 0.0000000000000000 0.0000000000000000
0.5000000000000000 0.5000000000000000 0.0000000000000000
0.2500000000000000 0.1250000000000000 0.04554000099999991
0.2500000000000000 0.6250000000000000 0.04554000099999991
0.7500000000000000 0.1250000000000000 0.04554000099999991
0.7500000000000000 0.6250000000000000 0.04554000099999991
0.2500000000000000 0.3750000000000000 0.04554000099999991
0.2500000000000000 0.8750000000000000 0.04554000099999991
0.7500000000000000 0.3750000000000000 0.04554000099999991
0.7500000000000000 0.8750000000000000 0.04554000099999991
0.0001078290072698 0.2500084350070182 0.0900205242004333

0.9999600433185449	0.7499759931281815	0.0899720967803859
0.4998921709927302	0.2500084350070182	0.0900205242004333
0.5000399566814551	0.7499759931281815	0.0899720967803859
0.2500000000000000	0.3745932040235331	0.1373081123486344
0.2500000000000000	0.8749701883417487	0.1369944770608029
0.7500000000000000	0.3749008495558144	0.1370232544821022
0.7500000000000000	0.8748254307526935	0.1369735576567095
0.2500000000000000	0.1252489403875643	0.1373250160251871
0.2500000000000000	0.6248851410558700	0.1369886847933017
0.7500000000000000	0.1249342737544410	0.1370193625363072
0.7500000000000000	0.6250006228616627	0.1369813873375918
0.0009989665083836	0.9999547352037865	0.1828196533545778
0.0010219526369752	0.4997271969726853	0.1828040418098453
0.4990010334916164	0.9999547352037865	0.1828196533545778
0.4989780473630248	0.4997271969726853	0.1828040418098453
0.2500000000000000	0.1230477796836809	0.2313183734001569
0.2500000000000000	0.6238987040970585	0.2305345110168346
0.7500000000000000	0.1240026379063011	0.2296677156523614
0.7500000000000000	0.6243784772298540	0.2295883777911669
0.2500000000000000	0.3764305097988228	0.2313008359996047
0.2500000000000000	0.8756325998810368	0.2305463199239242
0.7500000000000000	0.3755535746690057	0.2296474647022393
0.7500000000000000	0.8752159742969710	0.2295777000725892
0.9963555279485803	0.2497208924386385	0.2696874134232274
0.9988924270542796	0.7497428443627001	0.2693931321799639
0.5036444720514197	0.2497208924386385	0.2696874134232274
0.5011075729457204	0.7497428443627001	0.2693931321799639
0.2500000000000000	0.2494616689196221	0.2767600462054176

NiCo (25% Co) 220 Facet with Hydrogen supercell 2X2X1 - [Etot = -312.81780343 eV]

0.993794164815303

7.0900001526000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.0268001556000002	0.0000000000000000

0.0000000000000000 0.0000000000000000 27.5200996398999997

Fe Ni H

16 40 1

Direct

0.0000000000000000 0.2500000000000000 0.0000000000000000
0.0000000000000000 0.7500000000000000 0.0000000000000000
0.5000000000000000 0.2500000000000000 0.0000000000000000
0.5000000000000000 0.7500000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 0.09109000099999978
0.0000000000000000 0.5000000000000000 0.09109000099999978
0.5000000000000000 0.0000000000000000 0.09109000099999978
0.5000000000000000 0.5000000000000000 0.09109000099999978
0.9995699625617434 0.2496072000249328 0.1818526289782838
0.0010285848919125 0.7496037988165511 0.1820211611135747
0.5004300374382566 0.2496072000249328 0.1818526289782838
0.4989714151080875 0.7496037988165511 0.1820211611135747
0.9956285890604590 0.9971299766101467 0.2693336033956726
0.9956306453330868 0.5016037394544313 0.2693043656213518
0.5043714109395410 0.9971299766101467 0.2693336033956726
0.5043693546669132 0.5016037394544313 0.2693043656213518
0.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 0.5000000000000000 0.0000000000000000
0.5000000000000000 0.0000000000000000 0.0000000000000000
0.5000000000000000 0.5000000000000000 0.0000000000000000
0.2500000000000000 0.1250000000000000 0.04554000099999991
0.2500000000000000 0.6250000000000000 0.04554000099999991
0.7500000000000000 0.1250000000000000 0.04554000099999991
0.7500000000000000 0.6250000000000000 0.04554000099999991
0.2500000000000000 0.3750000000000000 0.04554000099999991
0.2500000000000000 0.8750000000000000 0.04554000099999991
0.7500000000000000 0.3750000000000000 0.04554000099999991
0.7500000000000000 0.8750000000000000 0.04554000099999991
0.0000187726282519 0.2499745570888123 0.0904050640911791

0.9997889611852173	0.7499169079668988	0.0903305388875921
0.4999812273717481	0.2499745570888123	0.0904050640911791
0.5002110388147827	0.7499169079668988	0.0903305388875921
0.2500000000000000	0.3741257034155865	0.1370745005004466
0.2500000000000000	0.8746687832388389	0.1366839610943558
0.7500000000000000	0.3744847453241320	0.1368106443502910
0.7500000000000000	0.8743194033791539	0.1366810497122373
0.2500000000000000	0.1254495066534247	0.1370646232226349
0.2500000000000000	0.6249694346554406	0.1366564469589235
0.7500000000000000	0.1250123659805951	0.1367831551988061
0.7500000000000000	0.6251860312127064	0.1367528457013307
0.0013932348660362	0.9996411665075016	0.1816744584331289
0.0014095639985143	0.4995232548079827	0.1816558177557397
0.4986067651339638	0.9996411665075016	0.1816744584331289
0.4985904360014857	0.4995232548079827	0.1816558177557397
0.2500000000000000	0.1223852431414159	0.2307600201222257
0.2500000000000000	0.6236831583020503	0.2298824438625502
0.7500000000000000	0.1236721650771528	0.2290747783130982
0.7500000000000000	0.6240557276823466	0.2290037913342999
0.2500000000000000	0.3763341344163678	0.2308453546761058
0.2500000000000000	0.8752055448864482	0.2299199710663800
0.7500000000000000	0.3753106638900405	0.2291109409751542
0.7500000000000000	0.8749234649075959	0.2289138971971880
0.9963636627068055	0.2493162161380909	0.2694011365407931
0.9988873119571906	0.7494371607125672	0.2690430971953006
0.5036363372931945	0.2493162161380909	0.2694011365407931
0.5011126880428094	0.7494371607125672	0.2690430971953006
0.2500000000000000	0.2489049699003516	0.2773664996741303

Pure-Ni 220 Facet with Hydrogen supercell 2X2X1 - [Etot = -287.67028384 eV]

1.01798110552312

7.0900001526000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.0268001556000002	0.0000000000000000

0.0000000000000000 0.0000000000000000 27.5200996398999997

Ni H

56 1

Direct

0.0000000000000000 0.2500000000000000 0.0000000000000000
0.0000000000000000 0.7500000000000000 0.0000000000000000
0.5000000000000000 0.2500000000000000 0.0000000000000000
0.5000000000000000 0.7500000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 0.09109000099999978
0.0000000000000000 0.5000000000000000 0.09109000099999978
0.5000000000000000 0.0000000000000000 0.09109000099999978
0.5000000000000000 0.5000000000000000 0.09109000099999978
0.0008991177178714 0.2507991071860403 0.1754344046120906
0.0008872333011567 0.7507967164746034 0.1753952294668366
0.4991008822821286 0.2507991071860403 0.1754344046120906
0.4991127666988433 0.7507967164746034 0.1753952294668366
0.9980049312911703 0.0013191283712075 0.2603704729862812
0.9995473013997227 0.5013820443035470 0.2601017439740616
0.5019950687088297 0.0013191283712075 0.2603704729862812
0.5004526986002773 0.5013820443035470 0.2601017439740616
0.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 0.5000000000000000 0.0000000000000000
0.5000000000000000 0.0000000000000000 0.0000000000000000
0.5000000000000000 0.5000000000000000 0.0000000000000000
0.2500000000000000 0.1250000000000000 0.04554000099999991
0.2500000000000000 0.6250000000000000 0.04554000099999991
0.7500000000000000 0.1250000000000000 0.04554000099999991
0.7500000000000000 0.6250000000000000 0.04554000099999991
0.2500000000000000 0.3750000000000000 0.04554000099999991
0.2500000000000000 0.8750000000000000 0.04554000099999991
0.7500000000000000 0.3750000000000000 0.04554000099999991
0.7500000000000000 0.8750000000000000 0.04554000099999991
0.0000409459785686 0.2500640399471550 0.0877854006564078

0.0000315011019651	0.7501648685496392	0.0877728418780990
0.4999590540214314	0.2500640399471550	0.0877854006564078
0.4999684988980349	0.7501648685496392	0.0877728418780990
0.2500000000000000	0.3749341507397617	0.1330885961682924
0.2500000000000000	0.8754609432183429	0.1334055381534540
0.7500000000000000	0.3751046394807602	0.1329866377897986
0.7500000000000000	0.8747898362458386	0.1330942690561656
0.2500000000000000	0.1255276974395159	0.1333830635404922
0.2500000000000000	0.6260325972331344	0.1330369947723469
0.7500000000000000	0.1261299769405184	0.1330781821714595
0.7500000000000000	0.6258179693702814	0.1329737571702339
0.9987908205870255	0.0008452025648111	0.1763348035357808
0.0002043627052544	0.5008322378673142	0.1764483349105319
0.5012091794129745	0.0008452025648111	0.1763348035357808
0.4997956372947456	0.5008322378673142	0.1764483349105319
0.2500000000000000	0.1278361755111845	0.2230633289886796
0.2500000000000000	0.6262780083445634	0.2221362656732069
0.7500000000000000	0.1260697424157797	0.2218353317329402
0.7500000000000000	0.6258900347179903	0.2215874624188956
0.2500000000000000	0.3761284225022195	0.2221858261676175
0.2500000000000000	0.8747250199766299	0.2230564889331887
0.7500000000000000	0.3766241534971186	0.2216234092413600
0.7500000000000000	0.8762516956676407	0.2218687886108768
0.9963295449584919	0.2537806296059699	0.2596080649182539
0.9965337694441061	0.7488695079978953	0.2595724703621087
0.5036704550415081	0.2537806296059699	0.2596080649182539
0.5034662305558939	0.7488695079978953	0.2595724703621087
0.2500000000000000	0.0018803017401936	0.2666742934591113

NiCu (25% Cu) 220 Facet with Hydrogen supercell 2X2X1 - [Etot = -262.44242067 eV]

0.998485100048875

7.0900001526000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.0268001556000002	0.0000000000000000

0.0000000000000000 0.0000000000000000 27.5200996398999997

Cu Ni H

16 40 1

Direct

0.0000000000000000 0.2500000000000000 0.0000000000000000

0.0000000000000000 0.7500000000000000 0.0000000000000000

0.5000000000000000 0.2500000000000000 0.0000000000000000

0.5000000000000000 0.7500000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 0.09109000099999978

0.0000000000000000 0.5000000000000000 0.09109000099999978

0.5000000000000000 0.0000000000000000 0.09109000099999978

0.5000000000000000 0.5000000000000000 0.09109000099999978

0.0005601668974862 0.2499790795158887 0.1812141746891882

0.0005498037900935 0.7499572785851640 0.1810931538614966

0.4994398331025138 0.2499790795158887 0.1812141746891882

0.4994501962099065 0.7499572785851640 0.1810931538614966

0.9952467663673445 0.9988085274751199 0.2730422560834782

0.9954942793702557 0.5010767691635820 0.2730435752126610

0.5047532336326555 0.9988085274751199 0.2730422560834782

0.5045057206297443 0.5010767691635820 0.2730435752126610

0.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 0.5000000000000000 0.0000000000000000

0.5000000000000000 0.0000000000000000 0.0000000000000000

0.5000000000000000 0.5000000000000000 0.0000000000000000

0.2500000000000000 0.1250000000000000 0.04554000099999991

0.2500000000000000 0.6250000000000000 0.04554000099999991

0.7500000000000000 0.1250000000000000 0.04554000099999991

0.7500000000000000 0.6250000000000000 0.04554000099999991

0.2500000000000000 0.3750000000000000 0.04554000099999991

0.2500000000000000 0.8750000000000000 0.04554000099999991

0.7500000000000000 0.3750000000000000 0.04554000099999991

0.7500000000000000 0.8750000000000000 0.04554000099999991

0.0001170622223086 0.2500134931016262 0.0905554439745586

0.9999019469203816	0.7499908839658715	0.0904923688397758
0.4998829377776914	0.2500134931016262	0.0905554439745586
0.5000980530796184	0.7499908839658715	0.0904923688397758
0.2500000000000000	0.3752993844733439	0.1369485105878212
0.2500000000000000	0.8751823150231601	0.1366557886368369
0.7500000000000000	0.3754150913853138	0.1366859538395815
0.7500000000000000	0.8754089134167344	0.1366428012583043
0.2500000000000000	0.1246490323278238	0.1369500519386975
0.2500000000000000	0.6246917012366637	0.1366648890222564
0.7500000000000000	0.1246458009332372	0.1366505730662340
0.7500000000000000	0.6246700205274465	0.1366481388646008
0.0014786152491340	0.9998683101714718	0.1824820088054864
0.0013638845698054	0.5000652985376206	0.1825008200934377
0.4985213847508660	0.9998683101714718	0.1824820088054864
0.4986361154301946	0.5000652985376206	0.1825008200934377
0.2500000000000000	0.1242003745486144	0.2301225174738164
0.2500000000000000	0.6255266551585947	0.2290287289865489
0.7500000000000000	0.1249139609684633	0.2278399075827906
0.7500000000000000	0.6258836124865823	0.2282001414667292
0.2500000000000000	0.3756893362927514	0.2300904428474837
0.2500000000000000	0.8744156099539566	0.2290441172242126
0.7500000000000000	0.3749713684390912	0.2279089767128397
0.7500000000000000	0.8740210847947694	0.2281571097804189
0.9941091978528078	0.2499018881870683	0.2700943655502357
0.9990505689725424	0.7499728733103836	0.2695841188470638
0.5058908021471922	0.2499018881870683	0.2700943655502357
0.5009494310274576	0.7499728733103836	0.2695841188470638
0.2500000000000000	0.2500897576940133	0.2749442492994660

NiZn (25% Zn) 220 Facet with Hydrogen supercell 2X2X1 - [Etot = -234.79860613 eV]

1.01038006037737

7.0900001526000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	10.0268001556000002	0.0000000000000000

0.0000000000000000 0.0000000000000000 27.5200996398999997

Zn Ni H

16 40 1

Direct

0.0000000000000000 0.2500000000000000 0.0000000000000000

0.0000000000000000 0.7500000000000000 0.0000000000000000

0.5000000000000000 0.2500000000000000 0.0000000000000000

0.5000000000000000 0.7500000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 0.09109000099999978

0.0000000000000000 0.5000000000000000 0.09109000099999978

0.5000000000000000 0.0000000000000000 0.09109000099999978

0.5000000000000000 0.5000000000000000 0.09109000099999978

0.0011414362837030 0.2491746221190638 0.1809814757180845

0.0002961669669546 0.7491322040834092 0.1806356730141232

0.4988585637162970 0.2491746221190638 0.1809814757180845

0.4997038330330454 0.7491322040834092 0.1806356730141232

0.9961826207250510 0.9974177986355812 0.2734578728747223

0.9964308260096146 0.4995888269453914 0.2734526928970737

0.5038173792749490 0.9974177986355812 0.2734578728747223

0.5035691739903854 0.4995888269453914 0.2734526928970737

0.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 0.5000000000000000 0.0000000000000000

