

Supporting Information

Hydrogen oxidation on Ni-based electrocatalysts: the effect of metal doping

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1. Experimental part

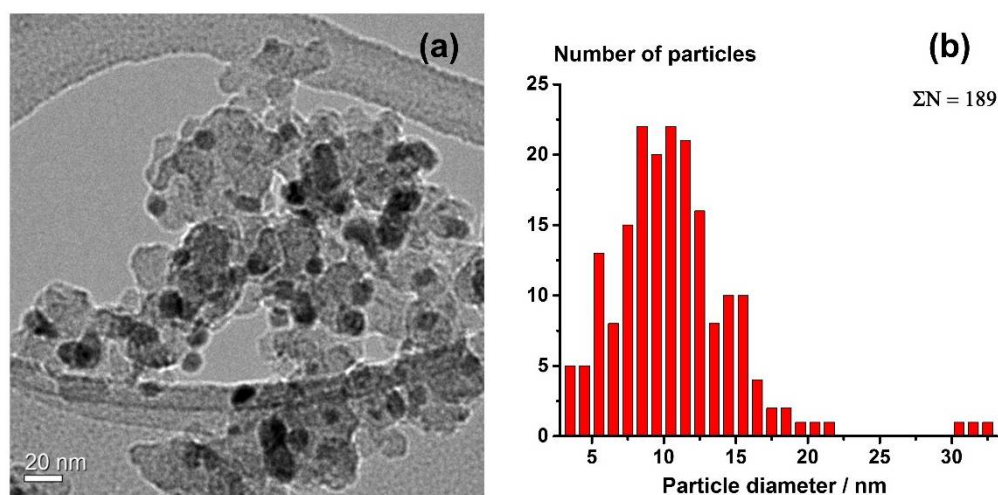


Figure S1. (a) Electron microscopy images of Ni₃Fe₁ catalyst; (b) particles size distribution for Ni₃Fe₁ catalyst.

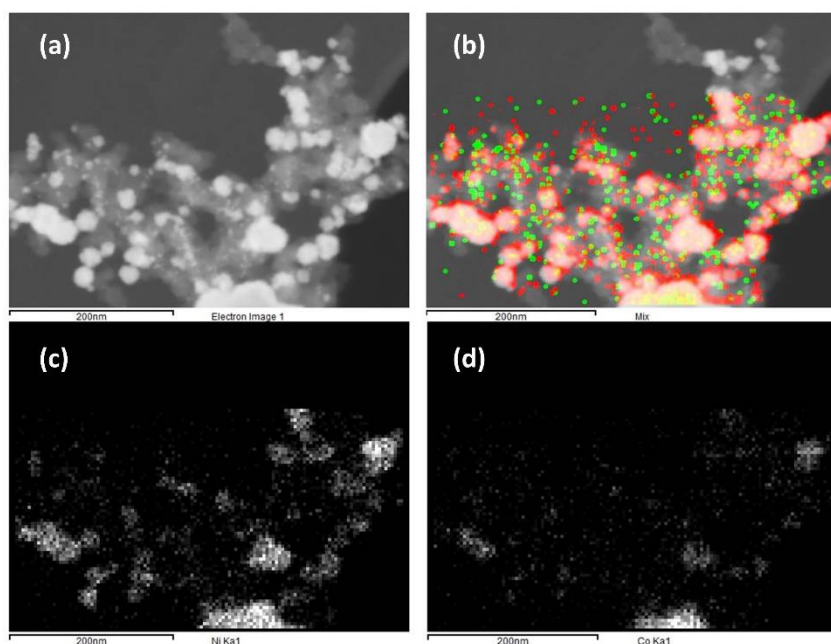


Figure 2S. STEM images of $\text{Ni}_3\text{Co}_1/\text{C}$: (a) electron image; (b) element map overlapping: Ni – red; Co – green; Ni + Co – yellow/orange; (c) mapping of Ni; (d) mapping of Co.

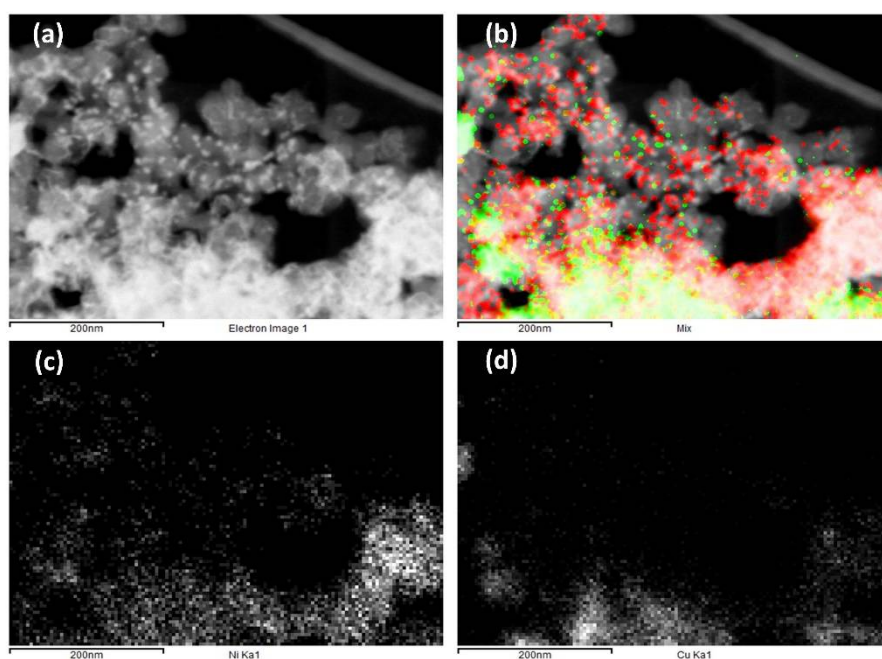


Figure S3. STEM images of $\text{Ni}_3\text{Cu}_1/\text{C}$: (a) electron image; (b) element map overlapping: Ni – red; Cu – green; Ni + Cu – yellow/orange; (c) mapping of Ni; (d) mapping of Cu.

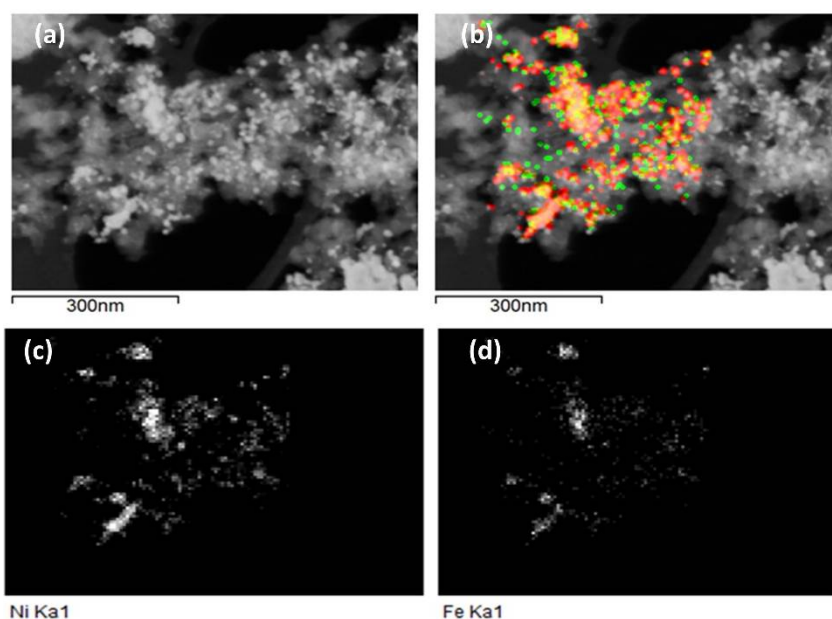


Figure S4. STEM images of $\text{Ni}_3\text{Fe}_1/\text{C}$: (a) electron image; (b) element map overlapping: Ni – red; Fe – green; Ni + Fe – yellow/orange; (c) mapping of Ni; (d) mapping of Fe.

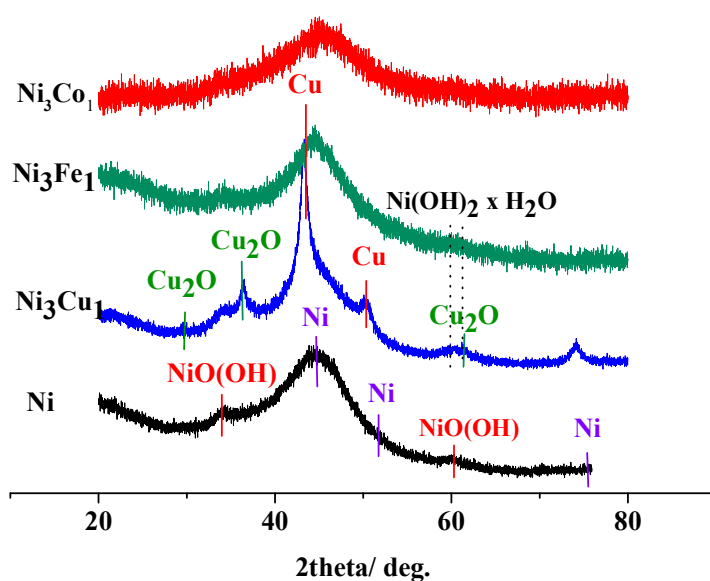


Figure S5. The main reflections of the XRD spectra for as-synthesized monometallic Ni/C catalyst and bimetallic $\text{Ni}_3\text{TM}_1/\text{C}$ composites.

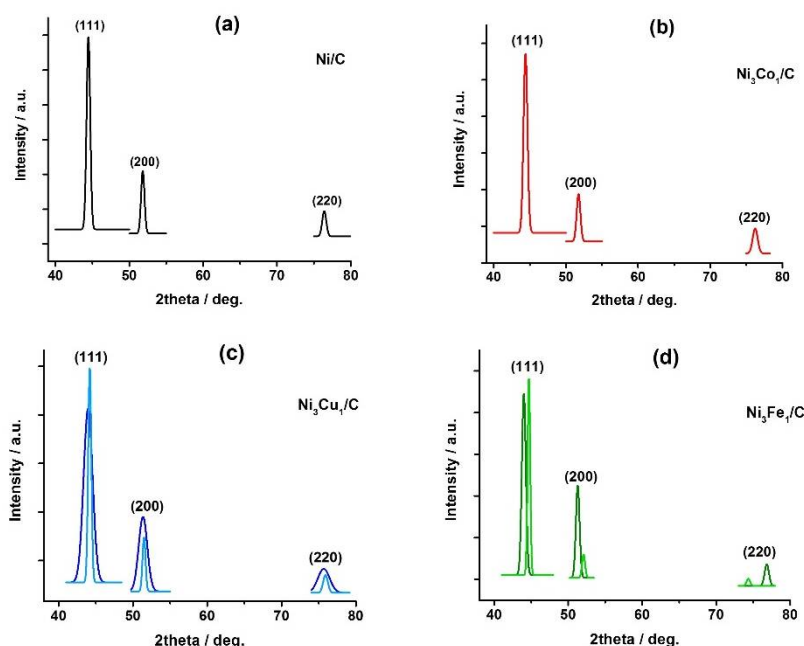


Figure S6. The main reflections of the XRD spectra for monometallic Ni/C catalyst and bimetallic $\text{Ni}_3\text{TM}_1/\text{C}$ composites after the thermal treatment at 450 °C in the mixture of 10% H_2/Ar .

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	-
$\text{Ni}_3\text{Fe}_1/\text{C}$	XPS	9.0	82.49	11.84	2.79	0.31
	EDS	2.7	72.22	14.14	9.02	3.38
$\text{Ni}_3\text{Co}_1/\text{C}$	XPS	17.3	81.11	12.43	4.16	0.24
	EDS	3.0	72.40	8.37	12.61	4.22
$\text{Ni}_3\text{Cu}_1/\text{C}$	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
$\text{Ni}_3\text{Fe}_1/\text{C}$	0.37	0.15	28.31	9.97	48.09	11.83
$\text{Ni}_3\text{Co}_1/\text{C}$	0.45	0.30	30.20	9.27	37.45	20.40
$\text{Ni}_3\text{Cu}_1/\text{C}$	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 $\text{Ni}_3\text{TM}_1/\text{C}$ 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.

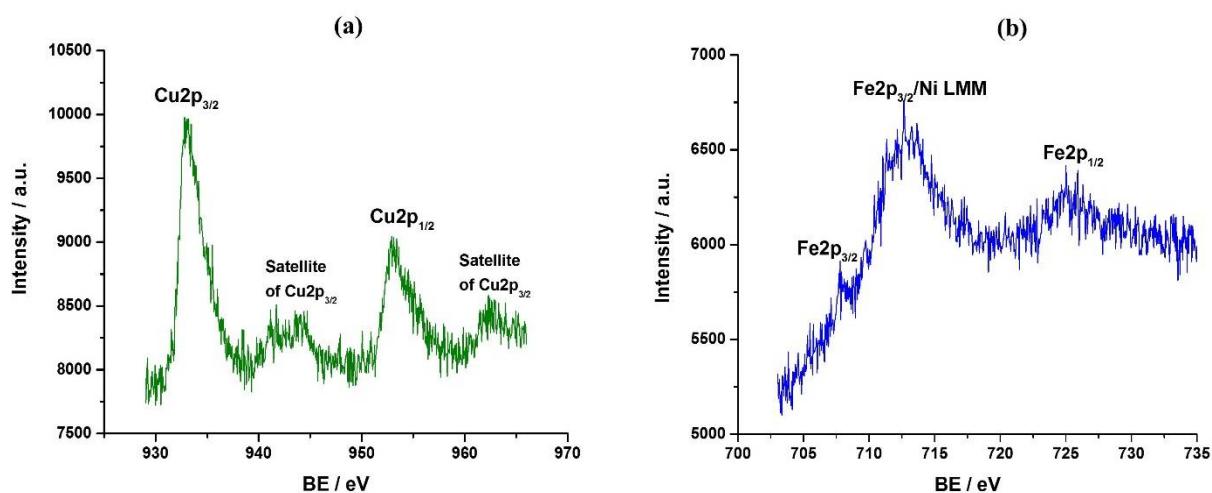


Figure S7. HR-XPS spectra for Cu of the catalyst $\text{Ni}_3\text{Cu}_1/\text{C}$ (a) and Fe of the catalyst $\text{Ni}_3\text{Fe}_1/\text{C}$ (b).

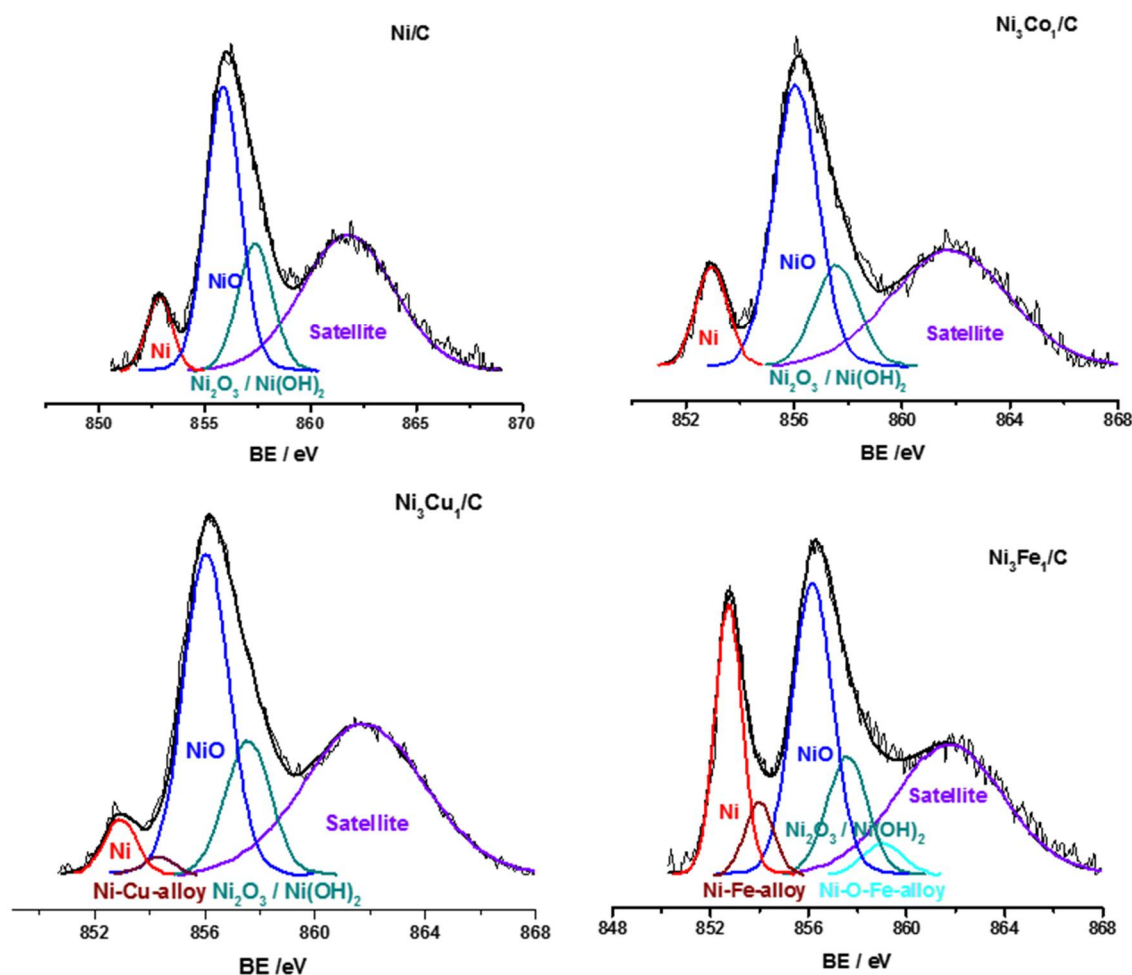


Figure S8. Deconvolution of HR XPS spectra of $\text{Ni } 2p_{3/2}$ for the chemically reduced electrocatalysts.

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 _Σ	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.

88 **2. Computational**

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94            Sc    Ni
95            20    60
96        Direct
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282	0.5000000000000000	0.5000000000000000	0.0726099979999972
283	0.3333330725788782	0.1666669414211158	0.1447204587991552
284	0.3333330725788782	0.6666669564211206	0.1447204587991552
285	0.8333331025788807	0.1666669414211158	0.1447204587991552
286	0.8333331025788807	0.6666669564211206	0.1447204587991552
287	0.1666688076781228	0.3333312223218797	0.2233001112196320
288	0.1666688076781228	0.8333311923218772	0.2233001112196320
289	0.6666688076781228	0.3333312223218797	0.2233001112196320
290	0.6666688076781228	0.8333311923218772	0.2233001112196320
291	0.0000021116020114	0.4999978843979883	0.2902124183829418
292	0.0000021116020114	0.9999978843979883	0.2902124183829418
293	0.5000021156020117	0.4999978843979883	0.2902124183829418
294	0.5000021156020117	0.9999978843979883	0.2902124183829418
295	0.1666650029999985	0.0833349970000015	0.0000000000000000

296	0.1666650029999985	0.5833349819999967	0.0000000000000000
297	0.6666650180000033	0.0833349970000015	0.0000000000000000
298	0.6666650180000033	0.5833349819999967	0.0000000000000000
299	0.4166649880000008	0.0833349970000015	0.0000000000000000
300	0.4166649880000008	0.5833349819999967	0.0000000000000000
301	0.9166649579999984	0.0833349970000015	0.0000000000000000
302	0.9166649579999984	0.5833349819999967	0.0000000000000000
303	0.4166649880000008	0.3333350119999992	0.0000000000000000
304	0.4166649880000008	0.8333350420000016	0.0000000000000000
305	0.9166649579999984	0.3333350119999992	0.0000000000000000
306	0.9166649579999984	0.8333350420000016	0.0000000000000000
307	0.0000000000000000	0.2500000000000000	0.0726099979999972
308	0.0000000000000000	0.7500000000000000	0.0726099979999972
309	0.5000000000000000	0.2500000000000000	0.0726099979999972
310	0.5000000000000000	0.7500000000000000	0.0726099979999972
311	0.2500000000000000	0.2500000000000000	0.0726099979999972
312	0.2500000000000000	0.7500000000000000	0.0726099979999972
313	0.7500000000000000	0.2500000000000000	0.0726099979999972
314	0.7500000000000000	0.7500000000000000	0.0726099979999972
315	0.2500000000000000	0.0000000000000000	0.0726099979999972
316	0.2500000000000000	0.5000000000000000	0.0726099979999972
317	0.7500000000000000	0.0000000000000000	0.0726099979999972
318	0.7500000000000000	0.5000000000000000	0.0726099979999972
319	0.3326008933568641	0.4162997158953582	0.1451924426269643
320	0.3326008933568641	0.9162997158953582	0.1451924426269643
321	0.8326008933568640	0.4162997158953582	0.1451924426269643
322	0.8326008933568640	0.9162997158953582	0.1451924426269643
323	0.0837009472096972	0.4162990307903010	0.1451922482236181
324	0.0837009472096972	0.9162990007903056	0.1451922482236181
325	0.5837009402096931	0.4162990307903010	0.1451922482236181
326	0.5837009402096931	0.9162990007903056	0.1451922482236181
327	0.0837002541046465	0.1673991066431359	0.1451924426269643
328	0.0837002541046465	0.6673991066431360	0.1451924426269643
329	0.5837002841046418	0.1673991066431359	0.1451924426269643
330	0.5837002841046418	0.6673991066431360	0.1451924426269643
331	0.1657226680597641	0.0828577557348174	0.2165934147351953
332	0.1657226680597641	0.5828577407348197	0.2165934147351953
333	0.6657226530597664	0.0828577557348174	0.2165934147351953
334	0.6657226530597664	0.5828577407348197	0.2165934147351953
335	0.4171415574776942	0.0828584285223046	0.2165935077324066
336	0.4171415574776942	0.5828584425223058	0.2165935077324066
337	0.9171415574776942	0.0828584285223046	0.2165935077324066
338	0.9171415574776942	0.5828584425223058	0.2165935077324066
339	0.4171422302651814	0.3342773469402336	0.2165934147351953
340	0.4171422302651814	0.8342773469402336	0.2165934147351953
341	0.9171422592651803	0.3342773469402336	0.2165934147351953
342	0.9171422592651803	0.8342773469402336	0.2165934147351953
343	0.0006181494091921	0.2503061182045195	0.2895166766633493
344	0.0006181494091921	0.7503061472045184	0.2895166766633493
345	0.5006181564091963	0.2503061182045195	0.2895166766633493
346	0.5006181564091963	0.7503061472045184	0.2895166766633493
347	0.2496950969927762	0.2503048880072262	0.2895162705686341

348	0.2496950969927762	0.7503048590072273	0.2895162705686341
349	0.7496950819927785	0.2503048880072262	0.2895162705686341
350	0.7496950819927785	0.7503048590072273	0.2895162705686341
351	0.2496938817954805	0.4993818435908037	0.2895166766633493
352	0.2496938817954805	0.9993818435908037	0.2895166766633493
353	0.7496938527954816	0.4993818435908037	0.2895166766633493
354	0.7496938527954816	0.9993818435908037	0.2895166766633493
355			
356	Bare- NiCr (25% Cr) 111 Facet supercell 2X2X1 - [Etot = -496.02028563 eV]		
357	0.995572721824907		
358	10.0268001556000002	0.0000000000000000	0.0000000000000000
359	-5.0134000778000001	8.6834636535000005	0.0000000000000000
360	0.0000000000000000	0.0000000000000000	28.1868000031000001
361	Cr Ni		
362	20 60		
363	Direct		
364	0.1666650029999985	0.3333350119999992	0.0000000000000000
365	0.1666650029999985	0.8333350420000016	0.0000000000000000
366	0.6666650180000033	0.3333350119999992	0.0000000000000000
367	0.6666650180000033	0.8333350420000016	0.0000000000000000
368	0.0000000000000000	0.0000000000000000	0.0726099979999972
369	0.0000000000000000	0.5000000000000000	0.0726099979999972
370	0.5000000000000000	0.0000000000000000	0.0726099979999972
371	0.5000000000000000	0.5000000000000000	0.0726099979999972
372	0.3333332074274225	0.1666668065725716	0.1453299403103543
373	0.3333332074274225	0.6666668215725764	0.1453299403103543
374	0.8333332374274249	0.1666668065725716	0.1453299403103543
375	0.8333332374274249	0.6666668215725764	0.1453299403103543
376	0.1666684834839174	0.3333315465160851	0.2221199165184728
377	0.1666684834839174	0.8333315165160826	0.2221199165184728
378	0.6666684834839174	0.3333315465160851	0.2221199165184728
379	0.6666684834839174	0.8333315165160826	0.2221199165184728
380	0.0000028796404550	0.4999971163595447	0.2921639793122779
381	0.0000028796404550	0.9999971163595447	0.2921639793122779
382	0.5000028836404553	0.4999971163595447	0.2921639793122779
383	0.5000028836404553	0.9999971163595447	0.2921639793122779
384	0.1666650029999985	0.0833349970000015	0.0000000000000000
385	0.1666650029999985	0.5833349819999967	0.0000000000000000
386	0.6666650180000033	0.0833349970000015	0.0000000000000000
387	0.6666650180000033	0.5833349819999967	0.0000000000000000
388	0.4166649880000008	0.0833349970000015	0.0000000000000000
389	0.4166649880000008	0.5833349819999967	0.0000000000000000
390	0.9166649579999984	0.0833349970000015	0.0000000000000000
391	0.9166649579999984	0.5833349819999967	0.0000000000000000
392	0.4166649880000008	0.3333350119999992	0.0000000000000000
393	0.4166649880000008	0.8333350420000016	0.0000000000000000
394	0.9166649579999984	0.3333350119999992	0.0000000000000000
395	0.9166649579999984	0.8333350420000016	0.0000000000000000
396	0.0000000000000000	0.2500000000000000	0.0726099979999972
397	0.0000000000000000	0.7500000000000000	0.0726099979999972
398	0.5000000000000000	0.2500000000000000	0.0726099979999972
399	0.5000000000000000	0.7500000000000000	0.0726099979999972