0.5000000000000000 0.0000000000000000 0.0000000000000000

0.5000000000000000 0.5000000000000000 0.0000000000000000

0.2500000000000000 0.1250000000000000 0.04554000099999991

0.2500000000000000 0.6250000000000000 0.04554000099999991

0.7500000000000000 0.1250000000000000 0.04554000099999991

0.7500000000000000 0.6250000000000000 0.04554000099999991

0.2500000000000000 0.3750000000000000 0.04554000099999991

0.2500000000000000 0.8750000000000000 0.04554000099999991

0.7500000000000000 0.3750000000000000 0.04554000099999991

0.7500000000000000 0.8750000000000000 0.04554000099999991

0.9999818553892581 0.2498864504379910 0.0909208461749387

0.9997976834624609	0.7498909564137364	0.0907777360590671
0.5000181446107419	0.2498864504379910	0.0909208461749387
0.5002023165375391	0.7498909564137364	0.0907777360590671
0.2500000000000000	0.3749962328761356	0.1367883982900935
0.2500000000000000	0.8749027254900739	0.1364610018954693
0.7500000000000000	0.3747836432560447	0.1365690591953452
0.7500000000000000	0.8751124851373149	0.1363716655234626
0.2500000000000000	0.1239646296146972	0.1368331943556029
0.2500000000000000	0.6241134700410100	0.1364765280787239
0.7500000000000000	0.1242201745669362	0.1365767378403149
0.7500000000000000	0.6239469987608715	0.1364077730813378
0.0012571608287004	0.9990170097217046	0.1820187990127948
0.0012513705563109	0.4991605201882052	0.1820284771642662
0.4987428391712996	0.9990170097217046	0.1820187990127948
0.4987486294436891	0.4991605201882052	0.1820284771642662
0.2500000000000000	0.1215448162650716	0.2299922391003264
0.2500000000000000	0.6232813639345522	0.2283380166196238
0.7500000000000000	0.1220222264653898	0.2275463440487115
0.7500000000000000	0.6233350359229775	0.2276546988009045
0.2500000000000000	0.3757183991158470	0.2299579351762020
0.2500000000000000	0.8741389084760840	0.2283357806315038
0.7500000000000000	0.3753872693380345	0.2276044020375565
0.7500000000000000	0.8740378002908145	0.2276371714741572
0.9938564149627140	0.2484794869604130	0.2689702725658449
0.9988257730730226	0.7485032063356272	0.2685214252010439
0.5061435850372860	0.2484794869604130	0.2689702725658449
0.5011742269269774	0.7485032063356272	0.2685214252010439
0.2500000000000000	0.2484857860653449	0.2724180490908168

NiCo (25% Co) 111 Facet with OH supercell 2X2X1 - [Etot = -458.05295eV]

0.993794164815303

10.0268001556000002	0.0000000000000000	0.0000000000000000
-5.0134000778000001	8.6834636535000005	0.0000000000000000

0.0000000000000000 0.0000000000000000 28.1868000031000001

Co Ni O H

20 60 1 1

Direct

0.1666650029999985 0.3333350119999992 0.0000000000000000
0.1666650029999985 0.8333350420000016 0.0000000000000000
0.6666650180000033 0.3333350119999992 0.0000000000000000
0.6666650180000033 0.8333350420000016 0.0000000000000000
0.0000000000000000 0.0000000000000000 0.0726099979999972
0.0000000000000000 0.5000000000000000 0.0726099979999972
0.5000000000000000 0.0000000000000000 0.0726099979999972
0.5000000000000000 0.5000000000000000 0.0726099979999972
0.3335879071261658 0.1670303600464962 0.1447805994397271
0.3334161797083439 0.6665971105573902 0.1452423986869817
0.8333786486886510 0.1666283961079245 0.1447079377571114
0.8329876557647111 0.6664238869960073 0.1447796141364677
0.1672605113241517 0.3346258950455976 0.2197373562535532
0.1667342572253148 0.8332879057402920 0.2186660245375691
0.6666340964298385 0.3334128168767094 0.2190005550488792
0.6654153173558015 0.8327813017434238 0.2197273979867305
0.9984163415560303 0.4995673932333133 0.2883792485927614
0.0000468401786691 0.0000047127815179 0.2884190499011297
0.5044643741418113 0.4955991357104850 0.2916265735617785
0.5004916842763194 0.0016390542863860 0.2883749528592219
0.1666650029999985 0.0833349970000015 0.0000000000000000
0.1666650029999985 0.5833349819999967 0.0000000000000000
0.6666650180000033 0.0833349970000015 0.0000000000000000
0.6666650180000033 0.5833349819999967 0.0000000000000000
0.4166649880000008 0.0833349970000015 0.0000000000000000
0.4166649880000008 0.5833349819999967 0.0000000000000000
0.9166649579999984 0.0833349970000015 0.0000000000000000
0.9166649579999984 0.5833349819999967 0.0000000000000000
0.4166649880000008 0.3333350119999992 0.0000000000000000

0.4166649880000000	0.8333350420000016	0.0000000000000000
0.9166649579999984	0.3333350119999992	0.0000000000000000
0.9166649579999984	0.8333350420000016	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0726099979999972
0.0000000000000000	0.7500000000000000	0.0726099979999972
0.5000000000000000	0.2500000000000000	0.0726099979999972
0.5000000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.2500000000000000	0.0726099979999972
0.2500000000000000	0.7500000000000000	0.0726099979999972
0.7500000000000000	0.2500000000000000	0.0726099979999972
0.7500000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.0000000000000000	0.0726099979999972
0.2500000000000000	0.5000000000000000	0.0726099979999972
0.7500000000000000	0.0000000000000000	0.0726099979999972
0.7500000000000000	0.5000000000000000	0.0726099979999972
0.3330875818648025	0.4165458152106325	0.1453166880310732
0.3331888633454412	0.9162744616059726	0.1451542400134613
0.8330937784614107	0.4165585359003643	0.1450202109862744
0.8329160687951997	0.9165887614678994	0.1450797710799208
0.0835889294058845	0.4166008968465178	0.1450906480582788
0.0834290865579490	0.9165934674011851	0.1449563550389286
0.5833999779305685	0.4166216702756955	0.1450905729154357
0.5834130600274037	0.9164296876483675	0.1450882315766009
0.0834320582813888	0.1671065860831931	0.1450814589752056
0.0837478130089977	0.6668294035311888	0.1451560104026086
0.5834541572503937	0.1669248377898640	0.1450198682868447
0.5834668289827007	0.6669310256733212	0.1453148687512567
0.1669224963945339	0.0835790333546882	0.2167493049753517
0.1672527935478811	0.5817671771172073	0.2177879659870428
0.6669543712631381	0.0836351860504863	0.2170560600861791
0.6658641435000732	0.5832714414053157	0.2175286158125900
0.4164025792984489	0.0832318068842923	0.2169767477929341
0.4170724300191111	0.5829668457792323	0.2176474962054442

0.9166062499063159	0.0834354143589806	0.2170092009924645
0.9168088860256987	0.5836341529864768	0.2169775119136617
0.4167684575890362	0.3341734789359805	0.2175325164503548
0.4182691540068788	0.8327848348167350	0.2177814726138152
0.9163996524511901	0.3330794906124979	0.2170596194698078
0.9164619980096234	0.8331119078903626	0.2167473554838040
0.9989026970385879	0.2490345380739214	0.2887078370822991
0.0007876982979553	0.7505030609232435	0.2885760507365092
0.5012883636658927	0.2495912116935841	0.2886566010953899
0.5013365653489359	0.7562213548388357	0.2914911045634625
0.2470181731004004	0.2457193317394086	0.2881296028341680
0.2468578145988758	0.7531964152518640	0.2881982506720533
0.7497025375109132	0.2503541781617002	0.2889275208873556
0.7543420803222460	0.7530425156061966	0.2881237077253260
0.2438455743695158	0.4987192626197725	0.2915073965658337
0.2495581305349788	0.9992700251164806	0.2885776035538470
0.7504632186620483	0.4987710278735165	0.2886541268985496
0.7510291216293510	0.0011607386220120	0.2887025948528006
0.4186808833885109	0.5814758039953105	0.3383530814900482
0.4196559890778531	0.5807856531970472	0.3730952250208759

NiCr (25% Cr) 111 Facet with OH supercell 2X2X1 - [Etot = -506.76655eV]

0.995572721824907

10.0268001556000002	0.0000000000000000	0.0000000000000000
-5.0134000778000001	8.6834636535000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.1868000031000001

Cr Ni O H

20 60 1 1

Direct

0.1666650029999985	0.3333350119999992	0.0000000000000000
0.1666650029999985	0.8333350420000016	0.0000000000000000
0.6666650180000033	0.3333350119999992	0.0000000000000000
0.6666650180000033	0.8333350420000016	0.0000000000000000

0.0000000000000000	0.0000000000000000	0.0726099979999972
0.0000000000000000	0.5000000000000000	0.0726099979999972
0.5000000000000000	0.0000000000000000	0.0726099979999972
0.5000000000000000	0.5000000000000000	0.0726099979999972
0.3333692873797816	0.1663596557447207	0.1450904693645114
0.3335718615307570	0.6663436559393006	0.1456462499225424
0.8333472406599753	0.1665589825240446	0.1450849261798695
0.8335897010532278	0.6665707063925268	0.1450881022575530
0.1663665569565111	0.3342589718879836	0.2217820030563900
0.1665120964213784	0.8333708568276279	0.2214590073231761
0.6660702379586141	0.3338185900616679	0.2216339647680101
0.6655649565177768	0.8334722620634381	0.2218129762746202
0.9986392502429737	0.4999014708745264	0.2914535133313265
0.9996970014469255	0.0001451370093761	0.2918460539693086
0.5031175960816725	0.4967461208370310	0.2945448402865054
0.4999551389215426	0.0011866154086064	0.2914588698903273
0.1666650029999985	0.0833349970000015	0.0000000000000000
0.1666650029999985	0.5833349819999967	0.0000000000000000
0.6666650180000033	0.0833349970000015	0.0000000000000000
0.6666650180000033	0.5833349819999967	0.0000000000000000
0.4166649880000008	0.0833349970000015	0.0000000000000000
0.4166649880000008	0.5833349819999967	0.0000000000000000
0.9166649579999984	0.0833349970000015	0.0000000000000000
0.9166649579999984	0.5833349819999967	0.0000000000000000
0.4166649880000008	0.3333350119999992	0.0000000000000000
0.4166649880000008	0.8333350420000016	0.0000000000000000
0.9166649579999984	0.3333350119999992	0.0000000000000000
0.9166649579999984	0.8333350420000016	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0726099979999972
0.0000000000000000	0.7500000000000000	0.0726099979999972
0.5000000000000000	0.2500000000000000	0.0726099979999972
0.5000000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.2500000000000000	0.0726099979999972

0.2500000000000000	0.7500000000000000	0.0726099979999972
0.7500000000000000	0.2500000000000000	0.0726099979999972
0.7500000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.0000000000000000	0.0726099979999972
0.2500000000000000	0.5000000000000000	0.0726099979999972
0.7500000000000000	0.0000000000000000	0.0726099979999972
0.7500000000000000	0.5000000000000000	0.0726099979999972
0.3327911831260693	0.4161948532215192	0.1458001224344088
0.3328564256189210	0.9158739803618303	0.1458418459017850
0.8327737616494844	0.4164370964841098	0.1455894650036953
0.8329153920124028	0.9165504337946828	0.1453932858053975
0.0835590506084785	0.4163364831929428	0.1456177303544806
0.0836405406962086	0.9162939715447536	0.1455350878042481
0.5834544077875137	0.4164606322615896	0.1458403765804661
0.5835724938312126	0.9163515993255231	0.1456201941647919
0.0833758600545096	0.1669973967427083	0.1453976458321975
0.0840828655638362	0.6670835713483996	0.1458429086539823
0.5835024125115922	0.1671622053309534	0.1455914046601308
0.5837546087711374	0.6671507419942060	0.1458010099131286
0.1665906105345911	0.0831929058364480	0.2171934379141405
0.1668622439184020	0.5819660760685466	0.2183237037644048
0.6669367560534880	0.0840854881659965	0.2174991163264437
0.6663480846555743	0.5834290942543419	0.2180887299371008
0.4165698001659521	0.0834551926861096	0.2176041057976477
0.4172297974073160	0.5826617612247418	0.2183301847896217
0.9166197730527017	0.0831721851930283	0.2174937755558091
0.9164142678543357	0.5833195271250915	0.2176007858599220
0.4164493427123475	0.3335136727155188	0.2180890810394587
0.4178539487539155	0.8329657733477305	0.2183153456781781
0.9157217303494107	0.3329018548903093	0.2174942730435205
0.9166573167017447	0.8332712393871162	0.2171875127094154
0.9991061528751572	0.2497368114021938	0.2900957022841624
0.0011205329508215	0.7512887042703866	0.2903498005520007


```

0.5010857045960577 0.2508253375844305 0.2906186910603736
0.5000273418890160 0.7533720900714655 0.2926319673605562
0.2472683533051381 0.2466889969904145 0.2892397089947920
0.2465520351900281 0.7533138623235871 0.2897856953329239
0.7487886431751036 0.2510424490240695 0.2904876885755954
0.7531587729814149 0.7525733195065740 0.2892566491677186
0.2464557953370274 0.4998803110081980 0.2926079826306207
0.2486007385674611 0.9987502815738267 0.2903552832409773
0.7490330810935362 0.4987916293286787 0.2906230621445545
0.7501078576515283 0.0007160849526002 0.2901189153781516
0.4202490712425515 0.5789113618114499 0.3412064539694413
0.4211042016766910 0.5766364017244712 0.3758988680640130
    
```

NiCu (25% Cu) 111 Facet with OH supercell 2X2X1 - [Etot = -391.57869eV]

```

0.998485100048875
10.0268001556000002 0.0000000000000000 0.0000000000000000
-5.0134000778000001 8.6834636535000005 0.0000000000000000
0.0000000000000000 0.0000000000000000 28.1868000031000001
Cu Ni O H
20 60 1 1
    
```

Direct

```

0.1666650029999985 0.3333350119999992 0.0000000000000000
0.1666650029999985 0.8333350420000016 0.0000000000000000
0.6666650180000033 0.3333350119999992 0.0000000000000000
0.6666650180000033 0.8333350420000016 0.0000000000000000
0.0000000000000000 0.0000000000000000 0.0726099979999972
0.0000000000000000 0.5000000000000000 0.0726099979999972
0.5000000000000000 0.0000000000000000 0.0726099979999972
0.5000000000000000 0.5000000000000000 0.0726099979999972
0.3332084363430354 0.1667212787196419 0.1454578270304054
0.3333252530012061 0.6669138278614497 0.1457367121403905
0.8332698227838762 0.1669636235457617 0.1455972018116185
0.8335345220705719 0.6670384877997151 0.1454533598402605
    
```

0.1678219901619116	0.3360704895161177	0.2183382006483825
0.1664692553247988	0.8339577516287449	0.2164486033404174
0.6667953502827473	0.3336407028949679	0.2170547608750582
0.6643901889634094	0.8326443769504337	0.2183319286729457
0.9987796079846092	0.4998542353508810	0.2925059327730040
0.0001479131960238	0.0003581122376417	0.2929952535110374
0.5037061732778412	0.4968236210648271	0.2911685592714832
0.5006566243838151	0.0017295142152847	0.2925009725340146
0.1666650029999985	0.0833349970000015	0.0000000000000000
0.1666650029999985	0.5833349819999967	0.0000000000000000
0.6666650180000033	0.0833349970000015	0.0000000000000000
0.6666650180000033	0.5833349819999967	0.0000000000000000
0.4166649880000008	0.0833349970000015	0.0000000000000000
0.4166649880000008	0.5833349819999967	0.0000000000000000
0.9166649579999984	0.0833349970000015	0.0000000000000000
0.9166649579999984	0.5833349819999967	0.0000000000000000
0.4166649880000008	0.3333350119999992	0.0000000000000000
0.4166649880000008	0.8333350420000016	0.0000000000000000
0.9166649579999984	0.3333350119999992	0.0000000000000000
0.9166649579999984	0.8333350420000016	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0726099979999972
0.0000000000000000	0.7500000000000000	0.0726099979999972
0.5000000000000000	0.2500000000000000	0.0726099979999972
0.5000000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.2500000000000000	0.0726099979999972
0.2500000000000000	0.7500000000000000	0.0726099979999972
0.7500000000000000	0.2500000000000000	0.0726099979999972
0.7500000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.0000000000000000	0.0726099979999972
0.2500000000000000	0.5000000000000000	0.0726099979999972
0.7500000000000000	0.0000000000000000	0.0726099979999972
0.7500000000000000	0.5000000000000000	0.0726099979999972
0.3332794326558428	0.4170984091256997	0.1454043191308330