400	0.2500000000000000	0.2500000000000000	0.0726099979999972
401	0.2500000000000000	0.7500000000000000	0.0726099979999972
402	0.7500000000000000	0.2500000000000000	0.0726099979999972
403	0.7500000000000000	0.7500000000000000	0.0726099979999972
404	0.2500000000000000	0.0000000000000000	0.0726099979999972
405	0.2500000000000000	0.5000000000000000	0.0726099979999972
406	0.7500000000000000	0.0000000000000000	0.0726099979999972
407	0.7500000000000000	0.5000000000000000	0.0726099979999972
408	0.3327292432529703	0.4163633881598585	0.1457636164680665
409	0.3327292432529703	0.9163633881598585	0.1457636164680665
410	0.8327292432529703	0.4163633881598585	0.1457636164680665
411	0.8327292432529703	0.9163633881598585	0.1457636164680665
412	0.0836343429218616	0.4163656350781366	0.1457635424375567
413	0.0836343429218616	0.9163656050781412	0.1457635424375567
414	0.5836343359218574	0.4163656350781366	0.1457635424375567
415	0.5836343359218574	0.9163656050781412	0.1457635424375567
416	0.0836365818401461	0.1672707567470297	0.1457636164680665
417	0.0836365818401461	0.6672707567470297	0.1457636164680665
418	0.5836366118401415	0.1672707567470297	0.1457636164680665
419	0.5836366118401415	0.6672707567470297	0.1457636164680665
420	0.1667022608071989	0.0833492381847876	0.2178230715861247
421	0.1667022608071989	0.5833492231847899	0.2178230715861247
422	0.6667022458072012	0.0833492381847876	0.2178230715861247
423	0.6667022458072012	0.5833492231847899	0.2178230715861247
424	0.4166501284783664	0.0833498575216325	0.2178229868053663
425	0.4166501284783664	0.5833498715216336	0.2178229868053663
426	0.9166501284783664	0.0833498575216325	0.2178229868053663
427	0.9166501284783664	0.5833498715216336	0.2178229868053663
428	0.4166507478152113	0.3332977541927988	0.2178230715861247
429	0.4166507478152113	0.8332977541927988	0.2178230715861247
430	0.9166507768152101	0.3332977541927988	0.2178230715861247
431	0.9166507768152101	0.8332977541927988	0.2178230715861247
432	0.0017294364182305	0.2508603656883892	0.2906462910142693
433	0.0017294364182305	0.7508603946883881	0.2906462910142693
434	0.5017294434182347	0.2508603656883892	0.2906462910142693
435	0.5017294434182347	0.7508603946883881	0.2906462910142693
436	0.2491390440141572	0.2508609409858451	0.2906458196759303
437	0.2491390440141572	0.7508609119858463	0.2906458196759303
438	0.7491390290141595	0.2508609409858451	0.2906458196759303
439	0.7491390290141595	0.7508609119858463	0.2906458196759303
440	0.2491396343116108	0.4982705565817653	0.2906462910142693
441	0.2491396343116108	0.9982705565817653	0.2906462910142693
442	0.7491396053116119	0.4982705565817653	0.2906462910142693
443	0.7491396053116119	0.9982705565817653	0.2906462910142693
444			
445	Bare- NiMn (25% Mn) 111 Facet supercell 2X2X1 - [Etot = -494.23957091 eV]		
446	1.0000000000000000		
447	9.9196901320999995	0.0000000000000000	0.0000000000000000
448	-4.9598426818999997	8.5906995225999996	0.0000000000000000
449	0.0000000000000000	0.0000000000000000	27.8856849669999995
450	Mn Ni		
451	20 60		

452	Direct		
453	0.1666650029999985	0.3333350119999992	0.0000000000000000
454	0.1666650029999985	0.8333350420000016	0.0000000000000000
455	0.6666650180000033	0.3333350119999992	0.0000000000000000
456	0.6666650180000033	0.8333350420000016	0.0000000000000000
457	0.0000000000000000	0.0000000000000000	0.0726099979999972
458	0.0000000000000000	0.5000000000000000	0.0726099979999972
459	0.5000000000000000	0.0000000000000000	0.0726099979999972
460	0.5000000000000000	0.5000000000000000	0.0726099979999972
461	0.3332655297792186	0.1666153471837717	0.1475653398308197
462	0.3332655297792186	0.6666153771837671	0.1475653398308197
463	0.8332655297792186	0.1666153471837717	0.1475653398308197
464	0.8332655297792186	0.6666153771837671	0.1475653398308197
465	0.1665489000084364	0.3332417222975437	0.2214153618003110
466	0.1665489000084364	0.8332417522975462	0.2214153618003110
467	0.6665489300084388	0.3332417222975437	0.2214153618003110
468	0.6665489300084388	0.8332417522975462	0.2214153618003110
469	0.4998042605921995	0.4998180188418289	0.2989863608164285
470	0.4998042605921995	0.9998180188418289	0.2989863608164285
471	0.9998042605921995	0.4998180188418289	0.2989863608164285
472	0.9998042605921995	0.9998180188418289	0.2989863608164285
473	0.1666650029999985	0.0833349970000015	0.0000000000000000
474	0.1666650029999985	0.5833349819999967	0.0000000000000000
475	0.6666650180000033	0.0833349970000015	0.0000000000000000
476	0.6666650180000033	0.5833349819999967	0.0000000000000000
477	0.0000000000000000	0.2500000000000000	0.0726099979999972
478	0.0000000000000000	0.7500000000000000	0.0726099979999972
479	0.5000000000000000	0.2500000000000000	0.0726099979999972
480	0.5000000000000000	0.7500000000000000	0.0726099979999972
481	0.4166649880000008	0.0833349970000015	0.0000000000000000
482	0.4166649880000008	0.5833349819999967	0.0000000000000000
483	0.9166649579999984	0.0833349970000015	0.0000000000000000
484	0.9166649579999984	0.5833349819999967	0.0000000000000000
485	0.2500000000000000	0.2500000000000000	0.0726099979999972
486	0.2500000000000000	0.7500000000000000	0.0726099979999972
487	0.7500000000000000	0.2500000000000000	0.0726099979999972
488	0.7500000000000000	0.7500000000000000	0.0726099979999972
489	0.4166649880000008	0.3333350119999992	0.0000000000000000
490	0.4166649880000008	0.8333350420000016	0.0000000000000000
491	0.9166649579999984	0.3333350119999992	0.0000000000000000
492	0.9166649579999984	0.8333350420000016	0.0000000000000000
493	0.2500000000000000	0.0000000000000000	0.0726099979999972
494	0.2500000000000000	0.5000000000000000	0.0726099979999972
495	0.7500000000000000	0.0000000000000000	0.0726099979999972
496	0.7500000000000000	0.5000000000000000	0.0726099979999972
497	0.3333865505946747	0.4166793897176788	0.1471594019476044
498	0.3333865505946747	0.9166794197176813	0.1471594019476044
499	0.8333865805946701	0.4166793897176788	0.1471594019476044
500	0.8333865805946701	0.9166794197176813	0.1471594019476044
501	0.1655331831062412	0.0827304573798884	0.2218632412338550
502	0.1655331831062412	0.5827304503798914	0.2218632412338550
503	0.6655331981062389	0.0827304573798884	0.2218632412338550

504	0.6655331981062389	0.5827304503798914	0.2218632412338550
505	0.4997703596160292	0.2498009190038673	0.2946061984893120
506	0.4997703596160292	0.7498009050038732	0.2946061984893120
507	0.9997703296160338	0.2498009190038673	0.2946061984893120
508	0.9997703296160338	0.7498009050038732	0.2946061984893120
509	0.0832032256285586	0.4166769875853618	0.1471597890047533
510	0.0832032256285586	0.9166769875853618	0.1471597890047533
511	0.5832032406285563	0.4166769875853618	0.1471597890047533
512	0.5832032406285563	0.9166769875853618	0.1471597890047533
513	0.4170602786834294	0.0827236536617448	0.2218613870855037
514	0.4170602786834294	0.5827236756617467	0.2218613870855037
515	0.9170602786834294	0.0827236536617448	0.2218613870855037
516	0.9170602786834294	0.5827236756617467	0.2218613870855037
517	0.2498345674826226	0.2497942679548117	0.2946056206265979
518	0.2498345674826226	0.7497942379548093	0.2946056206265979
519	0.7498345974826179	0.2497942679548117	0.2946056206265979
520	0.7498345974826179	0.7497942379548093	0.2946056206265979
521	0.0832041910890169	0.1664848653155246	0.1471606587475449
522	0.0832041910890169	0.6664848803155223	0.1471606587475449
523	0.5832042130890187	0.1664848653155246	0.1471606587475449
524	0.5832042130890187	0.6664848803155223	0.1471606587475449
525	0.4170608262194406	0.3342549782214732	0.2218627604183112
526	0.4170608262194406	0.8342549782214732	0.2218627604183112
527	0.9170608262194406	0.3342549782214732	0.2218627604183112
528	0.9170608262194406	0.8342549782214732	0.2218627604183112
529	0.2498333110093185	0.9998693950860940	0.2946083798932975
530	0.2498333110093185	0.4998693940860974	0.2946083798932975
531	0.7498333110093185	0.9998693950860940	0.2946083798932975
532	0.7498333110093185	0.4998693940860974	0.2946083798932975
533			
534	Bare- NiFe (25% Fe) 111 Facet supercell 2X2X1 - [Etot = -479.68023055 eV]		
535	1.000000000000000		
536	10.0268001556000002	0.0000000000000000	0.0000000000000000
537	-5.0134000778000001	8.6834636535000005	0.0000000000000000
538	0.0000000000000000	0.0000000000000000	28.1868000031000001
539	Fe Ni		
540	20 60		
541	Direct		
542	0.1666650029999985	0.3333350119999992	0.0000000000000000
543	0.1666650029999985	0.8333350420000016	0.0000000000000000
544	0.6666650180000033	0.3333350119999992	0.0000000000000000
545	0.6666650180000033	0.8333350420000016	0.0000000000000000
546	0.0000000000000000	0.0000000000000000	0.0726099979999972
547	0.0000000000000000	0.5000000000000000	0.0726099979999972
548	0.5000000000000000	0.0000000000000000	0.0726099979999972
549	0.5000000000000000	0.5000000000000000	0.0726099979999972
550	0.3333360210443530	0.1666639929556410	0.1447816711106995
551	0.3333360210443530	0.6666640079556458	0.1447816711106995
552	0.8333360510443555	0.1666639929556410	0.1447816711106995
553	0.8333360510443555	0.6666640079556458	0.1447816711106995
554	0.1666694936690902	0.3333305363309123	0.2193817578125845
555	0.1666694936690902	0.8333305063309098	0.2193817578125845

556	0.6666694936690902	0.3333305363309123	0.2193817578125845
557	0.6666694936690902	0.8333305063309098	0.2193817578125845
558	0.0000040302016373	0.4999959657983624	0.2885585145670859
559	0.0000040302016373	0.9999959657983624	0.2885585145670859
560	0.5000040342016376	0.4999959657983624	0.2885585145670859
561	0.5000040342016376	0.9999959657983624	0.2885585145670859
562	0.1666650029999985	0.0833349970000015	0.0000000000000000
563	0.1666650029999985	0.5833349819999967	0.0000000000000000
564	0.6666650180000033	0.0833349970000015	0.0000000000000000
565	0.6666650180000033	0.5833349819999967	0.0000000000000000
566	0.4166649880000008	0.0833349970000015	0.0000000000000000
567	0.4166649880000008	0.5833349819999967	0.0000000000000000
568	0.9166649579999984	0.0833349970000015	0.0000000000000000
569	0.9166649579999984	0.5833349819999967	0.0000000000000000
570	0.4166649880000008	0.3333350119999992	0.0000000000000000
571	0.4166649880000008	0.8333350420000016	0.0000000000000000
572	0.9166649579999984	0.3333350119999992	0.0000000000000000
573	0.9166649579999984	0.8333350420000016	0.0000000000000000
574	0.0000000000000000	0.2500000000000000	0.0726099979999972
575	0.0000000000000000	0.7500000000000000	0.0726099979999972
576	0.5000000000000000	0.2500000000000000	0.0726099979999972
577	0.5000000000000000	0.7500000000000000	0.0726099979999972
578	0.2500000000000000	0.2500000000000000	0.0726099979999972
579	0.2500000000000000	0.7500000000000000	0.0726099979999972
580	0.7500000000000000	0.2500000000000000	0.0726099979999972
581	0.7500000000000000	0.7500000000000000	0.0726099979999972
582	0.2500000000000000	0.0000000000000000	0.0726099979999972
583	0.2500000000000000	0.5000000000000000	0.0726099979999972
584	0.7500000000000000	0.0000000000000000	0.0726099979999972
585	0.7500000000000000	0.5000000000000000	0.0726099979999972
586	0.3330025544636754	0.4164974464143967	0.1452001606008508
587	0.3330025544636754	0.9164974464143967	0.1452001606008508
588	0.8330025544636754	0.4164974464143967	0.1452001606008508
589	0.8330025544636754	0.9164974464143967	0.1452001606008508
590	0.0835002407555834	0.4164997372444148	0.1451997975413732
591	0.0835002407555834	0.9164997072444194	0.1451997975413732
592	0.5835002337555792	0.4164997372444148	0.1451997975413732
593	0.5835002337555792	0.9164997072444194	0.1451997975413732
594	0.0835025235856079	0.1669974455363246	0.1452001606008508
595	0.0835025235856079	0.6669974455363246	0.1452001606008508
596	0.5835025535856033	0.1669974455363246	0.1452001606008508
597	0.5835025535856033	0.6669974455363246	0.1452001606008508
598	0.1669313964638022	0.0834601952999705	0.2172782882973081
599	0.1669313964638022	0.5834601802999728	0.2172782882973081
600	0.6669313814638045	0.0834601952999705	0.2172782882973081
601	0.6669313814638045	0.5834601802999728	0.2172782882973081
602	0.4165397231218151	0.0834602628781838	0.2172779930189321
603	0.4165397231218151	0.5834602768781849	0.2172779930189321
604	0.9165397231218151	0.0834602628781838	0.2172779930189321
605	0.9165397231218151	0.5834602768781849	0.2172779930189321
606	0.4165397907000283	0.3330686185361955	0.2172782882973081
607	0.4165397907000283	0.8330686185361955	0.2172782882973081

608	0.9165398197000272	0.3330686185361955	0.2172782882973081
609	0.9165398197000272	0.8330686185361955	0.2172782882973081
610	0.0011359679369107	0.2505585176516618	0.2889156470911729
611	0.0011359679369107	0.7505585466516607	0.2889156470911729
612	0.5011359749369149	0.2505585176516618	0.2889156470911729
613	0.5011359749369149	0.7505585466516607	0.2889156470911729
614	0.2494434796382308	0.2505565053617715	0.2889157699769100
615	0.2494434796382308	0.7505564763617727	0.2889157699769100
616	0.7494434646382331	0.2505565053617715	0.2889157699769100
617	0.7494434646382331	0.7505564763617727	0.2889157699769100
618	0.2494414823483382	0.4988640250630851	0.2889156470911729
619	0.2494414823483382	0.9988640250630851	0.2889156470911729
620	0.7494414533483393	0.4988640250630851	0.2889156470911729
621	0.7494414533483393	0.9988640250630851	0.2889156470911729
622			
623	Bare- NiCo (25% Co) 111 Facet supercell 2X2X1 - [Etot = -447.05815167 eV]		
624	0.993794164815303		
625	10.0268001556000002	0.0000000000000000	0.0000000000000000
626	-5.0134000778000001	8.6834636535000005	0.0000000000000000
627	0.0000000000000000	0.0000000000000000	28.1868000031000001
628	Co Ni		
629	20 60		
630	Direct		
631	0.1666650029999985	0.3333350119999992	0.0000000000000000
632	0.1666650029999985	0.8333350420000016	0.0000000000000000
633	0.6666650180000033	0.3333350119999992	0.0000000000000000
634	0.6666650180000033	0.8333350420000016	0.0000000000000000
635	0.0000000000000000	0.0000000000000000	0.0726099979999972
636	0.0000000000000000	0.5000000000000000	0.0726099979999972
637	0.5000000000000000	0.0000000000000000	0.0726099979999972
638	0.5000000000000000	0.5000000000000000	0.0726099979999972
639	0.3333356960742080	0.1666643179257861	0.1447750049574452
640	0.3333356960742080	0.6666643329257909	0.1447750049574452
641	0.8333357260742105	0.1666643179257861	0.1447750049574452
642	0.8333357260742105	0.6666643329257909	0.1447750049574452
643	0.1666704434869999	0.3333295865130026	0.2193115505540675
644	0.1666704434869999	0.8333295565130001	0.2193115505540675
645	0.6666704434869999	0.3333295865130026	0.2193115505540675
646	0.6666704434869999	0.8333295565130001	0.2193115505540675
647	0.0000045859499664	0.4999954100500332	0.2886886571841742
648	0.0000045859499664	0.9999954100500332	0.2886886571841742
649	0.5000045899499668	0.4999954100500332	0.2886886571841742
650	0.5000045899499668	0.9999954100500332	0.2886886571841742
651	0.1666650029999985	0.0833349970000015	0.0000000000000000
652	0.1666650029999985	0.5833349819999967	0.0000000000000000
653	0.6666650180000033	0.0833349970000015	0.0000000000000000
654	0.6666650180000033	0.5833349819999967	0.0000000000000000
655	0.4166649880000008	0.0833349970000015	0.0000000000000000
656	0.4166649880000008	0.5833349819999967	0.0000000000000000
657	0.9166649579999984	0.0833349970000015	0.0000000000000000
658	0.9166649579999984	0.5833349819999967	0.0000000000000000
659	0.4166649880000008	0.3333350119999992	0.0000000000000000

660	0.4166649880000008	0.8333350420000016	0.0000000000000000
661	0.9166649579999984	0.3333350119999992	0.0000000000000000
662	0.9166649579999984	0.8333350420000016	0.0000000000000000
663	0.0000000000000000	0.2500000000000000	0.0726099979999972
664	0.0000000000000000	0.7500000000000000	0.0726099979999972
665	0.5000000000000000	0.2500000000000000	0.0726099979999972
666	0.5000000000000000	0.7500000000000000	0.0726099979999972
667	0.2500000000000000	0.2500000000000000	0.0726099979999972
668	0.2500000000000000	0.7500000000000000	0.0726099979999972
669	0.7500000000000000	0.2500000000000000	0.0726099979999972
670	0.7500000000000000	0.7500000000000000	0.0726099979999972
671	0.2500000000000000	0.0000000000000000	0.0726099979999972
672	0.2500000000000000	0.5000000000000000	0.0726099979999972
673	0.7500000000000000	0.0000000000000000	0.0726099979999972
674	0.7500000000000000	0.5000000000000000	0.0726099979999972
675	0.3330524162472273	0.4165222175555243	0.1451676484252502
676	0.3330524162472273	0.9165222175555243	0.1451676484252502
677	0.8330524162472273	0.4165222175555243	0.1451676484252502
678	0.8330524162472273	0.9165222175555243	0.1451676484252502
679	0.0834775628387234	0.4165224151612748	0.1451674547121158
680	0.0834775628387234	0.9165223851612794	0.1451674547121158
681	0.5834775558387193	0.4165224151612748	0.1451674547121158
682	0.5834775558387193	0.9165223851612794	0.1451674547121158
683	0.0834777524444803	0.1669475837527727	0.1451676484252502
684	0.0834777524444803	0.6669475837527727	0.1451676484252502
685	0.5834777824444757	0.1669475837527727	0.1451676484252502
686	0.5834777824444757	0.6669475837527727	0.1451676484252502
687	0.1668770510505979	0.0834320915875821	0.2172445623688759
688	0.1668770510505979	0.5834320765875844	0.2172445623688759
689	0.6668770360506002	0.0834320915875821	0.2172445623688759
690	0.6668770360506002	0.5834320765875844	0.2172445623688759
691	0.4165669488927790	0.0834330371072198	0.2172446776818262
692	0.4165669488927790	0.5834330511072210	0.2172446776818262
693	0.9165669488927790	0.0834330371072198	0.2172446776818262
694	0.9165669488927790	0.5834330511072210	0.2172446776818262
695	0.4165678944124167	0.3331229639493998	0.2172445623688759
696	0.4165678944124167	0.8331229639493998	0.2172445623688759
697	0.9165679234124156	0.3331229639493998	0.2172445623688759
698	0.9165679234124156	0.8331229639493998	0.2172445623688759
699	0.0008713944834753	0.2504292352332769	0.2889490873343235
700	0.0008713944834753	0.7504292642332757	0.2889490873343235
701	0.5008714014834794	0.2504292352332769	0.2889490873343235
702	0.5008714014834794	0.7504292642332757	0.2889490873343235
703	0.2495694075417205	0.2504305774582818	0.2889482824187439
704	0.2495694075417205	0.7504305484582829	0.2889482824187439
705	0.7495693925417228	0.2504305774582818	0.2889482824187439
706	0.7495693925417228	0.7504305484582829	0.2889482824187439
707	0.2495707647667231	0.4991285985165206	0.2889490873343235
708	0.2495707647667231	0.9991285985165206	0.2889490873343235
709	0.7495707357667243	0.4991285985165206	0.2889490873343235
710	0.7495707357667243	0.9991285985165206	0.2889490873343235
711			

712	Pure-Ni 111 Facet supercell 2X2X1 - [Etot = -414.05399553 eV]		
713	1.01798110552312		
714	10.0268001556000002	0.0000000000000000	0.0000000000000000
715	-5.0134000778000001	8.6834636535000005	0.0000000000000000
716	0.0000000000000000	0.0000000000000000	28.1868000031000001
717	Ni		
718	80		
719	Direct		
720	0.1666650029999985	0.3333350119999992	0.0000000000000000
721	0.1666650029999985	0.8333350420000016	0.0000000000000000
722	0.6666650180000033	0.3333350119999992	0.0000000000000000
723	0.6666650180000033	0.8333350420000016	0.0000000000000000
724	0.0000000000000000	0.0000000000000000	0.0726099979999972
725	0.0000000000000000	0.5000000000000000	0.0726099979999972
726	0.5000000000000000	0.0000000000000000	0.0726099979999972
727	0.5000000000000000	0.5000000000000000	0.0726099979999972
728	0.3333379266307901	0.1666620873692040	0.1419871965719892
729	0.3333379266307901	0.6666621023692088	0.1419871965719892
730	0.8333379566307926	0.1666620873692040	0.1419871965719892
731	0.8333379566307926	0.6666621023692088	0.1419871965719892
732	0.1666705248782634	0.3333295051217391	0.2116348075142653
733	0.1666705248782634	0.8333294751217366	0.2116348075142653
734	0.6666705248782634	0.3333295051217391	0.2116348075142653
735	0.6666705248782634	0.8333294751217366	0.2116348075142653
736	0.0000050457843344	0.4999949502156653	0.2801756840107572
737	0.0000050457843344	0.9999949502156653	0.2801756840107572
738	0.5000050497843347	0.4999949502156653	0.2801756840107572
739	0.5000050497843347	0.9999949502156653	0.2801756840107572
740	0.1666650029999985	0.0833349970000015	0.0000000000000000
741	0.1666650029999985	0.5833349819999967	0.0000000000000000
742	0.6666650180000033	0.0833349970000015	0.0000000000000000
743	0.6666650180000033	0.5833349819999967	0.0000000000000000
744	0.4166649880000008	0.0833349970000015	0.0000000000000000
745	0.4166649880000008	0.5833349819999967	0.0000000000000000
746	0.9166649579999984	0.0833349970000015	0.0000000000000000
747	0.9166649579999984	0.5833349819999967	0.0000000000000000
748	0.4166649880000008	0.3333350119999992	0.0000000000000000
749	0.4166649880000008	0.8333350420000016	0.0000000000000000
750	0.9166649579999984	0.3333350119999992	0.0000000000000000
751	0.9166649579999984	0.8333350420000016	0.0000000000000000
752	0.0000000000000000	0.2500000000000000	0.0726099979999972
753	0.0000000000000000	0.7500000000000000	0.0726099979999972
754	0.5000000000000000	0.2500000000000000	0.0726099979999972
755	0.5000000000000000	0.7500000000000000	0.0726099979999972
756	0.2500000000000000	0.2500000000000000	0.0726099979999972
757	0.2500000000000000	0.7500000000000000	0.0726099979999972
758	0.7500000000000000	0.2500000000000000	0.0726099979999972
759	0.7500000000000000	0.7500000000000000	0.0726099979999972
760	0.2500000000000000	0.0000000000000000	0.0726099979999972
761	0.2500000000000000	0.5000000000000000	0.0726099979999972
762	0.7500000000000000	0.0000000000000000	0.0726099979999972
763	0.7500000000000000	0.5000000000000000	0.0726099979999972

764	0.3333734635052537	0.4166834890118736	0.1419692388587279
765	0.3333734635052537	0.9166834890118736	0.1419692388587279
766	0.8333734635052537	0.4166834890118736	0.1419692388587279
767	0.8333734635052537	0.9166834890118736	0.1419692388587279
768	0.0833184196422536	0.4166815583577446	0.1419683661446669
769	0.0833184196422536	0.9166815283577563	0.1419683661446669
770	0.5833184126422424	0.4166815583577446	0.1419683661446669
771	0.5833184126422424	0.9166815283577563	0.1419683661446669
772	0.0833164809881310	0.1666265364947463	0.1419692388587279
773	0.0833164809881310	0.6666265364947463	0.1419692388587279
774	0.5833165109881264	0.1666265364947463	0.1419692388587279
775	0.5833165109881264	0.6666265364947463	0.1419692388587279
776	0.1666671267871607	0.0833265077298861	0.2116606263748011
777	0.1666671267871607	0.5833264927298885	0.2116606263748011
778	0.6666671117871630	0.0833265077298861	0.2116606263748011
779	0.6666671117871630	0.5833264927298885	0.2116606263748011
780	0.4166717466262497	0.0833282393737491	0.2116617771692688
781	0.4166717466262497	0.5833282533737503	0.2116617771692688
782	0.9166717466262497	0.0833282393737491	0.2116617771692688
783	0.9166717466262497	0.5833282533737503	0.2116617771692688
784	0.4166734782701127	0.3333328882128370	0.2116606263748011
785	0.4166734782701127	0.8333328882128370	0.2116606263748011
786	0.9166735072701115	0.3333328882128370	0.2116606263748011
787	0.9166735072701115	0.8333328882128370	0.2116606263748011
788	0.0000075353253024	0.2499990047850531	0.2801213495404440
789	0.0000075353253024	0.7499990337850519	0.2801213495404440
790	0.5000075423253065	0.2499990047850531	0.2801213495404440
791	0.5000075423253065	0.7499990337850519	0.2801213495404440
792	0.2500038375296896	0.2499961474703127	0.2801228248185836
793	0.2500038375296896	0.7499961184703139	0.2801228248185836
794	0.7500038225296919	0.2499961474703127	0.2801228248185836
795	0.7500038225296919	0.7499961184703139	0.2801228248185836
796	0.2500009952149469	0.4999924576746935	0.2801213495404440
797	0.2500009952149469	0.9999924576746935	0.2801213495404440
798	0.7500009662149481	0.4999924576746935	0.2801213495404440
799	0.7500009662149481	0.9999924576746935	0.2801213495404440

800

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

802 0.998485100048875

803	10.0268001556000002	0.0000000000000000	0.0000000000000000
804	-5.0134000778000001	8.6834636535000005	0.0000000000000000
805	0.0000000000000000	0.0000000000000000	28.1868000031000001

806 Cu Ni

807 20 60

808 Direct

809	0.1666650029999985	0.3333350119999992	0.0000000000000000
810	0.1666650029999985	0.8333350420000016	0.0000000000000000
811	0.6666650180000033	0.3333350119999992	0.0000000000000000
812	0.6666650180000033	0.8333350420000016	0.0000000000000000
813	0.0000000000000000	0.0000000000000000	0.0726099979999972
814	0.0000000000000000	0.5000000000000000	0.0726099979999972
815	0.5000000000000000	0.0000000000000000	0.0726099979999972