0.3338963316251480	0.9168960024329280	0.1450518086799590
0.8336018316766456	0.4170285241695808	0.1451169117491773
0.8330042673260678	0.9170485166227351	0.1454022698593391
0.0834168472211303	0.4168618880319457	0.1453254659327712
0.0829089100243152	0.9173487017757793	0.1450169037516673
0.5832838095218804	0.4169666594283257	0.1450385041202509
0.5833502484557584	0.9167916778195959	0.1453288229181808
0.0831858206518277	0.1672364881378314	0.1454044934271579
0.0833555700417890	0.6663629778184799	0.1450554175790799
0.5832308860983844	0.1666413199001440	0.1451205238306486
0.5831413316371084	0.6669671281653606	0.1454066999927548
0.1651915180103742	0.0834463407960939	0.2180430237750102
0.1666582810500898	0.5830008688428521	0.2186786948846944
0.6654635161745688	0.0829584321545269	0.2182775671881956
0.6663107200207605	0.5836280117864092	0.2178775018946837
0.4169339068470279	0.0827271828588039	0.2180924328801694
0.4167440923579804	0.5836936897745630	0.2186297726236077
0.9171181580733574	0.0833497124205209	0.2184217093088208
0.9177000870054783	0.5835119975604997	0.2181003726737814
0.4168387958456350	0.3341633767130503	0.2178813101178463
0.4174376642220565	0.8337838464421807	0.2186777866655447
0.9174956861307066	0.3349834136610994	0.2182692522829015
0.9169931946365750	0.8352319329841436	0.2180391179927739
0.9990805455296083	0.2493536256712972	0.2890447703142556
0.9992341034024435	0.7505170825395524	0.2886911852810101
0.5000781697293277	0.2487671011404302	0.2888662188932472
0.5030165677575837	0.7527424335779713	0.2932550403717826
0.2500017203257130	0.2471729411891914	0.2887133392350094
0.2465278054735762	0.7539805977161933	0.2878928840709989
0.7505292686323912	0.2499753999966288	0.2890969273117960
0.7533619188454139	0.7505163044769887	0.2887087129232100
0.2477605927072801	0.4975176613845136	0.2932656502880135
0.2499717550168441	0.0012853714171825	0.2886839071258578

0.7517477646883037	0.5004224725054840	0.2888658556545991
0.7511665900786397	0.0014241317886743	0.2890501946144468
0.3751077801762221	0.6254749383274145	0.3446732444092007
0.3293880388768287	0.6714426979942800	0.3649075433239517

NiMn (25% Mn) 111 Facet with OH supercell 2X2X1 - [Etot = -504.68025eV]

1.0000000000000000

9.9196901320999995	0.0000000000000000	0.0000000000000000
-4.9598426818999997	8.5906995225999996	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.8856849669999995

Mn Ni O H

20 60 1 1

Direct

0.1666650029999985	0.3333350119999992	0.0000000000000000
0.1666650029999985	0.8333350420000016	0.0000000000000000
0.6666650180000033	0.3333350119999992	0.0000000000000000
0.6666650180000033	0.8333350420000016	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0726099979999972
0.0000000000000000	0.5000000000000000	0.0726099979999972
0.5000000000000000	0.0000000000000000	0.0726099979999972
0.5000000000000000	0.5000000000000000	0.0726099979999972
0.3332810206436960	0.1666637144775081	0.1474471141338469
0.3332782666197502	0.6665429695370690	0.1474564110985739
0.8333991997902288	0.1666630366862947	0.1474524703260869
0.8333169859078140	0.6666104628616480	0.1472255818401749
0.1666396354661757	0.3332409293663900	0.2219383829185730
0.1664115269902737	0.8331258781891009	0.2211689376316031
0.6667581820308399	0.3334712644966729	0.2211726145110262
0.6667507436587599	0.8331326955333580	0.2211708905470360
0.5040951514294818	0.5019442543587260	0.2973182429082684
0.4999695617142734	0.9998815024406724	0.2990854455834722
0.9979044127035195	0.5019410457486302	0.2973281966225798
0.9979116131218717	0.9957602303288482	0.2973009453725197

0.1666650029999985	0.0833349970000015	0.0000000000000000
0.1666650029999985	0.5833349819999967	0.0000000000000000
0.6666650180000033	0.0833349970000015	0.0000000000000000
0.6666650180000033	0.5833349819999967	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0726099979999972
0.0000000000000000	0.7500000000000000	0.0726099979999972
0.5000000000000000	0.2500000000000000	0.0726099979999972
0.5000000000000000	0.7500000000000000	0.0726099979999972
0.4166649880000008	0.0833349970000015	0.0000000000000000
0.4166649880000008	0.5833349819999967	0.0000000000000000
0.9166649579999984	0.0833349970000015	0.0000000000000000
0.9166649579999984	0.5833349819999967	0.0000000000000000
0.2500000000000000	0.2500000000000000	0.0726099979999972
0.2500000000000000	0.7500000000000000	0.0726099979999972
0.7500000000000000	0.2500000000000000	0.0726099979999972
0.7500000000000000	0.7500000000000000	0.0726099979999972
0.4166649880000008	0.3333350119999992	0.0000000000000000
0.4166649880000008	0.8333350420000016	0.0000000000000000
0.9166649579999984	0.3333350119999992	0.0000000000000000
0.9166649579999984	0.8333350420000016	0.0000000000000000
0.2500000000000000	0.0000000000000000	0.0726099979999972
0.2500000000000000	0.5000000000000000	0.0726099979999972
0.7500000000000000	0.0000000000000000	0.0726099979999972
0.7500000000000000	0.5000000000000000	0.0726099979999972
0.3334108377772154	0.4166730952653097	0.1473062413878878
0.3333494980898735	0.9166428056922413	0.1470021299777926
0.8334548862981634	0.4165212761638273	0.1470339150483184
0.8334569389551731	0.9168511049625394	0.1470307656084699
0.1666510557475647	0.0840190760320851	0.2220965249266484
0.1666505135403256	0.5824582678704786	0.2221184010856945
0.6653679530784729	0.0826141340050626	0.2214968883914636
0.6656093812863304	0.5827309504700082	0.2212558542958050
0.5008126771329131	0.2489528602803617	0.2942379645416580

0.5008009708456456	0.7516682040928657	0.2942376734341465
0.9956292995752278	0.2477016271821029	0.2974025750819109
0.9998879002245431	0.7498449037595236	0.2941707800398916
0.0832717760376696	0.4166705373216502	0.1473088122325095
0.0834083609549481	0.9168493009209513	0.1470290554441789
0.5830902210377360	0.4165269950779518	0.1470316377337610
0.5833083640933339	0.9166456976078123	0.1470035214618335
0.4172824936103581	0.0826134437556689	0.2214932071412505
0.4158443639989216	0.5824660809323987	0.2221151681800677
0.9174068816854515	0.0840256872801106	0.2221047493845845
0.9171593671570477	0.5827276202497700	0.2212592656708523
0.2521449206031576	0.2476828308272445	0.2973712860524600
0.2509060901714051	0.7516605521975279	0.2942379267053568
0.7482043216061456	0.2489576968735676	0.2942433705611904
0.7500144986070651	0.7498506585510114	0.2941710927087513
0.0832738124474588	0.1665383624567198	0.1473053679849201
0.0834111977262140	0.6664723346860981	0.1470336363355784
0.5833017854590921	0.1665855039685482	0.1470037061344271
0.5830799163454188	0.6664760505545644	0.1470335416049267
0.4158511571622299	0.3332290052713418	0.2221032670133170
0.4172764875701418	0.8345186520567580	0.2214948168152091
0.9174215951060418	0.3332242109370682	0.2221167835313693
0.9171565089416518	0.8342723849278144	0.2212491400290162
0.2509233316773205	0.9990497722809195	0.2942310868824265
0.2521447659464542	0.5042325909205090	0.2974216210421545
0.7481868669370826	0.9990602113069755	0.2942369721100491
0.7500053974188319	0.4999799288978153	0.2941731223703101
0.1666771834942935	0.3330220186817954	0.3453716488248730
0.1666757037428042	0.3325286048142289	0.3802666621488768

Pure Ni 111 Facet with OH supercell 2X2X1 - [Etot = -424.99061eV]

1.01798110552312

10.0268001556000002 0.0000000000000000 0.0000000000000000

-5.0134000778000001	8.6834636535000005	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.1868000031000001

Ni O H

80 1 1

Direct

0.1666650029999985	0.3333350119999992	0.0000000000000000
0.1666650029999985	0.8333350420000016	0.0000000000000000
0.6666650180000033	0.3333350119999992	0.0000000000000000
0.6666650180000033	0.8333350420000016	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0726099979999972
0.0000000000000000	0.5000000000000000	0.0726099979999972
0.5000000000000000	0.0000000000000000	0.0726099979999972
0.5000000000000000	0.5000000000000000	0.0726099979999972
0.3331978192353446	0.1668043909385020	0.1420796484226514
0.3331957649151107	0.6663694313217903	0.1420819451841027
0.8336372388023747	0.1668095636335352	0.1420822518903719
0.8333454179321507	0.6666612825324165	0.1419838415992487
0.1666890915227270	0.3333226281427528	0.2118297984514044
0.1665408936304473	0.8332478925045166	0.2114757405024932
0.6667626430043043	0.3334645218721235	0.2114752003967126
0.6667529466151549	0.8332587841524415	0.2114760042963937
0.9968720197625203	0.5031352373767959	0.2795372009096582
0.9968657710158908	0.9936818742259135	0.2795339877202991
0.5063339916988241	0.5031476081172030	0.2795333696346063
0.5000252529250133	0.9999886512241147	0.2803341681946208
0.1666650029999985	0.0833349970000015	0.0000000000000000
0.1666650029999985	0.5833349819999967	0.0000000000000000
0.6666650180000033	0.0833349970000015	0.0000000000000000
0.6666650180000033	0.5833349819999967	0.0000000000000000
0.4166649880000008	0.0833349970000015	0.0000000000000000
0.4166649880000008	0.5833349819999967	0.0000000000000000
0.9166649579999984	0.0833349970000015	0.0000000000000000
0.9166649579999984	0.5833349819999967	0.0000000000000000

0.4166649880000008	0.3333350119999992	0.0000000000000000
0.4166649880000008	0.8333350420000016	0.0000000000000000
0.9166649579999984	0.3333350119999992	0.0000000000000000
0.9166649579999984	0.8333350420000016	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0726099979999972
0.0000000000000000	0.7500000000000000	0.0726099979999972
0.5000000000000000	0.2500000000000000	0.0726099979999972
0.5000000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.2500000000000000	0.0726099979999972
0.2500000000000000	0.7500000000000000	0.0726099979999972
0.7500000000000000	0.2500000000000000	0.0726099979999972
0.7500000000000000	0.7500000000000000	0.0726099979999972
0.2500000000000000	0.0000000000000000	0.0726099979999972
0.2500000000000000	0.5000000000000000	0.0726099979999972
0.7500000000000000	0.0000000000000000	0.0726099979999972
0.7500000000000000	0.5000000000000000	0.0726099979999972
0.3336270681535680	0.4168028586862889	0.1422125958657077
0.3333834772816502	0.9166803867426268	0.1419415280847645
0.8332324905799240	0.4164045910411005	0.1419417227104205
0.8332237286750726	0.9168063898835968	0.1419429579639342
0.0832008633000640	0.4168039887684145	0.1422121427498979
0.0835967433714515	0.9168022510227942	0.1419403861178523
0.5832048022710339	0.4164077364812044	0.1419404618711795
0.5833225066952039	0.9166830234013901	0.1419431047841968
0.0832008286192121	0.1663773063715368	0.1422126109650321
0.0836001496502945	0.6667755788932155	0.1419416136531311
0.5833259305271241	0.1666216965488090	0.1419416019911210
0.5832000176716576	0.6667821180875819	0.1419425829468679
0.1678502053668893	0.0850149041216781	0.2122503387177446
0.1678466235648628	0.5827907160101375	0.2122548609236574
0.6665595871003376	0.0832633859975473	0.2115560703233612
0.6662569350511447	0.5831090847205687	0.2111404412869859
0.4167487696595344	0.0832589361385772	0.2115541713124429

0.4149915339639705 0.5827906805215690 0.2122538914797261
 0.9172186263293014 0.0850162931658147 0.2122551578183121
 0.9169036398496857 0.5831049658987908 0.2111417364869723
 0.4149978097377982 0.3321617507591910 0.2122498816623235
 0.4167468142190600 0.8334522111505720 0.2115556901165121
 0.9172227719207058 0.3321587388678751 0.2122563917858571
 0.9168996326247836 0.8337535278682253 0.2111405417208729
 0.9937729749984356 0.2468565766252837 0.2828507556583233
 0.9998241956158935 0.7498880991619217 0.2799303105706841
 0.5015530545299995 0.2493898858394630 0.2801108334008404
 0.5015506935694063 0.7521149627239012 0.2801166965261999
 0.2531615978364314 0.2468519339022492 0.2828366588008393
 0.2506137178680632 0.7521136429155391 0.2801166101732093
 0.7479050116553836 0.2493988947637291 0.2801170384785365
 0.7501230671593788 0.7498911916486790 0.2799294214378421
 0.2531590967669644 0.5062469690684566 0.2828470144063999
 0.2506218558863083 0.9984610217889625 0.2801113714383945
 0.7501252361770199 0.5001873371686543 0.2799301139355848
 0.7479019798082120 0.9984635376210491 0.2801174700170250
 0.1667434329099109 0.3333042060946809 0.3271159442361835
 0.1668634104475046 0.3332549480976752 0.3610473946072901

NiCr (25% Cr) 200 Facet with OH supercell 2X2X1 - [Etot = -263.03959 eV]

0.995572721824907

7.0844001770000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 7.0844001770000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 27.0844993591000005

Cr Ni O H

12 28 1 1

Direct

0.0000000000000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 0.5000000000000000 0.0000000000000000
 0.5000000000000000 0.0000000000000000 0.0000000000000000

0.5000000000000000	0.5000000000000000	0.0000000000000000
0.0001828165512734	0.9998783065314640	0.1316201145476938
0.0001833835819909	0.5001622154671566	0.1316129572063289
0.4998728500480567	0.0005534001380951	0.1318010605297388
0.4998689691657603	0.4994825384395796	0.1317995020356335
0.9972302843988459	0.9867536898507794	0.2650608272811326
0.9971541660491070	0.5133483560053875	0.2650555765233094
0.4991975895527858	0.0144422195483784	0.2693028837869704
0.4992912912400627	0.4856202229416908	0.2692828924203283
0.2500000000000000	0.2500000000000000	0.0000000000000000
0.2500000000000000	0.7500000000000000	0.0000000000000000
0.7500000000000000	0.2500000000000000	0.0000000000000000
0.7500000000000000	0.7500000000000000	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0653899980000006
0.0000000000000000	0.7500000000000000	0.0653899980000006
0.5000000000000000	0.2500000000000000	0.0653899980000006
0.5000000000000000	0.7500000000000000	0.0653899980000006
0.2500000000000000	0.0000000000000000	0.0653899980000006
0.2500000000000000	0.5000000000000000	0.0653899980000006
0.7500000000000000	0.0000000000000000	0.0653899980000006
0.7500000000000000	0.5000000000000000	0.0653899980000006
0.2503464097121366	0.2499904747589170	0.1310589496711003
0.2509596482517935	0.7500347781689172	0.1313804202886431
0.7508392084051891	0.2499996300421898	0.1311389666624478
0.7486940735175338	0.7500285021448576	0.1314105623349278
0.0033875391605989	0.2500312527027262	0.1961887824940973
0.9994350998555035	0.7500336230445868	0.1967521635464067
0.4996941687011258	0.2499948246349604	0.1968671026602777
0.4990890468890186	0.7500365370339139	0.1980895708644610
0.2506733450338459	0.0005915558835454	0.1973835291337807
0.2506682796890445	0.4994437705474866	0.1973733226183612
0.7484262186339592	0.9993353968342120	0.1971393740282110
0.7483850947220887	0.5006908540692834	0.1971349879413324