816	0.5000000000000000	0.5000000000000000	0.0726099979999972
817	0.3333288493490585	0.1666711646509356	0.1456301058409792
818	0.3333288493490585	0.6666711796509404	0.1456301058409792
819	0.8333288793490610	0.1666711646509356	0.1456301058409792
820	0.8333288793490610	0.6666711796509404	0.1456301058409792
821	0.1666825622939569	0.3333174677060455	0.2171562731733374
822	0.1666825622939569	0.8333174377060502	0.2171562731733374
823	0.6666825622939498	0.3333174677060455	0.2171562731733374
824	0.6666825622939498	0.8333174377060502	0.2171562731733374
825	0.0000009067924225	0.4999990892075772	0.2929619156089061
826	0.0000009067924225	0.9999990892075772	0.2929619156089061
827	0.5000009107924228	0.4999990892075772	0.2929619156089061
828	0.5000009107924228	0.9999990892075772	0.2929619156089061
829	0.1666650029999985	0.0833349970000015	0.0000000000000000
830	0.1666650029999985	0.5833349819999967	0.0000000000000000
831	0.6666650180000033	0.0833349970000015	0.0000000000000000
832	0.6666650180000033	0.5833349819999967	0.0000000000000000
833	0.4166649880000008	0.0833349970000015	0.0000000000000000
834	0.4166649880000008	0.5833349819999967	0.0000000000000000
835	0.9166649579999984	0.0833349970000015	0.0000000000000000
836	0.9166649579999984	0.5833349819999967	0.0000000000000000
837	0.4166649880000008	0.3333350119999992	0.0000000000000000
838	0.4166649880000008	0.8333350420000016	0.0000000000000000
839	0.9166649579999984	0.3333350119999992	0.0000000000000000
840	0.9166649579999984	0.8333350420000016	0.0000000000000000
841	0.0000000000000000	0.2500000000000000	0.0726099979999972
842	0.0000000000000000	0.7500000000000000	0.0726099979999972
843	0.5000000000000000	0.2500000000000000	0.0726099979999972
844	0.5000000000000000	0.7500000000000000	0.0726099979999972
845	0.2500000000000000	0.2500000000000000	0.0726099979999972
846	0.2500000000000000	0.7500000000000000	0.0726099979999972
847	0.7500000000000000	0.2500000000000000	0.0726099979999972
848	0.7500000000000000	0.7500000000000000	0.0726099979999972
849	0.2500000000000000	0.0000000000000000	0.0726099979999972
850	0.2500000000000000	0.5000000000000000	0.0726099979999972
851	0.7500000000000000	0.0000000000000000	0.0726099979999972
852	0.7500000000000000	0.5000000000000000	0.0726099979999972
853	0.3336236873540130	0.4168093850592030	0.1451601048952185
854	0.3336236873540130	0.9168093850592030	0.1451601048952185
855	0.8336236873540130	0.4168093850592030	0.1451601048952185
856	0.8336236873540130	0.9168093850592030	0.1451601048952185
857	0.0831839805429482	0.4168159974570500	0.1451607056646864
858	0.0831839805429482	0.9168159674570546	0.1451607056646864
859	0.5831839735429440	0.4168159974570500	0.1451607056646864
860	0.5831839735429440	0.9168159674570546	0.1451607056646864
861	0.0831905849408017	0.1663763126459870	0.1451601048952185
862	0.0831905849408017	0.6663763126459870	0.1451601048952185
863	0.5831906149407970	0.1663763126459870	0.1451601048952185
864	0.5831906149407970	0.6663763126459870	0.1451601048952185
865	0.1656654918832885	0.0828402366764962	0.2184374980008883
866	0.1656654918832885	0.5828402216764985	0.2184374980008883
867	0.6656654768832908	0.0828402366764962	0.2184374980008883

868	0.6656654768832908	0.5828402216764985	0.2184374980008883
869	0.4171840749882776	0.0828159110117213	0.2184311558397312
870	0.4171840749882776	0.5828159250117224	0.2184311558397312
871	0.9171840749882776	0.0828159110117213	0.2184311558397312
872	0.9171840749882776	0.5828159250117224	0.2184311558397312
873	0.4171597493235026	0.3343345231167092	0.2184374980008883
874	0.4171597493235026	0.8343345231167092	0.2184374980008883
875	0.9171597783235015	0.3343345231167092	0.2184374980008883
876	0.9171597783235015	0.8343345231167092	0.2184374980008883
877	0.9995421743006574	0.2497626512101760	0.2890967058856901
878	0.9995421743006574	0.7497626802101749	0.2890967058856901
879	0.4995421813006615	0.2497626512101760	0.2890967058856901
880	0.4995421813006615	0.7497626802101749	0.2890967058856901
881	0.2502352597840343	0.2497647252159680	0.2891030384579523
882	0.2502352597840343	0.7497646962159763	0.2891030384579523
883	0.7502352447840366	0.2497647252159680	0.2891030384579523
884	0.7502352447840366	0.7497646962159763	0.2891030384579523
885	0.2502373487898240	0.5004578186993385	0.2890967058856901
886	0.2502373487898240	0.0004578186993385	0.2890967058856901
887	0.7502373197898251	0.5004578186993385	0.2890967058856901
888	0.7502373197898251	0.0004578186993385	0.2890967058856901

889

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

891 1.01038006037737

892	10.0268001556000002	0.0000000000000000	0.0000000000000000
893	-5.0134000778000001	8.6834636535000005	0.0000000000000000
894	0.0000000000000000	0.0000000000000000	28.1868000031000001

895 Zn Ni

896 20 60

897 Direct

898	0.1666650029999985	0.3333350119999992	0.0000000000000000
899	0.1666650029999985	0.8333350420000016	0.0000000000000000
900	0.6666650180000033	0.3333350119999992	0.0000000000000000
901	0.6666650180000033	0.8333350420000016	0.0000000000000000
902	0.0000000000000000	0.0000000000000000	0.0726099979999972
903	0.0000000000000000	0.5000000000000000	0.0726099979999972
904	0.5000000000000000	0.0000000000000000	0.0726099979999972
905	0.5000000000000000	0.5000000000000000	0.0726099979999972
906	0.3333334697853161	0.1666665442146780	0.1451498879461255
907	0.3333334697853161	0.6666665592146828	0.1451498879461255
908	0.8333334997853186	0.1666665442146780	0.1451498879461255
909	0.8333334997853186	0.6666665592146828	0.1451498879461255
910	0.1666604477393747	0.3333395822606278	0.2163689804857754
911	0.1666604477393747	0.8333395522606253	0.2163689804857754
912	0.6666604477393747	0.3333395822606278	0.2163689804857754
913	0.6666604477393747	0.8333395522606253	0.2163689804857754
914	0.0000026806048652	0.4999973153951345	0.2940449738820448
915	0.0000026806048652	0.9999973153951345	0.2940449738820448
916	0.5000026846048655	0.4999973153951345	0.2940449738820448
917	0.5000026846048655	0.9999973153951345	0.2940449738820448
918	0.1666650029999985	0.0833349970000015	0.0000000000000000
919	0.1666650029999985	0.5833349819999967	0.0000000000000000

920	0.6666650180000033	0.0833349970000015	0.0000000000000000
921	0.6666650180000033	0.5833349819999967	0.0000000000000000
922	0.4166649880000008	0.0833349970000015	0.0000000000000000
923	0.4166649880000008	0.5833349819999967	0.0000000000000000
924	0.9166649579999984	0.0833349970000015	0.0000000000000000
925	0.9166649579999984	0.5833349819999967	0.0000000000000000
926	0.4166649880000008	0.3333350119999992	0.0000000000000000
927	0.4166649880000008	0.8333350420000016	0.0000000000000000
928	0.9166649579999984	0.3333350119999992	0.0000000000000000
929	0.9166649579999984	0.8333350420000016	0.0000000000000000
930	0.0000000000000000	0.2500000000000000	0.0726099979999972
931	0.0000000000000000	0.7500000000000000	0.0726099979999972
932	0.5000000000000000	0.2500000000000000	0.0726099979999972
933	0.5000000000000000	0.7500000000000000	0.0726099979999972
934	0.2500000000000000	0.2500000000000000	0.0726099979999972
935	0.2500000000000000	0.7500000000000000	0.0726099979999972
936	0.7500000000000000	0.2500000000000000	0.0726099979999972
937	0.7500000000000000	0.7500000000000000	0.0726099979999972
938	0.2500000000000000	0.0000000000000000	0.0726099979999972
939	0.2500000000000000	0.5000000000000000	0.0726099979999972
940	0.7500000000000000	0.0000000000000000	0.0726099979999972
941	0.7500000000000000	0.5000000000000000	0.0726099979999972
942	0.3335171787203564	0.4167555585831906	0.1449242104336150
943	0.3335171787203564	0.9167555585831906	0.1449242104336150
944	0.8335171787203564	0.4167555585831906	0.1449242104336150
945	0.8335171787203564	0.9167555585831906	0.1449242104336150
946	0.0832441902125893	0.4167557877874088	0.1449228372510021
947	0.0832441902125893	0.9167557577874135	0.1449228372510021
948	0.5832441832125852	0.4167557877874088	0.1449228372510021
949	0.5832441832125852	0.9167557577874135	0.1449228372510021
950	0.0832444114168140	0.1664828212796436	0.1449242104336150
951	0.0832444114168140	0.6664828212796436	0.1449242104336150
952	0.5832444414168094	0.1664828212796436	0.1449242104336150
953	0.5832444414168094	0.6664828212796436	0.1449242104336150
954	0.1647393718566619	0.0823626219034281	0.2175629257916043
955	0.1647393718566619	0.5823626069034304	0.2175629257916043
956	0.6647393568566642	0.0823626219034281	0.2175629257916043
957	0.6647393568566642	0.5823626069034304	0.2175629257916043
958	0.4176231126622056	0.0823768733377932	0.2175693514331911
959	0.4176231126622056	0.5823768873377944	0.2175693514331911
960	0.9176231126622056	0.0823768733377932	0.2175693514331911
961	0.9176231126622056	0.5823768873377944	0.2175693514331911
962	0.4176373640965707	0.3352606431433358	0.2175629257916043
963	0.4176373640965707	0.8352606431433358	0.2175629257916043
964	0.9176373930965696	0.3352606431433358	0.2175629257916043
965	0.9176373930965696	0.8352606431433358	0.2175629257916043
966	0.9991448969658023	0.2495698959031429	0.2876193404641398
967	0.9991448969658023	0.7495699249031418	0.2876193404641398
968	0.4991449039658065	0.2495698959031429	0.2876193404641398
969	0.4991449039658065	0.7495699249031418	0.2876193404641398
970	0.2504401862785528	0.2495597987214495	0.2876148099604308
971	0.2504401862785528	0.7495597697214507	0.2876148099604308

972	0.7504401712785551	0.2495597987214495	0.2876148099604308
973	0.7504401712785551	0.7495597697214507	0.2876148099604308
974	0.2504301040968571	0.5008550960341935	0.2876193404641398
975	0.2504301040968571	0.0008550960341935	0.2876193404641398
976	0.7504300750968582	0.5008550960341935	0.2876193404641398
977	0.7504300750968582	0.0008550960341935	0.2876193404641398
978			
979			
980			
981	NiSc (25% Sc) 111 Facet with Hydrogen supercell 2X2X1 - [Etot = -469.42312969 eV]		
982	1.04735280294076		
983	10.0268001556000002	0.0000000000000000	0.0000000000000000
984	-5.0134000778000001	8.6834636535000005	0.0000000000000000
985	0.0000000000000000	0.0000000000000000	28.1868000031000001
986	Sc Ni H		
987	20 60 1		
988	Direct		
989	0.1666650029999985	0.3333350119999992	0.0000000000000000
990	0.1666650029999985	0.8333350420000016	0.0000000000000000
991	0.6666650180000033	0.3333350119999992	0.0000000000000000
992	0.6666650180000033	0.8333350420000016	0.0000000000000000
993	0.0000000000000000	0.0000000000000000	0.0726099979999972
994	0.0000000000000000	0.5000000000000000	0.0726099979999972
995	0.5000000000000000	0.0000000000000000	0.0726099979999972
996	0.5000000000000000	0.5000000000000000	0.0726099979999972
997	0.3332157034126411	0.1667843105873530	0.1461440951587534
998	0.3332110822797887	0.6664284866183721	0.1461445878024250
999	0.8335715723816293	0.1667889317202054	0.1461445878024250
1000	0.8333319735473097	0.6666680854526916	0.1458929731354459
1001	0.1666616594958157	0.3333383705041868	0.2168609925525189
1002	0.1663582105674521	0.8331571752089459	0.2163834494898111
1003	0.6668428247910541	0.3336418194325503	0.2163834494898111
1004	0.6668223108235480	0.8331776891764520	0.2163869412283219
1005	0.9992632611655807	0.5007367348344189	0.2953256752275593
1006	0.9992525238378960	0.9985175813765252	0.2953224640372909
1007	0.5014824186234748	0.5007474721621037	0.2953224640372909
1008	0.5000046206424926	0.9999953793575074	0.2958359022196930
1009	0.1666650029999985	0.0833349970000015	0.0000000000000000
1010	0.1666650029999985	0.5833349819999967	0.0000000000000000
1011	0.6666650180000033	0.0833349970000015	0.0000000000000000
1012	0.6666650180000033	0.5833349819999967	0.0000000000000000
1013	0.4166649880000008	0.0833349970000015	0.0000000000000000
1014	0.4166649880000008	0.5833349819999967	0.0000000000000000
1015	0.9166649579999984	0.0833349970000015	0.0000000000000000
1016	0.9166649579999984	0.5833349819999967	0.0000000000000000
1017	0.4166649880000008	0.3333350119999992	0.0000000000000000
1018	0.4166649880000008	0.8333350420000016	0.0000000000000000
1019	0.9166649579999984	0.3333350119999992	0.0000000000000000
1020	0.9166649579999984	0.8333350420000016	0.0000000000000000
1021	0.0000000000000000	0.2500000000000000	0.0726099979999972
1022	0.0000000000000000	0.7500000000000000	0.0726099979999972
1023	0.5000000000000000	0.2500000000000000	0.0726099979999972