0.2251537991329045 0.2500968128520640 0.2625470428510752
 0.2576712556382930 0.7499682548108950 0.2601136452228943
 0.7684485048637342 0.2499978334007906 0.2586447029322940
 0.7386913068537311 0.7500238133867185 0.2606340820502595
 0.4366347931735390 0.2501172663532927 0.3124352450957062
 0.4063637054860578 0.2502123240385146 0.3477601987674745

NiMn (25% Mn) 200 Facet with OH supercell 2X2X1 - [Etot = - 263.06259 eV]

0.989317187668226

7.0844001770000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 7.0844001770000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 27.0844993591000005

Mn Ni O H

12 28 1 1

Direct

0.0000000000000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 0.5000000000000000 0.0000000000000000
 0.5000000000000000 0.0000000000000000 0.0000000000000000
 0.5000000000000000 0.5000000000000000 0.0000000000000000
 0.0000408579614657 0.0011007576853785 0.1338154634203832
 0.0000494441706849 0.4989729592890058 0.1338151490248833
 0.5000461883464595 0.9989179051630117 0.1336798824875913
 0.5000308950181989 0.5011390884454130 0.1336758911378908
 0.0001470688123817 0.9961689141690613 0.2711493071149960
 0.0001288408319624 0.5039806277288648 0.2711485886456515
 0.5001105993836177 0.9961070210383340 0.2719595527474681
 0.5001202518483154 0.5040490013375987 0.2719436202238512
 0.2500000000000000 0.2500000000000000 0.0000000000000000
 0.2500000000000000 0.7500000000000000 0.0000000000000000
 0.7500000000000000 0.2500000000000000 0.0000000000000000
 0.7500000000000000 0.7500000000000000 0.0000000000000000
 0.0000000000000000 0.2500000000000000 0.0653899980000006

0.0000000000000000	0.7500000000000000	0.0653899980000006
0.5000000000000000	0.2500000000000000	0.0653899980000006
0.5000000000000000	0.7500000000000000	0.0653899980000006
0.2500000000000000	0.0000000000000000	0.0653899980000006
0.2500000000000000	0.5000000000000000	0.0653899980000006
0.7500000000000000	0.0000000000000000	0.0653899980000006
0.7500000000000000	0.5000000000000000	0.0653899980000006
0.2501236106280587	0.2500359215735202	0.1336745863240552
0.2497434873648459	0.7500338070608734	0.1335946697820276
0.7499911587233967	0.2500266823977952	0.1336776078612090
0.7503189254691520	0.7500143466522005	0.1335995195174959
0.0000665876478081	0.2500460832569331	0.2032358957062002
0.0000879758879222	0.7500480127292377	0.2013019094926349
0.5000906448365399	0.2500537201875872	0.2006227293429319
0.5000904408294673	0.7500473515125137	0.2020392543428642
0.2505548551632302	0.0008765534619997	0.2016104112159312
0.2505393807300251	0.4992345753420935	0.2016069856844851
0.7496337150323811	0.0008705237510611	0.2016068964579958
0.7496180725113106	0.4992181399656488	0.2016086095366063
0.2454211421248971	0.2500892466440519	0.2678389506011385
0.2495414859168150	0.7500710218822562	0.2654864299198678
0.7548484247927263	0.2500690580183758	0.2678455074496497
0.7506692949083558	0.7500729448331143	0.2654757575806528
0.5006137517739333	0.2501631708363021	0.3147150412044013
0.5010982974341331	0.2502417684439351	0.3511623633369680

NiFe (25% Fe) 200 Facet with OH supercell 2X2X1 - [Etot = - 252.44736 eV]

1.0000000000000000		
7.0844001770000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.0844001770000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.0844993591000005
Fe	Ni	O H

12 28 1 1

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0000000000000000
0.9999989127999314	0.0010202053006125	0.1309399142835304
0.0000010055329511	0.4991142046146990	0.1309433230461323
0.5000006868528075	0.0002286663394031	0.1308244875994689
0.4999994903303957	0.4998988516584575	0.1308233233886966
0.0000019076106952	0.9944771772370871	0.2616857678614863
0.9999997908008140	0.5058281664941404	0.2616845126325558
0.4999999268924782	0.9893654357712691	0.2634307780202079
0.5000030281826966	0.5109344470116710	0.2634301361578366
0.2500000000000000	0.2500000000000000	0.0000000000000000
0.2500000000000000	0.7500000000000000	0.0000000000000000
0.7500000000000000	0.2500000000000000	0.0000000000000000
0.7500000000000000	0.7500000000000000	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0653899980000006
0.0000000000000000	0.7500000000000000	0.0653899980000006
0.5000000000000000	0.2500000000000000	0.0653899980000006
0.5000000000000000	0.7500000000000000	0.0653899980000006
0.2500000000000000	0.0000000000000000	0.0653899980000006
0.2500000000000000	0.5000000000000000	0.0653899980000006
0.7500000000000000	0.0000000000000000	0.0653899980000006
0.7500000000000000	0.5000000000000000	0.0653899980000006
0.2483411369163804	0.2500663815906208	0.1310597117981587
0.2503242941453934	0.7500790572661131	0.1309481710019895
0.7516565905352408	0.2500689121604083	0.1310590876640774
0.7496756520800005	0.7500776876434614	0.1309483979973507
0.9999983724679353	0.2501193602052112	0.1985453326869120
0.9999968144253017	0.7501155515738844	0.1960006499292675
0.4999993154127225	0.2501048412964906	0.1949014761303971

0.5000012756153254	0.7501076202639823	0.1966014127655384
0.2511894342571566	0.0016560759636874	0.1967175913540018
0.2511997105124308	0.4985693035950334	0.1967101297732725
0.7488075683802720	0.0016539389769150	0.1967173516676084
0.7488023629656411	0.4985724784266168	0.1967120526764106
0.2451000532189198	0.2501718387899459	0.2607982185099047
0.2484139293695051	0.7501238173053011	0.2586422755263982
0.7548965229483002	0.2501627781134417	0.2607994236559179
0.7515823150113690	0.7501337348853880	0.2586429928348437
0.4999772036446757	0.2502722215134909	0.3049868694034288
0.4999528068244743	0.2503993374766083	0.3411078489465709

Pure Ni 200 Facet with OH supercell 2X2X1 - [Etot = - 214.75562eV]

1.01798110552312

7.0844001770000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.0844001770000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.0844993591000005

Ni O H

40 1 1

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0000000000000000
0.9999587924866447	0.0009403294752204	0.1274923391196197
0.9999564036526678	0.4991202147535745	0.1274940949515084
0.4999526877556377	0.9991103570221469	0.1274048404838339
0.4999477529395193	0.5009806822114129	0.1274097761916764
0.9999138832649592	0.9966735038400358	0.2491427480733392
0.9999089734504309	0.5035188173597476	0.2491389262607200
0.4998985283779760	0.9972466887720657	0.2510834867361353
0.4998934022685759	0.5029395874709834	0.2510913596001743

0.2500000000000000	0.2500000000000000	0.0000000000000000
0.2500000000000000	0.7500000000000000	0.0000000000000000
0.7500000000000000	0.2500000000000000	0.0000000000000000
0.7500000000000000	0.7500000000000000	0.0000000000000000
0.0000000000000000	0.2500000000000000	0.0653899980000006
0.0000000000000000	0.7500000000000000	0.0653899980000006
0.5000000000000000	0.2500000000000000	0.0653899980000006
0.5000000000000000	0.7500000000000000	0.0653899980000006
0.2500000000000000	0.0000000000000000	0.0653899980000006
0.2500000000000000	0.5000000000000000	0.0653899980000006
0.7500000000000000	0.0000000000000000	0.0653899980000006
0.7500000000000000	0.5000000000000000	0.0653899980000006
0.2490146842940817	0.2500479555661954	0.1274095935077852
0.2508748968915171	0.7500383697643898	0.1274945325111716
0.7508826811125218	0.2500423773649914	0.1274046321018929
0.7490543903304854	0.7500407399088189	0.1274917977669858
0.9999060583976274	0.2500596416504166	0.1915934672644113
0.9999312186927725	0.7500581268702291	0.1891572277837312
0.4999535572618328	0.2500476277650989	0.1878218470015227
0.4999334476805686	0.7500813533484774	0.1915939832424982
0.2506380115822537	0.0007942548899393	0.1898903653000730
0.2506281307775140	0.4993644441366172	0.1898875289399768
0.7492019260991896	0.0007949295357648	0.1898951296291571
0.7491977805616870	0.4993560243730499	0.1898903156336473
0.2470507355281413	0.2501018116059370	0.2510897900326228
0.2464744620806485	0.7500884988586449	0.2491372011488693
0.7527403578731651	0.2500862833843200	0.2510830826067121
0.7533170696211258	0.7500769296430434	0.2491435493870142
0.4994160727591179	0.2505437994793880	0.2913844924620790
0.4990250050034035	0.2508910694479738	0.3268523504425147

1.01798110552312

7.090000152600000 0.000000000000000 0.000000000000000

0.000000000000000 10.026800155600002 0.000000000000000

0.000000000000000 0.000000000000000 27.520099639899997

Ni O H

56 1 1

Direct

0.000000000000000 0.250000000000000 0.000000000000000

0.000000000000000 0.750000000000000 0.000000000000000

0.500000000000000 0.250000000000000 0.000000000000000

0.500000000000000 0.750000000000000 0.000000000000000

0.000000000000000 0.000000000000000 0.0910900009999978

0.000000000000000 0.500000000000000 0.0910900009999978

0.500000000000000 0.000000000000000 0.0910900009999978

0.500000000000000 0.500000000000000 0.0910900009999978

0.9991125351668515 0.2500947452853808 0.1769408723561270

0.9989993456667960 0.7500140641999735 0.1751592997426314

0.5008860830838699 0.2500933388623707 0.1769406265504969

0.5009999450826186 0.7500153702779215 0.1751601060238031

0.9984580235094214 0.9965645613502829 0.2596869712100158

0.0000977557714990 0.5028461930059080 0.2597586974881807

0.5015420447978443 0.9965638523959086 0.2596836016282253

0.4999013677369035 0.5028415012490655 0.2597633577674756

0.000000000000000 0.000000000000000 0.000000000000000

0.000000000000000 0.500000000000000 0.000000000000000

0.500000000000000 0.000000000000000 0.000000000000000

0.500000000000000 0.500000000000000 0.000000000000000

0.250000000000000 0.125000000000000 0.0455400009999991

0.250000000000000 0.625000000000000 0.0455400009999991

0.750000000000000 0.125000000000000 0.0455400009999991

0.750000000000000 0.625000000000000 0.0455400009999991

0.250000000000000 0.375000000000000 0.0455400009999991

0.250000000000000 0.875000000000000 0.0455400009999991

0.7500000000000000	0.3750000000000000	0.04554000099999991
0.7500000000000000	0.8750000000000000	0.04554000099999991
0.9988202945637710	0.2499581319486666	0.0879543827421330
0.0005572659437121	0.7499798010882017	0.0876370984200321
0.5011782759217027	0.2499577261598560	0.0879542629362149
0.4994428624481344	0.7499796941262815	0.0876373519384401
0.2500003765595764	0.3738949986536255	0.1322215249025689
0.2500027917335501	0.8750552768610476	0.1330923824815926
0.7500004287440447	0.3741464892318120	0.1339725026075413
0.7500004987599453	0.8744426265579506	0.1327200138017375
0.2499988195475922	0.1261227945365491	0.1324237002221409
0.2500015926289336	0.6250076528334105	0.1330183915324383
0.7500007931595221	0.1258377070737211	0.1338928487599134
0.7499987461490747	0.6255672980591953	0.1327520014218493
0.9981419309639890	0.0000765062925581	0.1762506290308608
0.9977152232985631	0.5000876012400397	0.1763505145077602
0.5018572658680824	0.0000777481868326	0.1762525137152267
0.5022870776710704	0.5000854994851593	0.1763541328197178
0.2500018313043242	0.1183353561237439	0.2186043362754617
0.2500041471269085	0.6270458484206713	0.2216117656331775
0.7499978688080162	0.1288439880820818	0.2241480162098028
0.7499964988530010	0.6240786804443061	0.2217142931646165
0.2500014015687242	0.3818652205086721	0.2181320619603682
0.2500020446595101	0.8732208329621969	0.2218035278644592
0.7499976179296155	0.3702153738169187	0.2245795113980478
0.7499986722847751	0.8754268905524256	0.2215281371733582
0.0275517995477728	0.2504617986036308	0.2636801171770031
0.9986345719912819	0.7500033156969721	0.2593264831654807
0.4724422619599409	0.2504644895099730	0.2636795629464217
0.5013647121217417	0.7500026207932038	0.2593257796188979
0.2500011728370382	0.2470659352220466	0.3059679991537436
0.2500006997262645	0.1624907925790566	0.3224258734121221

Ground state structures-

Bare NiSc (25% Sc) 111 Facet- [Etot = -116.31350461 eV]

1.04735280294076

5.0134000778000001	0.0000000000000000	0.0000000000000000
-2.5067000389000000	4.3417318267000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.1868000031000001

Sc Ni

5 15

Direct

0.3333300050000005	0.6666700239999983	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0726099979999972
0.6666877336421848	0.3333122953578140	0.1459873532748972
0.3333762188998222	0.6666238101001767	0.2164783139378770
0.0000507295790015	0.9999492704209985	0.2957490578539534
0.3333300050000005	0.1666699949999995	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.1666699949999995	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.6666700239999983	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0726099979999972
0.6675867292467075	0.8337580549396435	0.1448025006386402
0.3244951446298074	0.1621871589671855	0.2184232164346014
0.9938454426948553	0.4968501859609660	0.2864575781851144
0.1662386074764086	0.8337613635235925	0.1448029635340617
0.8378251197993478	0.1621748512006533	0.2184229840010943
0.5031474713181439	0.4968525286818561	0.2864566601706287
0.1662419160603577	0.3324132997532843	0.1448025006386402
0.8378128120328157	0.6755048843701914	0.2184232164346014
0.5031498140390340	0.0061545573051447	0.2864575781851144

Bare NiTi (25% Ti) 111 Facet- [Etot = -124.73434036 eV]

1.01798110552312

5.0134000778000001	0.0000000000000000	0.0000000000000000
-2.5067000389000000	4.3417318267000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.1868000031000001

Ti Ni

5 15

Direct

0.3333300050000005	0.6666700239999983	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0726099979999972
0.6666793069973451	0.3333207220026537	0.1448438379804600
0.3333729845432885	0.6666270444567104	0.2212717471700429
0.0000571237841669	0.9999428762158331	0.2885532718654460
0.3333300050000005	0.1666699949999995	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.1666699949999995	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.6666700239999983	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0726099979999972
0.6654784271568062	0.8327179325382303	0.1454109468020590
0.3319878147385182	0.1659368522984224	0.2174517538036937
0.0019049934663400	0.5008618157720335	0.2894235859865404
0.1672817315973631	0.8327182394026380	0.1454111960729279
0.8340467638727063	0.1659532071272949	0.2174508073089640
0.4991320528685534	0.5008679471314466	0.2894245310976018
0.1672820384617708	0.3345216018431856	0.1454109468020590
0.8340631187015788	0.6680122142614806	0.2174517538036937
0.4991381842279665	0.9980950065336600	0.2894235859865404

Bare NiV (25% V) 111 Facet- [Etot = -125.17844066 eV]

1.00458661266245

5.0134000778000001	0.0000000000000000	0.0000000000000000
-2.5067000389000000	4.3417318267000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.1868000031000001

V Ni

5 15

Direct

0.3333300050000005	0.6666700239999983	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0726099979999972
0.6666692295599077	0.3333307994400911	0.1445396305549735
0.3333398326731682	0.6666601963268306	0.2234274135847869
0.0000045630584466	0.9999954369415534	0.2898302184578156
0.3333300050000005	0.1666699949999995	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.1666699949999995	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.6666700239999983	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0726099979999972
0.6650233937483918	0.8325007424903745	0.1452641759619269
0.3319281171412669	0.1659533965168691	0.2165596570391841
0.0015039216987134	0.5007439994255947	0.2895413134284368
0.1674923646062823	0.8325076063937189	0.1452640963818652
0.8340502266249672	0.1659497443750340	0.2165594108217448
0.4992538275403078	0.5007461724596922	0.2895413274732377
0.1674992285096266	0.3349766352516070	0.1452641759619269
0.8340465744831320	0.6680719118587319	0.2165596570391841
0.4992560005744053	0.9984960783012866	0.2895413134284368

Bare NiCr (25% Cr) 111 Facet- [Etot = -124.07166597 eV]

0.995572721824907

5.0134000778000001	0.0000000000000000	0.0000000000000000
-2.5067000389000000	4.3417318267000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.1868000031000001

Cr Ni

5 15

Direct

0.3333300050000005	0.6666700239999983	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0726099979999972

0.6666709300349183	0.3333290989650806	0.1453286339533264
0.3333359851905939	0.6666640438094049	0.2221376565740130
0.0000051748525465	0.9999948251474535	0.2919729278881178
0.3333300050000005	0.1666699949999995	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.1666699949999995	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.6666700239999983	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0726099979999972
0.6654319020265831	0.8327110100649975	0.1457344032481984
0.3334860648282429	0.1667392342672542	0.2177981924483845
0.0034209591524075	0.5017034910554301	0.2907214994538663
0.1672920494797694	0.8327079215202318	0.1457348632292366
0.8332617556769435	0.1667382153230577	0.2177980522885932
0.4982930932155156	0.5017069067844844	0.2907215316857119
0.1672889609350037	0.3345681269734158	0.1457344032481984
0.8332607367327469	0.6665139641717559	0.2177981924483845
0.4982965089445699	0.9965790408475925	0.2907214994538663

Bare NiMn (25% Mn) 111 Facet- [Etot = -122.45951645 eV]

0.989317187668226

5.0134000778000001	0.0000000000000000	0.0000000000000000
-2.5067000389000000	4.3417318267000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.1868000031000001

Mn Ni

5 15

Direct

0.3333300050000005	0.6666700239999983	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0726099979999972
0.6666754006061311	0.3333246283938678	0.1481797199843697
0.3333499804013016	0.6666500485986973	0.2214280037002112
0.0000127704186212	0.9999872295813788	0.2992758507027204
0.3333300050000005	0.1666699949999995	0.0000000000000000

0.0000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.1666699949999995	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.6666700239999983	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0726099979999972
0.6667130312094329	0.8333429009176569	0.1471516235290693
0.3307414124967210	0.1653475985996664	0.2219501611608408
0.9996680157056232	0.4998104885840107	0.2945941769954104
0.1666561543884768	0.8333438166115243	0.1471518570710799
0.8346494553992443	0.1653505156007569	0.2219501766185275
0.5001869591391355	0.4998130408608645	0.2945949970783062
0.1666570700823442	0.3332869977905659	0.1471516235290693
0.8346523724003347	0.6692586165032779	0.2219501611608408
0.5001895114159893	0.0003319842943768	0.2945941769954104

Bare NiFe (25% Fe) 111 Facet- [Etot = -119.96372461 eV]

1.0000000000000000		
5.0134000778000001	0.0000000000000000	0.0000000000000000
-2.5067000389000000	4.3417318267000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.1868000031000001

Fe Ni

5 15

Direct

0.3333300050000005	0.6666700239999983	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0726099979999972
0.6666726360278616	0.3333273929721372	0.1447967649929112
0.3333423114219514	0.6666577175780475	0.2193604419151782
0.0000080976197623	0.9999919023802377	0.2886120754165873
0.3333300050000005	0.1666699949999995	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.1666699949999995	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.6666700239999983	0.0000000000000000

0.5000000000000000	0.0000000000000000	0.0726099979999972
0.6660536756522646	0.8330188069870701	0.1451902134281298
0.3339734451528003	0.1669750504050498	0.2173258326549430
0.0021337141475897	0.5010506557787409	0.2889232790288290
0.1669811099709548	0.8330188610290463	0.1451901262245912
0.8330252113562580	0.1669747596437432	0.2173254096151567
0.4989465874791534	0.5010534125208466	0.2889235431396457
0.1669811640129311	0.3339463533477343	0.1451902134281298
0.8330249205949514	0.6660265838471986	0.2173258326549430
0.4989493442212591	0.9978662858524103	0.2889232790288290

Bare NiCo (25% Co) 111 Facet- [Etot = -111.83029501 eV]

0.993794164815303

5.0134000778000001	0.0000000000000000	0.0000000000000000
-2.5067000389000000	4.3417318267000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.1868000031000001

Co Ni

5 15

Direct

0.3333300050000005	0.6666700239999983	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0726099979999972
0.6666717378888123	0.3333282911111866	0.1448152646550867
0.3333406477954526	0.6666593812045463	0.2192765093165150
0.0000091533811926	0.9999908466188074	0.2886242599373503
0.3333300050000005	0.1666699949999995	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.1666699949999995	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.6666700239999983	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0726099979999972
0.6661088098468042	0.8330449172864931	0.1451968381070685
0.3338381522038247	0.1669071616841222	0.2173471283767867
0.0018635276826373	0.5009135025436535	0.2889571355090368

0.1669540440549895	0.8330459269450117	0.1451970160117071
0.8330923998837818	0.1669075711162193	0.2173453882124363
0.4990766115369141	0.5009233884630859	0.2889570728616917
0.1669550537135081	0.3338912191531946	0.1451968381070685
0.8330928093158789	0.6661618767961741	0.2173471283767867
0.4990864974563465	0.9981364723173627	0.2889571355090368

Pure Ni 111 Facet- [Etot = -104.25072995 eV]

0.993602894269297

5.0134000778000001	0.0000000000000000	0.0000000000000000
-2.5067000389000000	4.3417318267000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.1868000031000001

Ni

20

Direct

0.3333300050000005	0.6666700239999983	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0726099979999972
0.6666854930302293	0.3333145359697767	0.1450032888287893
0.3333782980021738	0.6666217309978251	0.2174623354386966
0.0000573956624237	0.9999426043375763	0.2888105590421830
0.3333300050000005	0.1666699949999995	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.1666699949999995	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.6666700239999983	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0726099979999972
0.6666691528736379	0.8333057862157176	0.1450053413381767
0.3333688017006651	0.1666220775352656	0.2174469088738320
0.0000512650298816	0.4999366113579811	0.2888165073459277
0.1666936310678437	0.8333063399321574	0.1450058067084257
0.8333782076748193	0.1666217633251819	0.2174453758734813
0.5000620971410044	0.4999379028589956	0.2888178002486796
0.1666941847842836	0.3333308761263538	0.1450053413381767
0.8333778934647356	0.6666312272993338	0.2174469088738320

0.5000633886420189 0.9999487349701184 0.2888165073459277

Bare NiCu (25% Cu) 111 Facet- [Etot = -95.24504276 eV]

0.998485100048875

5.0134000778000001 0.0000000000000000 0.0000000000000000

-2.5067000389000000 4.3417318267000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 28.1868000031000001

Cu Ni

5 15

Direct

0.3333300050000005 0.6666700239999983 0.0000000000000000

0.0000000000000000 0.0000000000000000 0.0726099979999972

0.6666691638760867 0.3333308651239122 0.1456779528850873

0.3333325519903738 0.6666674770096250 0.2172014328735301

0.0000001887715442 0.9999998112284558 0.2930262779943646

0.3333300050000005 0.1666699949999995 0.0000000000000000

0.0000000000000000 0.5000000000000000 0.0726099979999972

0.8333299760000017 0.1666699949999995 0.0000000000000000

0.5000000000000000 0.5000000000000000 0.0726099979999972

0.8333299760000017 0.6666700239999983 0.0000000000000000

0.5000000000000000 0.0000000000000000 0.0726099979999972

0.6672051723242802 0.8335887699879834 0.1451784090771540

0.3311497404969685 0.1655638979590535 0.2184795188845925

0.9990556861101467 0.4995178636112811 0.2891432952507174

0.1663998098371167 0.8336001611628845 0.1451792441383688

0.8344272803847019 0.1655726906152992 0.2184822265445661

0.5004884278843917 0.4995115721156083 0.2891240811401374

0.1664112010120178 0.3327948566757186 0.1451784090771540

0.8344360730409477 0.6688502885030303 0.2184795188845925

0.5004821363887189 0.0009443138898533 0.2891432952507174

Bare NiZn (25% Zn) 111 Facet- [Etot = -85.99800042 eV]

1.01038006037737

5.0134000778000001 0.0000000000000000 0.0000000000000000

-2.5067000389000000	4.3417318267000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.1868000031000001

Zn Ni

5 15

Direct

0.3333300050000005	0.6666700239999983	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0726099979999972
0.6666812614782387	0.3333187675217602	0.1451053471859396
0.3333871518183003	0.6666128771816986	0.2163052420120053
0.0000778136012300	0.9999221863987700	0.2937604876721309
0.3333300050000005	0.1666699949999995	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.1666699949999995	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.6666700239999983	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0726099979999972
0.6671208666371911	0.8335339273661830	0.1448729569854308
0.3294418968447985	0.1646459398167082	0.2175054318884833
0.9982571378226694	0.4990254376866190	0.2875059296465636
0.1664642246813202	0.8335357463186810	0.1448762549205611
0.8353669829719763	0.1646329880280248	0.2174974874269395
0.5009480523458691	0.4990519476541309	0.2875099961894492
0.1664660436338181	0.3328791623628007	0.1448729569854308
0.8353540311832930	0.6705581321552003	0.2175054318884833
0.5009745623133810	0.0017428621773306	0.2875059296465636

NiSc (25% Sc) 111 Facet with Hydrogen- [Etot = -132.27224645 eV]

1.04735280294076

5.0134000778000001	0.0000000000000000	0.0000000000000000
-2.5067000389000000	4.3417318267000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.1868000031000001

Sc Ni H

5 15 4

Direct

0.3333300050000005	0.6666700239999983	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0726099979999972
0.6665211837770002	0.3332157935581179	0.1450435113597237
0.3330955227570769	0.6664580150351682	0.2169453801214445
0.9996758633902658	0.9997260733370226	0.2896387922934878
0.3333300050000005	0.1666699949999995	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.1666699949999995	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.6666700239999983	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0726099979999972
0.6675838938586054	0.8337414503520790	0.1451635749965163
0.3320526062732370	0.1659394660855469	0.2183667090120593
0.9920372080620652	0.4959036922275786	0.2917688658009610
0.1659921184902160	0.8337387523564459	0.1451649932477252
0.8336058372007997	0.1659438160110085	0.2183686320391303
0.5034885871077606	0.4959083622924680	0.2917728336684462
0.1659859734106846	0.3321405098810573	0.1451652337096405
0.8336083331955564	0.6674925186855418	0.2183684492837017
0.5034729285087991	0.0073309140493620	0.2917745114139905
0.6663285496073286	0.3330396516644143	0.3206444901658259
0.5974963868901213	0.7986211875452227	0.3215653591710179
0.2007333972425371	0.7986131629954656	0.3215634936747875
0.2007477137855886	0.4018924255246148	0.3215607227309363

NiTi (25% Ti) 111 Facet with Hydrogen- [Etot = -140.22047452 eV]

1.01798110552312

5.0134000778000001	0.0000000000000000	0.0000000000000000
-2.5067000389000000	4.3417318267000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.1868000031000001

Ti Ni H

5 15 4

Direct

0.3333300050000005	0.6666700239999983	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0726099979999972
0.6665886887733876	0.3332729434318864	0.1432204078588768
0.3331363018879472	0.6664863363295623	0.2201972145199349
0.9997777346533283	0.9998011001463141	0.2861974412704882
0.3333300050000005	0.1666699949999995	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.1666699949999995	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.6666700239999983	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0726099979999972
0.6645780350819592	0.8322549112579196	0.1463508368927577
0.3357853388051808	0.1678262327901834	0.2178941756626642
0.9953063661863126	0.4975716941988040	0.2933692036781750
0.1675627376513518	0.8322409824555521	0.1463530713662706
0.8318271704116142	0.1678167463976763	0.2178925558355544
0.5019972378000759	0.4975565437455174	0.2933721612016029
0.1675722148390761	0.3352610899925139	0.1463546282540520
0.8318394827977187	0.6638669400733050	0.2178927631290222
0.5020008354907617	0.0042511724366179	0.2933746277521365
0.6664361861074255	0.3331239005185225	0.3247246107676958
0.6336724828422930	0.8167346576290697	0.3243729080684687
0.1828052054275346	0.8167380834548936	0.3243718663105994
0.1828136529975666	0.3658890508247481	0.3243719698050427

NiV (25% V) 111 Facet with Hydrogen- [Etot = -140.30623781 eV]

1.00458661266245

5.0134000778000001	0.0000000000000000	0.0000000000000000
-2.5067000389000000	4.3417318267000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.1868000031000001

V Ni H

5 15 4

Direct

0.3333300050000005	0.6666700239999983	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0726099979999972
0.6664405050046653	0.3331399587529091	0.1444546098310013
0.3329706424403724	0.6663686004402862	0.2211238704689862
0.9994331937250465	0.9995077151966711	0.2875598299293003
0.3333300050000005	0.1666699949999995	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.1666699949999995	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.6666700239999983	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0726099979999972
0.6648279534639698	0.8323431844312950	0.1458592167489385
0.3341049369926239	0.1669524132137994	0.2172806206386610
0.9959574317812354	0.4978362406656203	0.2932752631742730
0.1672761464885824	0.8323462914203006	0.1458585830384962
0.8324754251040360	0.1669405969001119	0.2172721865846441
0.5011927099232807	0.4977835095674408	0.2932752142236765
0.1672811578620923	0.3347924495205774	0.1458589475238057
0.8324820648622904	0.6653308955909267	0.2172716866224462
0.5011369289523557	0.0030276594308276	0.2932745124363976
0.6660773103403912	0.3328663668511780	0.3257221306171303
0.6453264694106267	0.8224775224042773	0.3246639143898378
0.1764607173631632	0.8224655523157764	0.3246532674870011
0.1764718368872096	0.3536401809623371	0.3246535588788291

NiCr (25% Cr) 111 Facet with Hydrogen- [Etot = -139.70832220 eV]

0.995572721824907

5.0134000778000001	0.0000000000000000	0.0000000000000000
-2.5067000389000000	4.3417318267000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.1868000031000001

Cr Ni H
5 15 4

Direct

0.3333300050000005	0.6666700239999983	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0726099979999972
0.6665057957647278	0.3332042942078388	0.1447094167208363
0.3329894996935963	0.6663803194318660	0.2201983316030294
0.9994868450642755	0.9995717544679366	0.2904975480174272
0.3333300050000005	0.1666699949999995	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.1666699949999995	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.6666700239999983	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0726099979999972
0.6661144293465142	0.8330025688381753	0.1458093720430469
0.3349347404919314	0.1673586488320424	0.2185466941693903
0.9958397026910006	0.4977672706881648	0.2944880970203982
0.1666979021180239	0.8330005975307628	0.1458096171367060
0.8320211129352018	0.1673656145736899	0.2185440970754797
0.5013202332026552	0.4977904079919924	0.2944895657317090
0.1666935843709965	0.3335774994935932	0.1458084716318169
0.8320284032702929	0.6644510312916978	0.2185429027649590
0.5012998007540901	0.0031801445492476	0.2944913668617204
0.6661180866442749	0.3328759090636311	0.3272120375744123
0.6439878640301302	0.8218112055512137	0.3264908972491511
0.1771884794149940	0.8217941854675956	0.3264877784184108
0.1772017634296859	0.3550529305170826	0.3264870345175481