1024	0.5000000000000000	0.7500000000000000	0.0726099979999972
1025	0.2500000000000000	0.2500000000000000	0.0726099979999972
1026	0.2500000000000000	0.7500000000000000	0.0726099979999972
1027	0.7500000000000000	0.2500000000000000	0.0726099979999972
1028	0.7500000000000000	0.7500000000000000	0.0726099979999972
1029	0.2500000000000000	0.0000000000000000	0.0726099979999972
1030	0.2500000000000000	0.5000000000000000	0.0726099979999972
1031	0.7500000000000000	0.0000000000000000	0.0726099979999972
1032	0.7500000000000000	0.5000000000000000	0.0726099979999972
1033	0.3335731167800517	0.4167856172447202	0.1449549724650439
1034	0.3335904246079551	0.9167906986824761	0.1448287089621871
1035	0.8338019211250511	0.4169052231331207	0.1447501326090119
1036	0.8338090393645956	0.9168979729429267	0.1447486525988140
1037	0.0832113216980375	0.4167886563019607	0.1449555171866521
1038	0.0830872481074749	0.9168937109432633	0.1447462682077827
1039	0.5831062300567353	0.4169127298925233	0.1447462682077827
1040	0.5832065522388490	0.9167933887611497	0.1448281647913632
1041	0.0832143527552844	0.1664268832199483	0.1449549724650439
1042	0.0830947468668839	0.6661980788749489	0.1447501326090119
1043	0.5832093013175239	0.1664095753920449	0.1448287089621871
1044	0.5831020270570733	0.6661909606354044	0.1447486525988140
1045	0.1625221739141125	0.0814690697808231	0.2186926973756798
1046	0.1625246375900744	0.5810644904024116	0.2186915904702715
1047	0.6619067309979059	0.0809589410260401	0.2183840931449481
1048	0.6621550277458610	0.5810815554035997	0.2182874286396626
1049	0.4190512814938927	0.0809487045061061	0.2183865368466726
1050	0.4185364872443884	0.5810588511521786	0.2186909177660823
1051	0.9189411488478214	0.0814634987556104	0.2186909177660823
1052	0.9189248189105257	0.5810751810894743	0.2182897425980954
1053	0.4185309162191757	0.3374778410858852	0.2186926973756798
1054	0.4190410449739588	0.8380932690020941	0.2183840931449481
1055	0.9189355095975884	0.3374753774099233	0.2186915904702715
1056	0.9189184445964003	0.8378449722541390	0.2182874286396626
1057	0.9975389592238173	0.2487662644318931	0.2879229200450339
1058	0.9968193480757961	0.7484080085846969	0.2864874287330039
1059	0.4966465313221420	0.2480368506968915	0.2862955124231021
1060	0.4966420882283558	0.7486080934216659	0.2862951460080652
1061	0.2512365512055794	0.2487634337944229	0.2879245067720433
1062	0.2519652969856878	0.7486084951680070	0.2862933279740361
1063	0.7513914458319988	0.2480346880143145	0.2862933279740361
1064	0.7515932367550633	0.7484067042449425	0.2864851606720435
1065	0.2512337355681069	0.5024610337761786	0.2879229200450339
1066	0.2519631493031085	0.0033534686778580	0.2862955124231021
1067	0.7515919914153031	0.5031806449241998	0.2864874287330039
1068	0.7513919065783341	0.0033579117716442	0.2862951460080652
1069	0.1666655946242912	0.3333344353757113	0.3145263549217248

1070

1071 NiTi (25% Ti) 111 Facet with Hydrogen supercell 2X2X1 - [Etot = -503.16328396 eV]

1072 1.01798110552312

1073	10.0268001556000002	0.0000000000000000	0.0000000000000000
1074	-5.0134000778000001	8.6834636535000005	0.0000000000000000
1075	0.0000000000000000	0.0000000000000000	28.1868000031000001

1076	Ti	Ni	H
1077	20	60	1
1078	Direct		
1079	0.1666650029999985	0.3333350119999992	0.0000000000000000
1080	0.1666650029999985	0.8333350420000016	0.0000000000000000
1081	0.6666650180000033	0.3333350119999992	0.0000000000000000
1082	0.6666650180000033	0.8333350420000016	0.0000000000000000
1083	0.0000000000000000	0.0000000000000000	0.0726099979999972
1084	0.0000000000000000	0.5000000000000000	0.0726099979999972
1085	0.5000000000000000	0.0000000000000000	0.0726099979999972
1086	0.5000000000000000	0.5000000000000000	0.0726099979999972
1087	0.3333656322824226	0.1666343817175715	0.1448202170617350
1088	0.3333653933298066	0.6667255880243346	0.1448200060016092
1089	0.8332744709756668	0.1666346206701874	0.1448200060016092
1090	0.8333342231517378	0.6666658358482636	0.1445422406821280
1091	0.1666698357194463	0.3333301942805562	0.2199677355473710
1092	0.1668350683446533	0.8334137056298871	0.2211471430159548
1093	0.6665862943701129	0.3331649616553491	0.2211471430159548
1094	0.6665868604972403	0.8334131395027597	0.2211473948185443
1095	0.9982545186839147	0.5017454773160850	0.2882521574497403
1096	0.9982534110215155	0.9965023452862454	0.2882521140126713
1097	0.5034976547137546	0.5017465849784841	0.2882521140126713
1098	0.5000026959805268	0.9999973040194732	0.2885688338890873
1099	0.1666650029999985	0.0833349970000015	0.0000000000000000
1100	0.1666650029999985	0.5833349819999967	0.0000000000000000
1101	0.6666650180000033	0.0833349970000015	0.0000000000000000
1102	0.6666650180000033	0.5833349819999967	0.0000000000000000
1103	0.4166649880000008	0.0833349970000015	0.0000000000000000
1104	0.4166649880000008	0.5833349819999967	0.0000000000000000
1105	0.9166649579999984	0.0833349970000015	0.0000000000000000
1106	0.9166649579999984	0.5833349819999967	0.0000000000000000
1107	0.4166649880000008	0.3333350119999992	0.0000000000000000
1108	0.4166649880000008	0.8333350420000016	0.0000000000000000
1109	0.9166649579999984	0.3333350119999992	0.0000000000000000
1110	0.9166649579999984	0.8333350420000016	0.0000000000000000
1111	0.0000000000000000	0.2500000000000000	0.0726099979999972
1112	0.0000000000000000	0.7500000000000000	0.0726099979999972
1113	0.5000000000000000	0.2500000000000000	0.0726099979999972
1114	0.5000000000000000	0.7500000000000000	0.0726099979999972
1115	0.2500000000000000	0.2500000000000000	0.0726099979999972
1116	0.2500000000000000	0.7500000000000000	0.0726099979999972
1117	0.7500000000000000	0.2500000000000000	0.0726099979999972
1118	0.7500000000000000	0.7500000000000000	0.0726099979999972
1119	0.2500000000000000	0.0000000000000000	0.0726099979999972
1120	0.2500000000000000	0.5000000000000000	0.0726099979999972
1121	0.7500000000000000	0.0000000000000000	0.0726099979999972
1122	0.7500000000000000	0.5000000000000000	0.0726099979999972
1123	0.3327889104263306	0.4163925509945301	0.1454205648104150
1124	0.3327730640108939	0.9163836305764619	0.1454144147596210
1125	0.8326775485126277	0.4162816655423143	0.1453982482391112
1126	0.8326773782424155	0.9163932211266612	0.1453987964386627
1127	0.0836073108676914	0.4163926671323068	0.1454204321149888

1128	0.0837193067880762	0.9163933258495049	0.1453986384704535
1129	0.5836066151504937	0.4162806712119220	0.1453986384704535
1130	0.5836155802427427	0.9163843607572559	0.1454145530057147
1131	0.0836074190054745	0.1672110895736694	0.1454205648104150
1132	0.0837183044576904	0.6673224514873723	0.1453982482391112
1133	0.5836163694235381	0.1672269359891061	0.1454144147596210
1134	0.5836067788733388	0.6673226217575845	0.1453987964386627
1135	0.1660755578064865	0.0835460073178069	0.2176489739163685
1136	0.1660752130801058	0.5825224308684227	0.2176488211018395
1137	0.6659993428122135	0.0829963708368240	0.2174893917803971
1138	0.6658980797121359	0.5829447332888691	0.2173759134149122
1139	0.4170027884957719	0.0829971975042270	0.2174888732595264
1140	0.4164540201615878	0.5825230589657622	0.2176490853723294
1141	0.9174769410342378	0.0835459658384110	0.2176490853723294
1142	0.9170554163133176	0.5829445836866824	0.2173756974535337
1143	0.4164539786821919	0.3339244571935112	0.2176489739163685
1144	0.4170036151631749	0.8340006571877865	0.2174893917803971
1145	0.9174775691315773	0.3339248019198919	0.2176488211018395
1146	0.9170552667111309	0.8341019202878641	0.2173759134149122
1147	0.0014171611850173	0.2507038830843769	0.2897021760739378
1148	0.0011235471611499	0.7505571438880452	0.2893573803590286
1149	0.5010338763320092	0.2507380738821254	0.2893645347821874
1150	0.5010333257810089	0.7502852264354800	0.2893646137349251
1151	0.2492983961748934	0.2507015888251090	0.2897037309668136
1152	0.2492605675579043	0.7502857222069181	0.2893647906887580
1153	0.7497142187930876	0.2507394174420980	0.2893647906887580
1154	0.7494438557176224	0.7505560852823834	0.2893582105713506
1155	0.2492961169156231	0.4985828318149785	0.2897021760739378
1156	0.2492619261178746	0.9989661236679908	0.2893645347821874
1157	0.7494428561119548	0.4988764458388459	0.2893573803590286
1158	0.7497147735645200	0.9989666742189911	0.2893646137349251
1159	0.1666718491714860	0.3333281808285165	0.3215108865330976

1160

1161 NiV (25% V) 111 Facet with Hydrogen supercell 2X2X1 - [Etot = -504.57052261 eV]

1162 1.00458661266245

1163 10.0268001556000002 0.0000000000000000 0.0000000000000000

1164 -5.0134000778000001 8.6834636535000005 0.0000000000000000

1165 0.0000000000000000 0.0000000000000000 28.1868000031000001

1166 V Ni H

1167 20 60 1

1168 Direct

1169 0.1666650029999985 0.3333350119999992 0.0000000000000000

1170 0.1666650029999985 0.8333350420000016 0.0000000000000000

1171 0.6666650180000033 0.3333350119999992 0.0000000000000000

1172 0.6666650180000033 0.8333350420000016 0.0000000000000000

1173 0.0000000000000000 0.0000000000000000 0.0726099979999972

1174 0.0000000000000000 0.5000000000000000 0.0726099979999972

1175 0.5000000000000000 0.0000000000000000 0.0726099979999972

1176 0.5000000000000000 0.5000000000000000 0.0726099979999972

1177 0.3333301184466464 0.1666698955533477 0.1448981377342875

1178 0.3333286299297669 0.6666646499822164 0.1448955867167356

1179 0.8333354090177849 0.1666713840702272 0.1448955867167356

1180	0.8333345160471524	0.6666655429528490	0.1448340749757193
1181	0.1666658440635800	0.3333341859364225	0.2211965002399126
1182	0.1669212901569139	0.8334639005814708	0.2230238801237263
1183	0.6665360994185292	0.3330787398430886	0.2230238801237263
1184	0.6665378635787391	0.8334621364212609	0.2230134468608895
1185	0.9980017036644355	0.5019982923355641	0.2906139465043793
1186	0.9980044327176785	0.9960084335917685	0.2906121350380459
1187	0.5039915664082315	0.5019955632823212	0.2906121350380459
1188	0.4999976979104233	0.0000023020895767	0.2905799431229283
1189	0.1666650029999985	0.0833349970000015	0.0000000000000000
1190	0.1666650029999985	0.5833349819999967	0.0000000000000000
1191	0.6666650180000033	0.0833349970000015	0.0000000000000000
1192	0.6666650180000033	0.5833349819999967	0.0000000000000000
1193	0.4166649880000008	0.0833349970000015	0.0000000000000000
1194	0.4166649880000008	0.5833349819999967	0.0000000000000000
1195	0.9166649579999984	0.0833349970000015	0.0000000000000000
1196	0.9166649579999984	0.5833349819999967	0.0000000000000000
1197	0.4166649880000008	0.3333350119999992	0.0000000000000000
1198	0.4166649880000008	0.8333350420000016	0.0000000000000000
1199	0.9166649579999984	0.3333350119999992	0.0000000000000000
1200	0.9166649579999984	0.8333350420000016	0.0000000000000000
1201	0.0000000000000000	0.2500000000000000	0.0726099979999972
1202	0.0000000000000000	0.7500000000000000	0.0726099979999972
1203	0.5000000000000000	0.2500000000000000	0.0726099979999972
1204	0.5000000000000000	0.7500000000000000	0.0726099979999972
1205	0.2500000000000000	0.2500000000000000	0.0726099979999972
1206	0.2500000000000000	0.7500000000000000	0.0726099979999972
1207	0.7500000000000000	0.2500000000000000	0.0726099979999972
1208	0.7500000000000000	0.7500000000000000	0.0726099979999972
1209	0.2500000000000000	0.0000000000000000	0.0726099979999972
1210	0.2500000000000000	0.5000000000000000	0.0726099979999972
1211	0.7500000000000000	0.0000000000000000	0.0726099979999972
1212	0.7500000000000000	0.5000000000000000	0.0726099979999972
1213	0.3326775621994358	0.4163370485560520	0.1453100580979623
1214	0.3326621209375844	0.9163355229081276	0.1451933901666536
1215	0.8326964954754601	0.4162431908216035	0.1451611434559936
1216	0.8327039453509713	0.9164650276105633	0.1451597753528162
1217	0.0836584629309414	0.4163415150690568	0.1453103080043832
1218	0.0837584402428320	0.9164589864270667	0.1451618902026865
1219	0.5835409545729320	0.4162415377571662	0.1451618902026865
1220	0.5836617201395882	0.9163382208604105	0.1451919242036297
1221	0.0836629214439526	0.1673224378005642	0.1453100580979623
1222	0.0837567791784011	0.6673035045245399	0.1451611434559936
1223	0.5836644770918724	0.1673378790624156	0.1451933901666536
1224	0.5835349723894367	0.6672960546490287	0.1451597753528162
1225	0.1657434519348300	0.0831848542674720	0.2168699947632575
1226	0.1657371928086988	0.5825528969774396	0.2168727503556696
1227	0.6656944551644628	0.0828463488996150	0.2166215705339809
1228	0.6653636245526471	0.5826941806869996	0.2165570116630704
1229	0.4171534877885605	0.0828464982114383	0.2166233601035614
1230	0.4168165545973679	0.5825701330529398	0.2168681555999186
1231	0.9174298669470602	0.0831834314026310	0.2168681555999186

1232	0.9173198395597879	0.5826801604402121	0.2165595330505852
1233	0.4168151317325268	0.3342565630651677	0.2168699947632575
1234	0.4171536371003839	0.8343055448355372	0.2166215705339809
1235	0.9174471030225604	0.3342628221912989	0.2168727503556696
1236	0.9173058193130004	0.8346363754473529	0.2165570116630704
1237	0.0012332152911370	0.2506063418375746	0.2896517111915884
1238	0.0005985256932348	0.7503008316861397	0.2893820379231187
1239	0.5004177451767617	0.2502870361621419	0.2894327944396480
1240	0.5004549871522315	0.7501541306089763	0.2894305919577889
1241	0.2493925522542924	0.2506074327457100	0.2896552434281787
1242	0.2497119894375430	0.7501471905450998	0.2894308837673307
1243	0.7498527504549060	0.2502879955624593	0.2894308837673307
1244	0.7496864632957951	0.7503134777042106	0.2893790945784005
1245	0.2493936581624254	0.4987667777088589	0.2896517111915884
1246	0.2497129638378581	0.9995822548232383	0.2894327944396480
1247	0.7496991683138603	0.4994014673067610	0.2893820379231187
1248	0.7498458693910237	0.9995450128477685	0.2894305919577889
1249	0.1666659171826765	0.3333341128173259	0.3229928306355134

1250

1251 NiCr (25% Cr) 111 Facet with Hydrogen supercell 2X2X1 - [Etot = -500.10268842 eV]

1252 0.995572721824907

1253	10.0268001556000002	0.0000000000000000	0.0000000000000000
1254	-5.0134000778000001	8.6834636535000005	0.0000000000000000
1255	0.0000000000000000	0.0000000000000000	28.1868000031000001

1256 Cr Ni H

1257 20 60 1

1258 Direct

1259	0.1666650029999985	0.3333350119999992	0.0000000000000000
1260	0.1666650029999985	0.8333350420000016	0.0000000000000000
1261	0.6666650180000033	0.3333350119999992	0.0000000000000000
1262	0.6666650180000033	0.8333350420000016	0.0000000000000000
1263	0.0000000000000000	0.0000000000000000	0.0726099979999972
1264	0.0000000000000000	0.5000000000000000	0.0726099979999972
1265	0.5000000000000000	0.0000000000000000	0.0726099979999972
1266	0.5000000000000000	0.5000000000000000	0.0726099979999972
1267	0.3333043069231607	0.1666957070768333	0.1454685715034145
1268	0.3333028558953472	0.6666028353348565	0.1454605657118506
1269	0.8333972236651448	0.1666971581046468	0.1454605657118506
1270	0.8333358504808714	0.6666642085191299	0.1453180658616375
1271	0.1666651767929679	0.3333348532070346	0.2205440015647397
1272	0.1668018368366688	0.8334023422922954	0.2220762215036487
1273	0.6665976577077046	0.3331981931633337	0.2220762215036487
1274	0.6666047659466088	0.8333952340533912	0.2220519471662143
1275	0.9986602887845777	0.5013397072154220	0.2919959677516246
1276	0.9986470746719505	0.9973174889890117	0.2920037396882122
1277	0.5026825110109883	0.5013529213280492	0.2920037396882122
1278	0.5000110330907575	0.9999889669092425	0.2921565986567813
1279	0.1666650029999985	0.0833349970000015	0.0000000000000000
1280	0.1666650029999985	0.5833349819999967	0.0000000000000000
1281	0.6666650180000033	0.0833349970000015	0.0000000000000000
1282	0.6666650180000033	0.5833349819999967	0.0000000000000000
1283	0.4166649880000008	0.0833349970000015	0.0000000000000000

1284	0.4166649880000008	0.5833349819999967	0.0000000000000000
1285	0.9166649579999984	0.0833349970000015	0.0000000000000000
1286	0.9166649579999984	0.5833349819999967	0.0000000000000000
1287	0.4166649880000008	0.3333350119999992	0.0000000000000000
1288	0.4166649880000008	0.8333350420000016	0.0000000000000000
1289	0.9166649579999984	0.3333350119999992	0.0000000000000000
1290	0.9166649579999984	0.8333350420000016	0.0000000000000000
1291	0.0000000000000000	0.2500000000000000	0.0726099979999972
1292	0.0000000000000000	0.7500000000000000	0.0726099979999972
1293	0.5000000000000000	0.2500000000000000	0.0726099979999972
1294	0.5000000000000000	0.7500000000000000	0.0726099979999972
1295	0.2500000000000000	0.2500000000000000	0.0726099979999972
1296	0.2500000000000000	0.7500000000000000	0.0726099979999972
1297	0.7500000000000000	0.2500000000000000	0.0726099979999972
1298	0.7500000000000000	0.7500000000000000	0.0726099979999972
1299	0.2500000000000000	0.0000000000000000	0.0726099979999972
1300	0.2500000000000000	0.5000000000000000	0.0726099979999972
1301	0.7500000000000000	0.0000000000000000	0.0726099979999972
1302	0.7500000000000000	0.5000000000000000	0.0726099979999972
1303	0.3331628195923528	0.4165825767133811	0.1457198222095712
1304	0.3328132233450845	0.9163996760587736	0.1457509139982278
1305	0.8325453426295297	0.4162866652824988	0.1456764528316441
1306	0.8325505527609494	0.9162547005697945	0.1456733851389771
1307	0.0834277118197875	0.4165722661802107	0.1457189886524617
1308	0.0837020056946400	0.9162605384759814	0.1456775984215639
1309	0.5837394025240172	0.4162979723053581	0.1456775984215639
1310	0.5836046218193047	0.9163953191806939	0.1457474009011790
1311	0.0834173932866236	0.1668371804076472	0.1457198222095712
1312	0.0837133047175058	0.6674546573704703	0.1456764528316441
1313	0.5836003239412264	0.1671867766549155	0.1457509139982278
1314	0.5837452994302055	0.6674494472390506	0.1456733851389771
1315	0.1668112117157463	0.0832938527073424	0.2181138366019226
1316	0.1668136963960691	0.5835205227939966	0.2181033871296449
1317	0.6665823376732689	0.0832839435758643	0.2178215510274839
1318	0.6666401954014702	0.5833179446497638	0.2175735783990476
1319	0.4167102265821683	0.0832897594178306	0.2178310083349970
1320	0.4167159265102001	0.5835165385646235	0.2181050806162688
1321	0.9164834614353765	0.0832840594897988	0.2181050806162688
1322	0.9166785920620200	0.5833214079379800	0.2175719964834713
1323	0.4167061332926565	0.3331888032842514	0.2181138366019226
1324	0.4167160424241345	0.8334176623267311	0.2178215510274839
1325	0.9164794772060034	0.3331863186039286	0.2181033871296449
1326	0.9166820553502362	0.8333598045985298	0.2175735783990476
1327	0.0014219758281371	0.2507040197395582	0.2913555304404341
1328	0.0017401541398385	0.7508767575766555	0.2905149960084188
1329	0.5015813175689914	0.2507564451446029	0.2907113585173136
1330	0.5015884495826697	0.7508275961233295	0.2906983170611568
1331	0.2492814082761399	0.2507185767238624	0.2913601554536598
1332	0.2492654866057649	0.7508247152742911	0.2907039158631974
1333	0.7491752257257147	0.2507344983942374	0.2907039158631974
1334	0.7491168524454253	0.7508830885545805	0.2905077774978224
1335	0.2492959802604418	0.4985780171718588	0.2913555304404341

1336	0.2492435548553971	0.9984186824310086	0.2907113585173136
1337	0.7491232424233445	0.4982598388601573	0.2905149960084188
1338	0.7491724038766705	0.9984115504173303	0.2906983170611568
1339	0.1666694615119368	0.3333305684880656	0.3252121545763558
1340			
1341	NiMn (25% Mn) 111 Facet with Hydrogen supercell 2X2X1 - [Etot = -498.31615918 eV]		
1342	1.0000000000000000		
1343	9.9196901320999995	0.0000000000000000	0.0000000000000000
1344	-4.9598426818999997	8.5906995225999996	0.0000000000000000
1345	0.0000000000000000	0.0000000000000000	27.8856849669999995
1346	Mn Ni H		
1347	20 60 1		
1348	Direct		
1349	0.1666650029999985	0.3333350119999992	0.0000000000000000
1350	0.1666650029999985	0.8333350420000016	0.0000000000000000
1351	0.6666650180000033	0.3333350119999992	0.0000000000000000
1352	0.6666650180000033	0.8333350420000016	0.0000000000000000
1353	0.0000000000000000	0.0000000000000000	0.0726099979999972
1354	0.0000000000000000	0.5000000000000000	0.0726099979999972
1355	0.5000000000000000	0.0000000000000000	0.0726099979999972
1356	0.5000000000000000	0.5000000000000000	0.0726099979999972
1357	0.3332152805190205	0.1666249272505027	0.1474970528066493
1358	0.3332075461619084	0.6665128102487330	0.1475087046767953
1359	0.8333139861045638	0.1666217293897461	0.1475029852596705
1360	0.8332412555039497	0.6665829898579645	0.1474620154961599
1361	0.1665330588684029	0.3332195536757041	0.2215247626687429
1362	0.1662850880851821	0.8330813174706009	0.2213153974296063
1363	0.6666506151812399	0.3334355325707250	0.2213354563734455
1364	0.6666529457420438	0.8330829318883701	0.2213237539929906
1365	0.5010638596955275	0.5004495229202206	0.2986612130846282
1366	0.4998245165996309	0.9998371284264138	0.2989912409073767
1367	0.9992109468608348	0.5004522983942294	0.2986546629069693
1368	0.9992149309950094	0.9986160877571493	0.2986664251206719
1369	0.1666650029999985	0.0833349970000015	0.0000000000000000
1370	0.1666650029999985	0.5833349819999967	0.0000000000000000
1371	0.6666650180000033	0.0833349970000015	0.0000000000000000
1372	0.6666650180000033	0.5833349819999967	0.0000000000000000
1373	0.0000000000000000	0.2500000000000000	0.0726099979999972
1374	0.0000000000000000	0.7500000000000000	0.0726099979999972
1375	0.5000000000000000	0.2500000000000000	0.0726099979999972
1376	0.5000000000000000	0.7500000000000000	0.0726099979999972
1377	0.4166649880000008	0.0833349970000015	0.0000000000000000
1378	0.4166649880000008	0.5833349819999967	0.0000000000000000
1379	0.9166649579999984	0.0833349970000015	0.0000000000000000
1380	0.9166649579999984	0.5833349819999967	0.0000000000000000
1381	0.2500000000000000	0.2500000000000000	0.0726099979999972
1382	0.2500000000000000	0.7500000000000000	0.0726099979999972
1383	0.7500000000000000	0.2500000000000000	0.0726099979999972
1384	0.7500000000000000	0.7500000000000000	0.0726099979999972
1385	0.4166649880000008	0.3333350119999992	0.0000000000000000
1386	0.4166649880000008	0.8333350420000016	0.0000000000000000
1387	0.9166649579999984	0.3333350119999992	0.0000000000000000

1388	0.9166649579999984	0.8333350420000016	0.0000000000000000
1389	0.2500000000000000	0.0000000000000000	0.0726099979999972
1390	0.2500000000000000	0.5000000000000000	0.0726099979999972
1391	0.7500000000000000	0.0000000000000000	0.0726099979999972
1392	0.7500000000000000	0.5000000000000000	0.0726099979999972
1393	0.3332981174893632	0.4166203261066741	0.1471506872131059
1394	0.3333312295363058	0.9166253790002870	0.1470864759523351
1395	0.8333114404160753	0.4165796646240167	0.1470855622914726
1396	0.8333213107684188	0.9166654599763859	0.1470849393475220
1397	0.1658157498661907	0.0829549203203115	0.2218214088676191
1398	0.1658111842960253	0.5827466644036434	0.2218330857335360
1399	0.6653992437291265	0.0826403477761346	0.2216695327908837
1400	0.6655260459919674	0.5826946745918562	0.2216634767946317
1401	0.4996322461642535	0.2493898815412905	0.2943530018927021
1402	0.4996437768301831	0.7500972492315796	0.2943503539451555
1403	0.9998256534778847	0.2498563364977144	0.2957126215906456
1404	0.9997824560060522	0.7498179489096373	0.2945142400713010
1405	0.0832282337087236	0.4166204821292396	0.1471521690955555
1406	0.0832435061018018	0.9166543197274777	0.1470813051335469
1407	0.5831872267769285	0.4165839174493797	0.1470866379492506
1408	0.5832084624170051	0.9166314382794027	0.1470885999994707
1409	0.4170946781893434	0.0826493004383622	0.2216648130135823
1410	0.4167899865261617	0.5827445258718669	0.2218357633980617
1411	0.9169900638545485	0.0829513769403505	0.2218313070680509
1412	0.9170110412900527	0.5826983284781164	0.2216518788302864
1413	0.2498376046750508	0.2498533839477730	0.2957032635391030
1414	0.2502674365566833	0.7501045154156500	0.2943467532020065
1415	0.7495865953234926	0.2493994155319825	0.2943543708836671
1416	0.7498561440633082	0.7498196924561213	0.2945237671374556
1417	0.0832269368857510	0.1665504276571497	0.1471503843089152
1418	0.0832477503599520	0.6665081346528936	0.1470821691353379
1419	0.5832204496928028	0.1665193386221588	0.1470903721353523
1420	0.5831717110221319	0.6665154844621100	0.1470852794561708
1421	0.4167935999467431	0.3339130292015966	0.2218231423273807
1422	0.4170948570168136	0.8343264081234949	0.2216688721660560
1423	0.9169769269966039	0.3339184438276703	0.2218247151727724
1424	0.9170195632705003	0.8341927077647071	0.2216577323958830
1425	0.2502594666885045	0.0000368125885046	0.2943360639044386
1426	0.2498501938526374	0.4998824719268100	0.2957220345250562
1427	0.7495908811284835	0.0000446835412191	0.2943462673916102
1428	0.7498652239567818	0.4998950763080998	0.2945250404038973
1429	0.1664830330437539	0.3331463125528700	0.3291019479052295
1430			
1431	NiFe (25% Fe) 111 Facet with Hydrogen supercell 2X2X1 - [Etot = -483.63851074 eV]		
1432	1.000000000000000		
1433	10.0268001556000002	0.0000000000000000	0.0000000000000000
1434	-5.0134000778000001	8.6834636535000005	0.0000000000000000
1435	0.0000000000000000	0.0000000000000000	28.1868000031000001
1436	Fe Ni H		
1437	20 60 1		
1438	Direct		
1439	0.1666650029999985	0.3333350119999992	0.0000000000000000