NiMn (25% Mn) 111 Facet with Hydrogen- [Etot = -139.17664835 eV]

0.989317187668226

5.0134000778000001	0.0000000000000000	0.0000000000000000
-2.5067000389000000	4.3417318267000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.1868000031000001

Mn	Ni	H
5	15	4

Direct

0.3333300050000005	0.6666700239999983	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0726099979999972
0.6664816028378411	0.3331734672289528	0.1467584417558072
0.3328892482036707	0.6662711763302696	0.2224131334905479
0.9994083569845813	0.9994917117569386	0.2941701139517718
0.3333300050000005	0.1666699949999995	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.1666699949999995	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.6666700239999983	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0726099979999972
0.6664237560577604	0.8331148315022077	0.1472516356529141
0.3347150886301336	0.1671986742976586	0.2216587028895063
0.9975331289614289	0.4985522252363594	0.2981997891982360
0.1664579819136520	0.8331184231156428	0.1472531815539568
0.8320202789556035	0.1671976655457712	0.2216551159962776
0.5003458941583787	0.4985385534834776	0.2982034743173116
0.1664716690242827	0.3331591680943049	0.1472532709978935
0.8320412351286137	0.6645272035418230	0.2216529894198871
0.5003459234035645	0.0013612527476923	0.2982051450107335
0.6660579718969473	0.3327991185170944	0.3300147611266695
0.6458936681803422	0.8227080974651670	0.3302791283271560
0.1761233598814087	0.8227024309599997	0.3302745270411691
0.1761278575058611	0.3529745162184383	0.3302710612194772

NiFe (25% Fe) 111 Facet with Hydrogen- [Etot = -135.21095788 eV]

1.0000000000000000		
5.0134000778000001	0.0000000000000000	0.0000000000000000
-2.5067000389000000	4.3417318267000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.1868000031000001

Fe Ni H

5 15 4

Direct

0.3333300050000005	0.6666700239999983	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0726099979999972
0.6662828763873208	0.3330235014170100	0.1447311138440668
0.3327231973685159	0.6661829303083664	0.2177619708974845
0.9991927560594149	0.9993184186496649	0.2886579181628193
0.3333300050000005	0.1666699949999995	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.1666699949999995	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.6666700239999983	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0726099979999972
0.6661210868015957	0.8329479620283919	0.1453801238364392
0.3324523708088520	0.1660421566173227	0.2176519850724006
0.9987301075191723	0.4991022366432531	0.2916035467694869
0.1663816620648362	0.8329449420730910	0.1453809034130060
0.8328791697473150	0.1660456819429328	0.2176503514642860
0.4994275638290020	0.4991017308609074	0.2915997318325552
0.1663776527502492	0.3332144498479508	0.1453817915961011
0.8328748786328575	0.6664674635172929	0.2176487809767167
0.4994480053002519	0.9998018203794885	0.2916006667510587
0.665835888629223	0.3326384178016468	0.3222131573983802
0.6501206759460700	0.8247834612875096	0.3223958586999132
0.1737083350049815	0.8247921736975812	0.3223926994141593
0.1736878244908695	0.3483404851620904	0.3223881491305676

NiCo (25% Co) 111 Facet with Hydrogen- [Etot = -127.17202572 eV]

0.993794164815303

5.0134000778000001	0.0000000000000000	0.0000000000000000
-2.5067000389000000	4.3417318267000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.1868000031000001

Co Ni H
5 15 4

Direct

0.3333300050000005	0.6666700239999983	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0726099979999972
0.6664509065868529	0.3331470285872626	0.1455569304960562
0.3328838536997765	0.6662885924160733	0.2182646706096492
0.9991828333305222	0.9993560239047028	0.2894908644645042
0.3333300050000005	0.1666699949999995	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.1666699949999995	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.6666700239999983	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0726099979999972
0.6665422253828197	0.8331940018247153	0.1451464456016609
0.3324625712476035	0.1660740811147150	0.2173674754383867
0.9983036350110837	0.4988759029581473	0.2916189651640764
0.1664297071023597	0.8331891184786073	0.1451468819401498
0.8330504602905435	0.1660756290318233	0.2173701755539952
0.4995541794590608	0.4988876721814961	0.2916179578271638
0.1664306594817617	0.3330947399576729	0.1451465485786727
0.8330487718090254	0.6666538731670215	0.2173725991651168
0.4994959982047575	0.0001049264441519	0.2916097662221233
0.6658409291943812	0.3326507899467117	0.3226898938395379
0.6686929380935140	0.8340926570365639	0.3220070308102834
0.1644057143732098	0.8340573066844001	0.3220190428317053
0.1644329838595269	0.3298411151418605	0.3220196652433884

Pure Ni 111 Facet with Hydrogen- [Etot = -119.88927303 eV]

0.993602894269297

5.0134000778000001	0.0000000000000000	0.0000000000000000
-2.5067000389000000	4.3417318267000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.1868000031000001

Ni H

20 4

Direct

0.3333300050000005	0.6666700239999983	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0726099979999972
0.6666208622973642	0.3332971810225587	0.1447034909988005
0.3331436905877894	0.6664968355097969	0.2172928857295702
0.9996043162200721	0.9996576830244805	0.2909376149045144
0.3333300050000005	0.1666699949999995	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.1666699949999995	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.6666700239999983	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0726099979999972
0.6665973775892340	0.8332794472477758	0.1447586648177079
0.3332273208333660	0.1665387361151076	0.2172300408248802
0.9995610167718638	0.4996303378062592	0.2910084048294124
0.1666172577705751	0.8332725549696391	0.1447561486094031
0.8330938726272450	0.1665330491718251	0.2172356930721975
0.4996478067441501	0.4996083718177076	0.2910069419982193
0.1666193479634117	0.3333114927210516	0.1447551000173632
0.8330911909203493	0.6664060103010101	0.2172382548398843
0.4996497913759796	0.9997545894704274	0.2910071872704236
0.6662830919158154	0.3330046133606643	0.3215130235367738
0.6665897818466462	0.8331538324765688	0.3214095782127870
0.1661518285414303	0.8331968354946682	0.3214132773072507
0.1661478991905696	0.3326677660822028	0.3214158444132380

NiCu (25% Cu) 111 Facet with Hydrogen- [Etot = -110.72417251 eV]

0.998485100048875

5.0134000778000001	0.0000000000000000	0.0000000000000000
-2.5067000389000000	4.3417318267000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.1868000031000001

Cu Ni H
5 15 4

Direct

0.3333300050000005	0.6666700239999983	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0726099979999972
0.6664517347050065	0.3331599770790845	0.1456153219306415
0.3329174736570195	0.6663192941991269	0.2176978360136559
0.9993370259116077	0.9994630440118115	0.2939016243843966
0.3333300050000005	0.1666699949999995	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.1666699949999995	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.6666700239999983	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0726099979999972
0.6666986443899887	0.8332760722964991	0.1448516968942428
0.3304230350210204	0.1650815876276610	0.2178670999307926
0.9998771938100788	0.4997405750080119	0.2914499359195304
0.1663526842725815	0.8332667268250091	0.1448520245316161
0.8341511409224864	0.1651081646733417	0.2178757173438655
0.4992175629840929	0.4997949620170559	0.2914494712974829
0.1663625432440696	0.3329706385620526	0.1448516381694702
0.8341418725824852	0.6687592152532815	0.2178791384339718
0.4992244058331252	0.9990446150064543	0.2914493226960175
0.6660740255735718	0.3328460666529125	0.3209286673490084
0.6391268737773927	0.8193626416441049	0.3229180678013819
0.1795241766552351	0.8193986265271107	0.3229211612605383
0.1795035607552435	0.3597054939093951	0.3229207532906528

NiZn (25% Zn) 111 Facet with Hydrogen- [Etot = -101.48473710 eV]

1.01038006037737

5.0134000778000001	0.0000000000000000	0.0000000000000000
-2.5067000389000000	4.3417318267000002	0.0000000000000000
0.0000000000000000	0.0000000000000000	28.1868000031000001

Zn Ni H
5 15 4

Direct

0.3333300050000005	0.6666700239999983	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0726099979999972
0.6665112169105143	0.3332228912293900	0.1453121807534288
0.3329752147847316	0.6663679056071743	0.2174056230466093
0.9995744657170746	0.9996297098943572	0.2907585762757279
0.3333300050000005	0.1666699949999995	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.1666699949999995	0.0000000000000000
0.5000000000000000	0.5000000000000000	0.0726099979999972
0.8333299760000017	0.6666700239999983	0.0000000000000000
0.5000000000000000	0.0000000000000000	0.0726099979999972
0.6657456658664813	0.8328126719616904	0.1447571551476230
0.3326569671536959	0.1662181924857720	0.2172112927635936
0.0015234963119966	0.5006388164551794	0.2913906555288648
0.1669351426730756	0.8328521677456990	0.1447597019669615
0.8332082477984528	0.1661986593163007	0.2172170527759718
0.4986832686427931	0.5006473095651032	0.2913934134931679
0.1669461006573343	0.3339870994302530	0.1447566950928092
0.8332083241538655	0.6667932527634832	0.2172125801249010
0.4986716927588546	0.9977427611548464	0.2913953306519019
0.6663009849460337	0.3330125628800715	0.3191221450760864
0.6194891486179657	0.8096093056399880	0.3232250080973813
0.1896746214357279	0.8096318438448051	0.3232290211557682
0.1896656652726563	0.3797521076237871	0.3232285239802337

Bare NiSc (30% Sc) 200 Facet - [Etot = -59.26045307 eV]

1.04735280294076

3.5422000885000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	3.5422000885000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.0844993591000005

Sc Ni

3 7

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.1312859042261749
0.0000000000000000	0.0000000000000000	0.2652545561185349
0.5000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0653899980000006
0.5000000000000000	0.0000000000000000	0.0653899980000006
0.5000000000000000	0.5000000000000000	0.1310034635120658
0.0000000000000000	0.5000000000000000	0.1976849372197407
0.5000000000000000	0.0000000000000000	0.1976849372197407
0.5000000000000000	0.5000000000000000	0.2516505255088433

Bare NiTi (30% Ti) 200 Facet - [Etot = -63.02218105 eV]

1.01798110552312

3.542200885000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	3.542200885000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.0844993591000005

Ti Ni

3 7

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000
-0.0000000000000000	0.0000000000000000	0.1312426529275885
-0.0000000000000000	-0.0000000000000000	0.2648892700000515
0.5000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0653899980000006
0.5000000000000000	0.0000000000000000	0.0653899980000006
0.5000000000000000	0.5000000000000000	0.1309601012622824
-0.0000000000000000	0.5000000000000000	0.1966007751060960
0.5000000000000000	-0.0000000000000000	0.1966007751060960
0.5000000000000000	0.5000000000000000	0.2572003691964161

Bare NiV (25% V) 200 Facet - [Etot = -62.75957795 eV]

1.00458661266245

3.542200885000000	0.000000000000000	0.000000000000000
0.000000000000000	3.542200885000000	0.000000000000000
0.000000000000000	0.000000000000000	27.084499359100005

V Ni

3 7

Direct

0.000000000000000	0.000000000000000	0.000000000000000
0.000000000000000	0.000000000000000	0.1313102592749544
0.000000000000000	0.000000000000000	0.2649128679249202
0.500000000000000	0.500000000000000	0.000000000000000
0.000000000000000	0.500000000000000	0.0653899980000006
0.500000000000000	0.000000000000000	0.0653899980000006
0.500000000000000	0.500000000000000	0.1307333918986089
0.000000000000000	0.500000000000000	0.1959074836131549
0.500000000000000	0.000000000000000	0.1959074836131549
0.500000000000000	0.500000000000000	0.2581471483085878

Bare NiCr (30% Cr) 200 Facet - [Etot = -62.87764789 eV]

0.995572721824907

3.542200885000000	0.000000000000000	0.000000000000000
0.000000000000000	3.542200885000000	0.000000000000000
0.000000000000000	0.000000000000000	27.084499359100005

Cr Ni

3 7

Direct

0.000000000000000	0.000000000000000	0.000000000000000
0.000000000000000	0.000000000000000	0.1317328421960511
0.000000000000000	0.000000000000000	0.2671042513257831
0.500000000000000	0.500000000000000	0.000000000000000
0.000000000000000	0.500000000000000	0.0653899980000006
0.500000000000000	0.000000000000000	0.0653899980000006

0.5000000000000000	0.5000000000000000	0.1315838659237869
0.0000000000000000	0.5000000000000000	0.1975189857674522
0.5000000000000000	0.0000000000000000	0.1975189857674522
0.5000000000000000	0.5000000000000000	0.2604284135161024

Bare NiMn (25% Mn) 200 Facet - [Etot = -62.92430140 eV]

0.989317187668226

3.542200885000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	3.542200885000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.0844993591000005

Mn Ni

3 7

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.1337845967442135
0.0000000000000000	0.0000000000000000	0.2720593563633571
0.5000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0653899980000006
0.5000000000000000	0.0000000000000000	0.0653899980000006
0.5000000000000000	0.5000000000000000	0.1334605811899010
0.0000000000000000	0.5000000000000000	0.2015201312150339
0.5000000000000000	0.0000000000000000	0.2015201312150339
0.5000000000000000	0.5000000000000000	0.2655143964691931

Bare NiFe (30% Fe) 200 Facet - [Etot = -60.48459440 eV]

1.0000000000000000

3.542200885000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	3.542200885000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.0844993591000005

Fe Ni

3 7

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000
--------------------	--------------------	--------------------

0.0000000000000000	0.0000000000000000	0.1310262016318333
0.0000000000000000	0.0000000000000000	0.2623047982847879
0.5000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0653899980000006
0.5000000000000000	0.0000000000000000	0.0653899980000006
0.5000000000000000	0.5000000000000000	0.1309871519793404
0.0000000000000000	0.5000000000000000	0.1967624143260949
0.5000000000000000	0.0000000000000000	0.1967624143260949
0.5000000000000000	0.5000000000000000	0.2594996221837036

Bare NiCo (30% Co) 200 Facet - [Etot = -55.55706988 eV]

0.993794164815303

3.542200885000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	3.542200885000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.0844993591000005

Co Ni

3 7

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.1310206751132910
0.0000000000000000	0.0000000000000000	0.2612143230630863
0.5000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0653899980000006
0.5000000000000000	0.0000000000000000	0.0653899980000006
0.5000000000000000	0.5000000000000000	0.1310844068296859
0.0000000000000000	0.5000000000000000	0.1970354134184120
0.5000000000000000	0.0000000000000000	0.1970354134184120
0.5000000000000000	0.5000000000000000	0.2602208148552378

Pure Ni 200 Facet - [Etot = -50.89616180 eV]

1.01798110552312

3.542200885000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	3.542200885000000	0.0000000000000000

0.0000000000000000 0.0000000000000000 27.0844993591000005

Ni

10

Direct

0.0000000000000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 0.1273596480353731
 0.0000000000000000 0.0000000000000000 0.2494919539913170
 0.5000000000000000 0.5000000000000000 0.0000000000000000
 0.0000000000000000 0.5000000000000000 0.0653899980000006
 0.5000000000000000 0.0000000000000000 0.0653899980000006
 0.5000000000000000 0.5000000000000000 0.1273483065571952
 0.0000000000000000 0.5000000000000000 0.1900511076671521
 0.5000000000000000 0.0000000000000000 0.1900511076671521
 0.5000000000000000 0.5000000000000000 0.2495026632962265

Bare NiCu (30% Cu) 200 Facet - [Etot = -46.17902883 eV]

0.998485100048875

3.542200885000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 3.542200885000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 27.0844993591000005

Cu Ni

3 7

Direct

0.0000000000000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 0.1313632986931665
 0.0000000000000000 0.0000000000000000 0.2633617604973750
 0.5000000000000000 0.5000000000000000 0.0000000000000000
 0.0000000000000000 0.5000000000000000 0.0653899980000006
 0.5000000000000000 0.0000000000000000 0.0653899980000006
 0.5000000000000000 0.5000000000000000 0.1311633260883127
 0.0000000000000000 0.5000000000000000 0.1973624566677401
 0.5000000000000000 0.0000000000000000 0.1973624566677401
 0.5000000000000000 0.5000000000000000 0.2592972507347255

Bare NiZn (30% Zn) 200 Facet - [Etot = -41.11663348 eV]

1.01038006037737

3.5422000885000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	3.5422000885000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.0844993591000005

Zn Ni

3 7

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.1314133226571528
0.0000000000000000	0.0000000000000000	0.2652804859278888
0.5000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0653899980000006
0.5000000000000000	0.0000000000000000	0.0653899980000006
0.5000000000000000	0.5000000000000000	0.1311807051115821
0.0000000000000000	0.5000000000000000	0.1973788415422959
0.5000000000000000	0.0000000000000000	0.1973788415422959
0.5000000000000000	0.5000000000000000	0.2579351728787103

NiSc (30% Sc) 200 Facet with Hydrogen- [Etot = -67.03527104 eV]

1.04735280294076

3.5422000885000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	3.5422000885000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.0844993591000005

Sc Ni H

3 7 2

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000517642777567	0.0001076935102020	0.1312756564973228
0.0001540908572224	0.0000173334462445	0.2662601816194226
0.5000000000000000	0.5000000000000000	0.0000000000000000

0.0000000000000000	0.5000000000000000	0.0653899980000006
0.5000000000000000	0.0000000000000000	0.0653899980000006
0.5000372546099925	0.5000937613436278	0.1308769681616866
0.0000580093529905	0.5001344838060930	0.1987846428183886
0.5001388356236873	0.0001089271383066	0.1972875155083216
0.5001518299279581	0.4999642795064219	0.2565432901606144
0.7542064239182480	0.5001187646399572	0.2986957229746992
0.2465146217720431	0.4994482165003262	0.2987382819841073

NiTi (30% Ti) 200 Facet with Hydrogen- [Etot = -70.35968884 eV]

1.01798110552312

3.5422000885000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	3.5422000885000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.0844993591000005

Ti Ni H

3 7 2

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000407950432617	0.0000185822378853	0.1311559569658769
0.0000577550735912	0.9999783822625616	0.2633925300940518
0.5000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0653899980000006
0.5000000000000000	0.0000000000000000	0.0653899980000006
0.5000343944288446	0.5000236870681718	0.1309098578560324
0.0000661415424972	0.5000286613433644	0.1963468885494493
0.5000578416998991	0.0000295409504076	0.1963571798055526
0.5000647652736916	0.5000044507151955	0.2596071578579782
0.6995089695718946	0.6972678772666541	0.3031421193651056
0.3006164132269475	0.3026715770286614	0.3031361338455412

NiV (30% V) 200 Facet with Hydrogen- [Etot = -70.48830245 eV]

1.00458661266245

3.5422000885000000	0.0000000000000000	0.0000000000000000
--------------------	--------------------	--------------------

0.0000000000000000	3.5422000885000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.0844993591000005

V Ni H

3 7 2

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0001646146820491	0.9998911400705168	0.1322127633544099
0.0006540084180671	0.9996718519031731	0.2656140809625924
0.5000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0653899980000006
0.5000000000000000	0.0000000000000000	0.0653899980000006
0.5001054402758243	0.4999328110211252	0.1302693240673776
0.0001253327637230	0.4999158335989691	0.1952501153034234
0.5001697954210087	0.9999404548861293	0.1952497886494911
0.5001541401233922	0.5000159507093613	0.2628201369126302
0.5008128722048610	0.9986967131592692	0.2894330383783768
0.0020808836916117	0.4995637554556751	0.2894307157568647

NiCr (30% Cr) 200 Facet with Hydrogen- [Etot = -70.69361570 eV]

0.995572721824907

3.5422000885000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	3.5422000885000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.0844993591000005

Cr Ni H

3 7 2

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0001127060387986	0.9999070388309477	0.1315446257106174
0.0004406733756497	0.9996922995738302	0.2657877565467217
0.5000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0653899980000006
0.5000000000000000	0.0000000000000000	0.0653899980000006
0.5001015913228670	0.4999543733385465	0.1314379698166945

0.0002026670038902 0.4998749192674055 0.1977589336876520
 0.5002506630393739 0.9998358889145962 0.1977588444135918
 0.5003994124556712 0.4997531899952747 0.2680138491720854
 0.5005756581370164 0.9992265851946627 0.2915923980874879
 0.0013032068978163 0.4996527847697436 0.2915901763759194

NiMn (30% Mn) 200 Facet with Hydrogen- [Etot = -70.68252715 eV]

0.989317187668226
 3.5422000885000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 3.5422000885000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 27.0844993591000005

Mn Ni H
 3 7 2

Direct

0.0000000000000000 0.0000000000000000 0.0000000000000000
 0.0001836385068970 0.9999170523314689 0.1337435197797632
 0.0004730655001097 0.9997410415264198 0.2715774266753215
 0.5000000000000000 0.5000000000000000 0.0000000000000000
 0.0000000000000000 0.5000000000000000 0.0653899980000006
 0.5000000000000000 0.0000000000000000 0.0653899980000006
 0.5001842032488000 0.4999035711441735 0.1343632002431221
 0.0002762977896964 0.4998464828861486 0.2022446587750011
 0.5002934814986517 0.9998603736401890 0.2022429474637448
 0.5004289264169728 0.4997911203137448 0.2717082868419922
 0.5005321777287008 0.9993895158493302 0.2958970725193026
 0.0009997011536313 0.4996740243047952 0.2958967202145288

NiFe (30% Fe) 200 Facet with Hydrogen- [Etot = -64.31742027 eV]

1.0000000000000000
 3.5422000885000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 3.5422000885000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 27.0844993591000005

Fe Ni H

3 7 2

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0006907491286031	0.9997258110894944	0.1303186326476950
0.0013652580979092	0.9990569964874932	0.2626581305521456
0.5000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0653899980000006
0.5000000000000000	0.0000000000000000	0.0653899980000006
0.5007342091677482	0.4996618160056331	0.1314489825240394
0.0010717460937783	0.4993391868699448	0.1963529672235798
0.5011382742240513	0.9993262071561976	0.1963641260749912
0.5013010413536825	0.4992311793354717	0.2639345393209585
0.5015885550649007	0.9988492452206363	0.2838743503153899
0.0019130523435243	0.4991432475134888	0.2838820249225652

NiCo (30% Co) 200 Facet with Hydrogen- [Etot = -63.33402605 eV]

0.993794164815303

3.5422000885000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	3.5422000885000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.0844993591000005

Co Ni H

3 7 2

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0002569082904245	0.9998379049835577	0.1314167072751644
0.0006148345969095	0.9996334983620301	0.2632815133692503
0.5000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0653899980000006
0.5000000000000000	0.0000000000000000	0.0653899980000006
0.5002612504532067	0.4998568974363522	0.1313249638275806
0.0004440903827287	0.4997498360635149	0.1964041040849764
0.5004270155483965	0.9997295336240555	0.1964038407410413
0.5006230143338328	0.4996300131835056	0.2635938551959214

0.5007405011364270 0.9996506497489577 0.2812594986706500
 0.0007097765832142 0.4996023179219549 0.2812573656913600

Pure Ni 200 Facet with Hydrogen- [Etot = -58.01666781 eV]

1.01798110552312

3.5422000885000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 3.5422000885000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 27.0844993591000005

Ni H

10 2

Direct

0.0000000000000000 0.0000000000000000 0.0000000000000000
 0.0000331273925909 0.9999737049389807 0.1275634442078228
 0.0000676394244579 0.9999296566902984 0.2485699110005726
 0.5000000000000000 0.5000000000000000 0.0000000000000000
 0.0000000000000000 0.5000000000000000 0.0653899980000006
 0.5000000000000000 0.0000000000000000 0.0653899980000006
 0.5000289063123162 0.4999813833875848 0.1268402821457428
 0.0000676849283181 0.4999432724318709 0.1896360106868045
 0.5000651046115863 0.9999540934593369 0.1896322954618981
 0.5000664984250278 0.4999247888854512 0.2526911626051103
 0.5879024323548094 0.5861695052393117 0.3079721527077837
 0.4122199999215113 0.4138576833145464 0.3079768214322129

NiCu (30% Cu) 200 Facet with Hydrogen- [Etot = -53.77002599 eV]

0.998485100048875

3.5422000885000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 3.5422000885000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 27.0844993591000005

Cu Ni H

3 7 2

Direct

0.0000000000000000 0.0000000000000000 0.0000000000000000

0.0004750546013668	0.9996894528271199	0.1314202166295644
0.0011957462777730	0.9992821758343382	0.2661845044205364
0.5000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0653899980000006
0.5000000000000000	0.0000000000000000	0.0653899980000006
0.5004739234317555	0.4997330704985501	0.1315848105200601
0.0008384116497453	0.4995230820232592	0.1968234985293549
0.5008125355304145	0.9994851655604009	0.1968238507762905
0.5011268276712073	0.4993304598247263	0.2655097765972201
0.5013440898142605	0.9991142878898032	0.2818169470759955
0.0015048429765514	0.4991980545378780	0.2818205938126681

NiZn (30% Zn) 200 Facet with Hydrogen- [Etot = -48.26799493 eV]

1.01038006037737

3.5422000885000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	3.5422000885000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.0844993591000005

Zn Ni H

3 7 2

Direct

0.0000000000000000	0.0000000000000000	0.0000000000000000
-0.0001000990030342	0.0003806786205839	0.1312847376188165
-0.0001953917743792	0.0003451177264793	0.2621722241881438
0.5000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.5000000000000000	0.0653899980000006
0.5000000000000000	0.0000000000000000	0.0653899980000006
0.4999768877092408	0.5004000331043875	0.1311246958887670
-0.0000956458499871	0.5004789064502541	0.1969041008951693
0.4997291529015526	0.0002966051735593	0.1968895917328777
0.4999010504543327	0.5002938249053722	0.2641710190135788
0.5880727494360842	0.5850200771673191	0.3208355948047200
0.4127291958212252	0.4142228057435987	0.3208103028303055

Bare NiSc (28.57% Sc) 220 Facet - [Etot = -82.19892257 eV]

1.04735280294076

3.5450000763000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.0134000778000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.5200996398999997

Ti Ni

4 10

Direct

0.0000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.09109000099999978
0.0000000000000000	0.5000000000000000	0.1814129549948973
0.0000000000000000	0.0000000000000000	0.2737207834881445
0.0000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.2500000000000000	0.04554000099999991
0.5000000000000000	0.7500000000000000	0.04554000099999991
0.0000000000000000	0.5000000000000000	0.09109000099999978
0.5000000000000000	0.7520103422324809	0.1370254515899845
0.5000000000000000	0.2479896577675191	0.1370254515899845
0.0000000000000000	0.0000000000000000	0.1845186708041098
0.5000000000000000	0.2461441991371771	0.2301315707850335
0.5000000000000000	0.7538558008628229	0.2301315707850335
0.0000000000000000	0.5000000000000000	0.2667671605914421

Bare NiTi (28.57% Ti) 220 Facet - [Etot = -87.22227187 eV]

1.01798110552312

3.5450000763000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.0134000778000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.5200996398999997

Ti Ni

4 10

Direct

0.0000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0910900009999978
0.0000000000000000	0.5000000000000000	0.1833059258352989
0.0000000000000000	0.0000000000000000	0.2696591452685482
0.0000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.2500000000000000	0.0455400009999991
0.5000000000000000	0.7500000000000000	0.0455400009999991
0.0000000000000000	0.5000000000000000	0.0910900009999978
0.5000000000000000	0.7499617181842524	0.1375903862375409
0.5000000000000000	0.2500382818157476	0.1375903862375409
0.0000000000000000	0.0000000000000000	0.1838549078102503
0.5000000000000000	0.2454038667961100	0.2307959998963938
0.5000000000000000	0.7545961332038900	0.2307959998963938
0.0000000000000000	0.5000000000000000	0.2685540049113442

Bare NiV (28.57% V) 220 Facet - [Etot = -87.15577727 eV]

1.01798110552312

3.5450000763000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.0134000778000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.5200996398999997

Ti Ni

4 10

Direct

0.0000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0910900009999978
0.0000000000000000	0.5000000000000000	0.1817785925848625
0.0000000000000000	0.0000000000000000	0.2680857924438840
0.0000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.2500000000000000	0.0455400009999991
0.5000000000000000	0.7500000000000000	0.0455400009999991
0.0000000000000000	0.5000000000000000	0.0910900009999978
0.5000000000000000	0.7494768084158636	0.1352267940461829
0.5000000000000000	0.2505231915841364	0.1352267940461829

0.0000000000000000	0.0000000000000000	0.1792037315087782
0.5000000000000000	0.2445923261349066	0.2251595608406518
0.5000000000000000	0.7554076738650934	0.2251595608406518
0.0000000000000000	0.5000000000000000	0.2641561484325621

Bare NiCr (28.57% Cr) 220 Facet - [Etot = -87.39538807 eV]

0.995572721824907

3.5450000763000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.0134000778000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.5200996398999997

Cr Ni
4 10

Direct

0.0000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.09109000099999978
0.0000000000000000	0.5000000000000000	0.1841174964431147
0.0000000000000000	0.0000000000000000	0.2755097899507106
0.0000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.2500000000000000	0.04554000099999991
0.5000000000000000	0.7500000000000000	0.04554000099999991
0.0000000000000000	0.5000000000000000	0.09109000099999978
0.5000000000000000	0.7491851831162890	0.1371621917744363
0.5000000000000000	0.2508148168837110	0.1371621917744363
0.0000000000000000	0.0000000000000000	0.1818701758089034
0.5000000000000000	0.2485455198952877	0.2291487382866109
0.5000000000000000	0.7514544801047123	0.2291487382866109
0.0000000000000000	0.5000000000000000	0.2703211703465271

Bare NiMn (28.57% Mn) 220 Facet - [Etot = -87.18222007 eV]

1.01798110552312

3.5450000763000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.0134000778000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.5200996398999997

Ti Ni
4 10

Direct

0.0000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0910900009999978
0.0000000000000000	0.5000000000000000	0.1796695249021951
0.0000000000000000	0.0000000000000000	0.2691625721429673
0.0000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.2500000000000000	0.0455400009999991
0.5000000000000000	0.7500000000000000	0.0455400009999991
0.0000000000000000	0.5000000000000000	0.0910900009999978
0.5000000000000000	0.7502404582143285	0.1355969428589532
0.5000000000000000	0.2497595417856715	0.1355969428589532
0.0000000000000000	0.0000000000000000	0.1803489673500636
0.5000000000000000	0.2496042979322937	0.2260279615156833
0.5000000000000000	0.7503957020677063	0.2260279615156833
0.0000000000000000	0.5000000000000000	0.2648725973890151

Bare NiFe (28.57% Fe) 220 Facet - [Etot = -83.94041813 eV]

1.0000000000000000		
3.5450000763000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.0134000778000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.5200996398999997

Fe Ni
4 10

Direct

0.0000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0910900009999978
0.0000000000000000	0.5000000000000000	0.1827931444331625
0.0000000000000000	0.0000000000000000	0.2701758164477894
0.0000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.2500000000000000	0.0455400009999991
0.5000000000000000	0.7500000000000000	0.0455400009999991

0.0000000000000000	0.5000000000000000	0.0910900009999978
0.5000000000000000	0.7500119520163935	0.1372950642117701
0.5000000000000000	0.2499880479836065	0.1372950642117701
0.0000000000000000	0.0000000000000000	0.1830476252628443
0.5000000000000000	0.2486959908710560	0.2304854736194244
0.5000000000000000	0.7513040091289440	0.2304854736194244
0.0000000000000000	0.5000000000000000	0.2697993978265814

Bare NiCo (28.57% Co) 220 Facet - [Etot = -77.30883532 eV]

0.993794164815303

3.5450000763000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.0134000778000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.5200996398999997

Co Ni

4 10

Direct

0.0000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0910900009999978
0.0000000000000000	0.5000000000000000	0.1826907547229766
0.0000000000000000	0.0000000000000000	0.2696660201127727
0.0000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.2500000000000000	0.0455400009999991
0.5000000000000000	0.7500000000000000	0.0455400009999991
0.0000000000000000	0.5000000000000000	0.0910900009999978
0.5000000000000000	0.7493507901032075	0.1370025999022246
0.5000000000000000	0.2506492098967925	0.1370025999022246
0.0000000000000000	0.0000000000000000	0.1819664213974974
0.5000000000000000	0.2487151031307917	0.2299591562094037
0.5000000000000000	0.7512848968692083	0.2299591562094037
0.0000000000000000	0.5000000000000000	0.2697273579343289

Bare Pure-Ni 220 Facet - [Etot = -70.95118829 eV]

1.01798110552312

3.5450000763000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.0134000778000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.5200996398999997

Ni

14

Direct

0.0000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.09109000099999978
0.0000000000000000	0.5000000000000000	0.1770422364030537
0.0000000000000000	0.0000000000000000	0.2608398138929076
0.0000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.2500000000000000	0.04554000099999991
0.5000000000000000	0.7500000000000000	0.04554000099999991
0.0000000000000000	0.5000000000000000	0.09109000099999978
0.5000000000000000	0.7499626033605793	0.1338818603876248
0.5000000000000000	0.2500373966394207	0.1338818603876248
0.0000000000000000	0.0000000000000000	0.1770081288543039
0.5000000000000000	0.2500232954063648	0.2230343063240099
0.5000000000000000	0.7499767045936352	0.2230343063240099
0.0000000000000000	0.5000000000000000	0.2608656262583082

Bare NiCu (28.57% Cu) 220 Facet - [Etot = -64.65470018 eV]

0.998485100048875

3.5450000763000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.0134000778000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.5200996398999997

Cu Ni

4 10

Direct

0.0000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.09109000099999978
0.0000000000000000	0.5000000000000000	0.1814407851904036

0.0000000000000000	0.0000000000000000	0.2732427264603103
0.0000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.2500000000000000	0.0455400009999991
0.5000000000000000	0.7500000000000000	0.0455400009999991
0.0000000000000000	0.5000000000000000	0.0910900009999978
0.5000000000000000	0.7508344608217214	0.1368888301452316
0.5000000000000000	0.2491655391782786	0.1368888301452316
0.0000000000000000	0.0000000000000000	0.1827482707795909
0.5000000000000000	0.2512558193052570	0.2289303671017677
0.5000000000000000	0.7487441806947430	0.2289303671017677
0.0000000000000000	0.5000000000000000	0.2698793109472390

Bare NiZn (28.57% Zn) 220 Facet - [Etot = -57.70415899 eV]

1.01038006037737

3.5450000763000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.0134000778000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.5200996398999997

Zn Ni

4 10

Direct

0.0000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0910900009999978
0.0000000000000000	0.5000000000000000	0.1811932639445004
0.0000000000000000	0.0000000000000000	0.2738217275372961
0.0000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.2500000000000000	0.0455400009999991
0.5000000000000000	0.7500000000000000	0.0455400009999991
0.0000000000000000	0.5000000000000000	0.0910900009999978
0.5000000000000000	0.7506666104335764	0.1366888405304465
0.5000000000000000	0.2493333895664236	0.1366888405304465
0.0000000000000000	0.0000000000000000	0.1823815719361903
0.5000000000000000	0.2480670550393498	0.2285578138307471
0.5000000000000000	0.7519329449606502	0.2285578138307471

0.0000000000000000 0.5000000000000000 0.2689292886038714

NiSc (28.57% Sc) 220 Facet with Hydrogen- [Etot = -86.22694515 eV]

1.04735280294076

3.5450000763000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 5.0134000778000001 0.0000000000000000
 0.0000000000000000 0.0000000000000000 27.5200996398999997

Ti Ni H
 4 10 1

Direct

0.0000000000000000 0.5000000000000000 0.0000000000000000
 0.0000000000000000 0.0000000000000000 0.09109000099999978
 0.0000000000000000 0.5006156562202335 0.1803074518768426
 0.0000000000000000 0.0009265686610220 0.2742702427132144
 0.0000000000000000 0.0000000000000000 0.0000000000000000
 0.5000000000000000 0.2500000000000000 0.04554000099999991
 0.5000000000000000 0.7500000000000000 0.04554000099999991
 0.0000000000000000 0.5000000000000000 0.09109000099999978
 0.5000000000000000 0.7528116475667588 0.1372439226789055
 0.5000000000000000 0.2479268130705492 0.1372286140753332
 0.0000000000000000 0.0006665742537706 0.1854128314653565
 0.5000000000000000 0.2435312571991517 0.2312203995928144
 0.5000000000000000 0.7581292775655086 0.2312147036036976
 0.0000000000000000 0.5009368390732050 0.2670653684875290
 0.5000000000000000 0.5009052849659454 0.2693518237170878

NiTi (28.57% Ti) 220 Facet with Hydrogen- [Etot = -90.56844229 eV]

1.01798110552312

3.5450000763000000 0.0000000000000000 0.0000000000000000
 0.0000000000000000 5.0134000778000001 0.0000000000000000
 0.0000000000000000 0.0000000000000000 27.5200996398999997

Ti Ni H
 4 10 1

Direct

0.0000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0910900009999978
0.0000000000000000	0.5004396523593755	0.1817389398222886
0.0000000000000000	0.0007568305826595	0.2732976233555036
0.0000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.2500000000000000	0.0455400009999991
0.5000000000000000	0.7500000000000000	0.0455400009999991
0.0000000000000000	0.5000000000000000	0.0910900009999978
0.5000000000000000	0.7508216659517828	0.1377733946018935
0.5000000000000000	0.2497908856160436	0.1377809712270235
0.0000000000000000	0.0005875996001237	0.1841498514523821
0.5000000000000000	0.2435361570216088	0.2303341756020316
0.5000000000000000	0.7578697427998051	0.2303266964048092
0.0000000000000000	0.5007865941741230	0.2694182615203005
0.5000000000000000	0.5010060690450189	0.2741360535429820

NiV (28.57% V) 220 Facet with Hydrogen- [Etot = -90.73268590 eV]

1.01798110552312

3.5450000763000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.0134000778000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.5200996398999997

Ti Ni H

4 10 1

Direct

0.0000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0910900009999978
0.0000000000000000	0.5004155288131500	0.1794392912242273
0.0000000000000000	0.0007952116385681	0.2697318379972273
0.0000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.2500000000000000	0.0455400009999991
0.5000000000000000	0.7500000000000000	0.0455400009999991
0.0000000000000000	0.5000000000000000	0.0910900009999978

0.5000000000000000	0.7503244523076162	0.1354391602529290
0.5000000000000000	0.2502223371901451	0.1354378216511662
0.0000000000000000	0.0005089078136606	0.1799285628230862
0.5000000000000000	0.2449585502163458	0.2255441182003892
0.5000000000000000	0.7565045005275621	0.2255334014921999
0.0000000000000000	0.5008092505014403	0.2642344246699224
0.5000000000000000	0.5011428366572801	0.2690981329499493

NiCr (28.57% Cr) 220 Facet with Hydrogen- [Etot = -91.18828281 eV]

0.995572721824907

3.5450000763000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.0134000778000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.5200996398999997

Cr Ni H

4 10 1

Direct

0.0000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0910900009999978
0.0000000000000000	0.5005928459111786	0.1824263349284365
0.0000000000000000	0.0009469068285171	0.2768359428721681
0.0000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.2500000000000000	0.0455400009999991
0.5000000000000000	0.7500000000000000	0.0455400009999991
0.0000000000000000	0.5000000000000000	0.0910900009999978
0.5000000000000000	0.7500256209979668	0.1373861175386324
0.5000000000000000	0.2506499651781340	0.1373824745066869
0.0000000000000000	0.0005928537548172	0.1824483648522204
0.5000000000000000	0.2484367574184319	0.2295967273708541
0.5000000000000000	0.7533358554561218	0.2296021261864709
0.0000000000000000	0.5008913799408177	0.2709969933303213
0.5000000000000000	0.5017140655950101	0.2762917420319368

NiMn (28.57% Mn) 220 Facet with Hydrogen- [Etot = -91.11217186 eV]

1.01798110552312

3.5450000763000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.0134000778000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.5200996398999997

Ti Ni H

4 10 1

Direct

0.0000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.09109000099999978
0.0000000000000000	0.5005859063218310	0.1791657418979469
0.0000000000000000	0.0008774712756363	0.2698645286406247
0.0000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.2500000000000000	0.04554000099999991
0.5000000000000000	0.7500000000000000	0.04554000099999991
0.0000000000000000	0.5000000000000000	0.09109000099999978
0.5000000000000000	0.7507004521380196	0.1357621244219303
0.5000000000000000	0.2499908442078365	0.1357575024005939
0.0000000000000000	0.0006701567114220	0.1805834788524479
0.5000000000000000	0.2480935047717452	0.2269381325686837
0.5000000000000000	0.7536901421922479	0.2269436923782138
0.0000000000000000	0.5009391619907078	0.2654099180810263
0.5000000000000000	0.5009993740461525	0.2698124332647041

NiFe (28.57% Fe) 220 Facet with Hydrogen- [Etot = -87.68000922 eV]

1.0000000000000000

3.5450000763000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.0134000778000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.5200996398999997

Fe Ni H

4 10 1

Direct

0.0000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.09109000099999978

0.0000000000000000	0.5006674538188065	0.1816213631462489
0.0000000000000000	0.0011434869506814	0.2705856558411242
0.0000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.2500000000000000	0.0455400009999991
0.5000000000000000	0.7500000000000000	0.0455400009999991
0.0000000000000000	0.5000000000000000	0.0910900009999978
0.5000000000000000	0.7500813655165572	0.1375012094126262
0.5000000000000000	0.2502176953858779	0.1375169688247766
0.0000000000000000	0.0009090184406588	0.1834368880791004
0.5000000000000000	0.2474551700604763	0.2312548558982925
0.5000000000000000	0.7549227083700103	0.2311636349134503
0.0000000000000000	0.5014226833279380	0.2704856048295099
0.5000000000000000	0.5021489462762219	0.2773796174304124

NiCo (28.57% Co) 220 Facet with Hydrogen- [Etot = -81.06656270 eV]

0.993794164815303

3.5450000763000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.0134000778000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.5200996398999997

Co Ni H

4 10 1

Direct

0.0000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0910900009999978
0.0000000000000000	0.5006076576684748	0.1817539678007449
0.0000000000000000	0.0010080352707078	0.2702541568500294
0.0000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.2500000000000000	0.0455400009999991
0.5000000000000000	0.7500000000000000	0.0455400009999991
0.0000000000000000	0.5000000000000000	0.0910900009999978
0.5000000000000000	0.7497053031272642	0.1371837000970970
0.5000000000000000	0.2509801844542423	0.1371856544743224
0.0000000000000000	0.0006244354208533	0.1821400377001510

0.5000000000000000	0.2467803464317697	0.2302754645082814
0.5000000000000000	0.7550103988112227	0.2302757940889606
0.0000000000000000	0.5009881099977349	0.2702853248725603
0.5000000000000000	0.5014031044564788	0.2776670678421667

Pure-Ni 220 Facet with Hydrogen- [Etot = -74.80999210 eV]

1.01798110552312

3.5450000763000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.0134000778000001	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.5200996398999997

Ni H

14 1

Direct

0.0000000000000000	0.5000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.09109000099999978
0.0000000000000000	0.5005528740471661	0.1765879707314681
0.0000000000000000	0.0010249932991115	0.2613633713841779
0.0000000000000000	0.0000000000000000	0.0000000000000000
0.5000000000000000	0.2500000000000000	0.04554000099999991
0.5000000000000000	0.7500000000000000	0.04554000099999991
0.0000000000000000	0.5000000000000000	0.09109000099999978
0.5000000000000000	0.7503478228563694	0.1340716236893016
0.5000000000000000	0.2502320783952854	0.1340781500641768
0.0000000000000000	0.0005610433605483	0.1773058967092851
0.5000000000000000	0.2477519478970081	0.2235940306424027
0.5000000000000000	0.7540811635547158	0.2235751529770909
0.0000000000000000	0.5010386575672570	0.2614494377713896
0.5000000000000000	0.5010357849091207	0.2672000694472558

NiCu (28.57% Cu) 220 Facet with Hydrogen- [Etot = -68.59221313 eV]

0.998485100048875

3.5450000763000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	5.0134000778000001	0.0000000000000000

0.0000000000000000 0.0000000000000000 27.5200996398999997

Cu Ni H

4 10 1

Direct

0.0000000000000000 0.5000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 0.09109000099999978
0.0000000000000000 0.5005952249441492 0.1814391025104172
0.0000000000000000 0.0009420864809329 0.2733180413450214
0.0000000000000000 0.0000000000000000 0.0000000000000000
0.5000000000000000 0.2500000000000000 0.04554000099999991
0.5000000000000000 0.7500000000000000 0.04554000099999991
0.0000000000000000 0.5000000000000000 0.09109000099999978
0.5000000000000000 0.7510627687985263 0.1370116293832382
0.5000000000000000 0.2495018696824189 0.1370111217303034
0.0000000000000000 0.0005481720202027 0.1824709950709291
0.5000000000000000 0.2486801224617352 0.2291948314310375
0.5000000000000000 0.7529847458723182 0.2291889466524424
0.0000000000000000 0.5008973721816758 0.2706697324607603
0.5000000000000000 0.5009225677613642 0.2752888216974085

NiZn (28.57% Zn) 220 Facet with Hydrogen- [Etot = -61.77210979 eV]

1.01038006037737

3.5450000763000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 5.0134000778000001 0.0000000000000000
0.0000000000000000 0.0000000000000000 27.5200996398999997

Zn Ni H

4 10 1

Direct

0.0000000000000000 0.5000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 0.09109000099999978
0.0000000000000000 0.5005942121141658 0.1811787728503376
0.0000000000000000 0.0010278485597297 0.2731298547248286
0.0000000000000000 0.0000000000000000 0.0000000000000000

```

0.5000000000000000 0.2500000000000000 0.0455400009999991
0.5000000000000000 0.7500000000000000 0.0455400009999991
0.0000000000000000 0.5000000000000000 0.0910900009999978
0.5000000000000000 0.7509025681759525 0.1366843666784519
0.5000000000000000 0.2497757469533468 0.1366803870621922
0.0000000000000000 0.0006162028286738 0.1820940390095771
0.5000000000000000 0.2470386689075426 0.2289708177712555
0.5000000000000000 0.7546793530245139 0.2289680871672530
0.0000000000000000 0.5010034424687220 0.2694342630780824
0.5000000000000000 0.5009137777060246 0.2727681571483842

```

Sample VASP INCAR file -

SYSTEM = Ni Alloy (111)

```

LAECHG = .TRUE.      ##### for bader charge analysis
LCHARG = .TRUE.      ##### to write charge densities
NSIM=3              ##### NSIM>1, performance enhancement.
ISYM = 2            ##### switches on the use of symmetry, memory conserving symmetrisation
#NPAR=16           ##### vasp band parallelization
#KPAR=16           ##### vasp k points parallelization

ALGO = Fast         ##### Damped or default for hybrid functionals, Fast otherwise
PREC = Accurate
EDIFF = 1e-5        ##### electronic convergence criteria
EDIFFG = -0.01     ##### ionic convergence criteria
NELM=40            ##### maximum number of electronic SC (selfconsistency) steps
#ISMear = -5       ##### 0: Gaussian smearing, -5 : tetrahedron method with Blöchl corrections
#SIGMA = 0.05      ##### width of the smearing in eV

GGA = PE           ##### optional for HSE if the POTCAR are PBE
ENCUT = 400        ##### energy cut off

```

```
LREAL = Auto      ##### start Auto-REAL and finish FALSE
ISPIN=2           ##### 2: spin polarized 1: non-spin polarized

#Ionic relaxation
NSW = 50          ##### number of ionic steps
IBRION=2          ##### 2: conjug
```