1440	0.1666650029999985	0.8333350420000016	0.0000000000000000
1441	0.6666650180000033	0.3333350119999992	0.0000000000000000
1442	0.6666650180000033	0.8333350420000016	0.0000000000000000
1443	0.0000000000000000	0.0000000000000000	0.0726099979999972
1444	0.0000000000000000	0.5000000000000000	0.0726099979999972
1445	0.5000000000000000	0.0000000000000000	0.0726099979999972
1446	0.5000000000000000	0.5000000000000000	0.0726099979999972
1447	0.3332864487836318	0.1667135652163552	0.1447407954409172
1448	0.3332863200037366	0.6665683516545968	0.1447388140892087
1449	0.8334317073454045	0.1667136939962575	0.1447388140892087
1450	0.8333348157035800	0.6666652432964213	0.1445708350706454
1451	0.1666698080254676	0.3333302219745349	0.2186093740334840
1452	0.1666331018730034	0.8333112403534031	0.2192801760214209
1453	0.6666887596465969	0.3333669281269991	0.2192801760214209
1454	0.6666893367888136	0.8333106632111864	0.2192738538399936
1455	0.9988574387126548	0.5011425572873449	0.2883904590212438
1456	0.9988527222929520	0.9976988106921496	0.2883886008130929
1457	0.5023011893078504	0.5011472737070477	0.2883886008130929
1458	0.500082613860002	0.9999917386139998	0.2885596595686835
1459	0.1666650029999985	0.0833349970000015	0.0000000000000000
1460	0.1666650029999985	0.5833349819999967	0.0000000000000000
1461	0.6666650180000033	0.0833349970000015	0.0000000000000000
1462	0.6666650180000033	0.5833349819999967	0.0000000000000000
1463	0.4166649880000008	0.0833349970000015	0.0000000000000000
1464	0.4166649880000008	0.5833349819999967	0.0000000000000000
1465	0.9166649579999984	0.0833349970000015	0.0000000000000000
1466	0.9166649579999984	0.5833349819999967	0.0000000000000000
1467	0.4166649880000008	0.3333350119999992	0.0000000000000000
1468	0.4166649880000008	0.8333350420000016	0.0000000000000000
1469	0.9166649579999984	0.3333350119999992	0.0000000000000000
1470	0.9166649579999984	0.8333350420000016	0.0000000000000000
1471	0.0000000000000000	0.2500000000000000	0.0726099979999972
1472	0.0000000000000000	0.7500000000000000	0.0726099979999972
1473	0.5000000000000000	0.2500000000000000	0.0726099979999972
1474	0.5000000000000000	0.7500000000000000	0.0726099979999972
1475	0.2500000000000000	0.2500000000000000	0.0726099979999972
1476	0.2500000000000000	0.7500000000000000	0.0726099979999972
1477	0.7500000000000000	0.2500000000000000	0.0726099979999972
1478	0.7500000000000000	0.7500000000000000	0.0726099979999972
1479	0.2500000000000000	0.0000000000000000	0.0726099979999972
1480	0.2500000000000000	0.5000000000000000	0.0726099979999972
1481	0.7500000000000000	0.0000000000000000	0.0726099979999972
1482	0.7500000000000000	0.5000000000000000	0.0726099979999972
1483	0.3330940551442296	0.4165453983449154	0.1451619252346248
1484	0.3330350339102424	0.9165150226703602	0.1451416801023626
1485	0.8329675908063763	0.4165264386715748	0.1451184455136385
1486	0.8329694685162323	0.9164362560097032	0.1451151147447618
1487	0.0834573998302872	0.4165425781697110	0.1451644202864060
1488	0.0834736822845841	0.9164346002995387	0.1451170904642183
1489	0.5835653407004600	0.4165262957154141	0.1451170904642183
1490	0.5834845221220561	0.9165154188779425	0.1451394025013428
1491	0.0834545716550892	0.1669059448557704	0.1451619252346248

1492	0.0834735313284298	0.6670324091936237	0.1451184455136385
1493	0.5834849773296398	0.1669649660897576	0.1451416801023626
1494	0.5835637439902968	0.6670305314837677	0.1451151147447618
1495	0.1670406591114570	0.0836571307091774	0.2172678979155194
1496	0.1670375889402038	0.5833707698189627	0.2172644959062353
1497	0.6670860917710826	0.0835349189626342	0.2172659981264289
1498	0.6668934561213291	0.5834447742436737	0.2171900051023457
1499	0.4164607756266392	0.0835392103733597	0.2172687194071869
1500	0.4163466445973896	0.5833756934098417	0.2172625613281696
1501	0.9166243065901583	0.0836533414026093	0.2172625613281696
1502	0.9165591584848443	0.5834408415151557	0.2171912402572715
1503	0.4163428552908215	0.3329593558885406	0.2172678979155194
1504	0.4164650670373646	0.8329139082289174	0.2172659981264289
1505	0.9166292301810373	0.3329624260597939	0.2172644959062353
1506	0.916552257563263	0.8331065438786709	0.2171900051023457
1507	0.0008858945131109	0.2504329110219032	0.2896219568735603
1508	0.0011495172518039	0.7505691576909470	0.2888645089054194
1509	0.5010825211934673	0.2504199385465000	0.2888194131155757
1510	0.5010878089298600	0.7506496579410111	0.2888176969973344
1511	0.2495654974452748	0.2504344875547275	0.2896221121050289
1512	0.2495832189911056	0.7506495515644644	0.2888199597999375
1513	0.7493503894355413	0.2504167660088967	0.2888199597999375
1514	0.7494277807947398	0.7505721602052660	0.2888628845088661
1515	0.2495670889780897	0.4991140984868849	0.2896219568735603
1516	0.2495800614535000	0.9989174788065327	0.2888194131155757
1517	0.7494308423090530	0.4988504757481920	0.2888645089054194
1518	0.7493503420589889	0.9989121910701400	0.2888176969973344
1519	0.1666725584862760	0.3333274715137264	0.3226365107435143

1520

1521 NiCo (25% Co) 111 Facet with Hydrogen supercell 2X2X1 - [Etot = -450.92529772 eV]

1522 0.993794164815303

1523	10.0268001556000002	0.0000000000000000	0.0000000000000000
1524	-5.0134000778000001	8.6834636535000005	0.0000000000000000
1525	0.0000000000000000	0.0000000000000000	28.1868000031000001

1526 Co Ni H

1527 20 60 1

1528 Direct

1529	0.1666650029999985	0.3333350119999992	0.0000000000000000
1530	0.1666650029999985	0.8333350420000016	0.0000000000000000
1531	0.6666650180000033	0.3333350119999992	0.0000000000000000
1532	0.6666650180000033	0.8333350420000016	0.0000000000000000
1533	0.0000000000000000	0.0000000000000000	0.0726099979999972
1534	0.0000000000000000	0.5000000000000000	0.0726099979999972
1535	0.5000000000000000	0.0000000000000000	0.0726099979999972
1536	0.5000000000000000	0.5000000000000000	0.0726099979999972
1537	0.3333115464162120	0.1666884675837821	0.1448063774476154
1538	0.3333120560670864	0.6666169870011061	0.1448055002542006
1539	0.8333830719988953	0.1666879579329077	0.1448055002542006
1540	0.8333368026015435	0.6666632563984578	0.1447225110932280
1541	0.1666712069710741	0.3333288230289284	0.2187410534966290
1542	0.1666256356508455	0.8333083986986125	0.2192288648150225
1543	0.6666916013013875	0.3333743943491569	0.2192288648150225

1544	0.6666925795041934	0.8333074204958066	0.2192290668675199
1545	0.9989016449818209	0.5010983510181788	0.2885658982458139
1546	0.9988983357927310	0.9977877118672467	0.2885550037033582
1547	0.5022122881327533	0.5011016602072687	0.2885550037033582
1548	0.5000042712214139	0.9999957287785861	0.2887727888223495
1549	0.1666650029999985	0.0833349970000015	0.0000000000000000
1550	0.1666650029999985	0.5833349819999967	0.0000000000000000
1551	0.6666650180000033	0.0833349970000015	0.0000000000000000
1552	0.6666650180000033	0.5833349819999967	0.0000000000000000
1553	0.4166649880000008	0.0833349970000015	0.0000000000000000
1554	0.4166649880000008	0.5833349819999967	0.0000000000000000
1555	0.9166649579999984	0.0833349970000015	0.0000000000000000
1556	0.9166649579999984	0.5833349819999967	0.0000000000000000
1557	0.4166649880000008	0.3333350119999992	0.0000000000000000
1558	0.4166649880000008	0.8333350420000016	0.0000000000000000
1559	0.9166649579999984	0.3333350119999992	0.0000000000000000
1560	0.9166649579999984	0.8333350420000016	0.0000000000000000
1561	0.0000000000000000	0.2500000000000000	0.0726099979999972
1562	0.0000000000000000	0.7500000000000000	0.0726099979999972
1563	0.5000000000000000	0.2500000000000000	0.0726099979999972
1564	0.5000000000000000	0.7500000000000000	0.0726099979999972
1565	0.2500000000000000	0.2500000000000000	0.0726099979999972
1566	0.2500000000000000	0.7500000000000000	0.0726099979999972
1567	0.7500000000000000	0.2500000000000000	0.0726099979999972
1568	0.7500000000000000	0.7500000000000000	0.0726099979999972
1569	0.2500000000000000	0.0000000000000000	0.0726099979999972
1570	0.2500000000000000	0.5000000000000000	0.0726099979999972
1571	0.7500000000000000	0.0000000000000000	0.0726099979999972
1572	0.7500000000000000	0.5000000000000000	0.0726099979999972
1573	0.3330922747296299	0.4165435212254209	0.1452145309818320
1574	0.3330914069868811	0.9165425767741766	0.1451066199353903
1575	0.8330089015528230	0.4165698926017143	0.1450486446093819
1576	0.8330126722352134	0.9164327490106672	0.1450489687484833
1577	0.0834572581237296	0.4165427198762686	0.1452131951888092
1578	0.0834284900581892	0.9164336474636841	0.1450492897256623
1579	0.5835662935363146	0.4165714879418090	0.1450492897256623
1580	0.5834572317584303	0.9165427092415683	0.1451078551227525
1581	0.0834564487745837	0.1669077252703701	0.1452145309818320
1582	0.0834300773982903	0.6669910984471770	0.1450486446093819
1583	0.5834574232258234	0.1669085930131189	0.1451066199353903
1584	0.5835672509893328	0.6669873277647866	0.1450489687484833
1585	0.1670122114426107	0.0836470542652634	0.2172869122777286
1586	0.1669996784385219	0.5833458090207415	0.2172858901192782
1587	0.6669254206733015	0.0834597861742381	0.2172244016201077
1588	0.6666432510903633	0.5833148574746048	0.2172255328866513
1589	0.4165432652405627	0.0834567207594361	0.2172239342490769
1590	0.4163516937061971	0.5833495464785159	0.2172861325763620
1591	0.9166504535214841	0.0836482922938018	0.2172861325763620
1592	0.9166902695169057	0.5833097304830943	0.2172267878798451
1593	0.4163529317347354	0.3329878035573870	0.2172869122777286
1594	0.4165401998257607	0.8330745793266985	0.2172244016201077
1595	0.9166541909792585	0.3330003365614758	0.2172858901192782

1596	0.9166851425253952	0.8333567489096367	0.2172255328866513
1597	0.0006625042214878	0.2503328508106151	0.2899234785878306
1598	0.0009943795936493	0.7504834353336491	0.2888547153609053
1599	0.5008255055983710	0.2502892974332411	0.2887927417645813
1600	0.5008153723475104	0.7505186037107308	0.2887911985466616
1601	0.2496727691263629	0.2503272158736394	0.2899200883998461
1602	0.2497053249650349	0.7505098403953028	0.2887926077038969
1603	0.7494901006047030	0.2502946600349674	0.2887926077038969
1604	0.7495076124547708	0.7504923285452350	0.2888542547801052
1605	0.2496671491893849	0.4993374887785080	0.2899234785878306
1606	0.2497107025667589	0.9991744944016290	0.2887927417645813
1607	0.7495165646663509	0.4990056134063465	0.2888547153609053
1608	0.7494813962892692	0.9991846276524896	0.2887911985466616
1609	0.1666678644409814	0.3333321655590211	0.3235403276261124
1610			
1611	Pure-Ni 111 Facet with Hydrogen supercell 2X2X1 - [Etot = -417.97240235 eV]		
1612	1.01798110552312		
1613	10.0268001556000002	0.0000000000000000	0.0000000000000000
1614	-5.0134000778000001	8.6834636535000005	0.0000000000000000
1615	0.0000000000000000	0.0000000000000000	28.1868000031000001
1616	Ni H		
1617	80 1		
1618	Direct		
1619	0.1666650029999985	0.3333350119999992	0.0000000000000000
1620	0.1666650029999985	0.8333350420000016	0.0000000000000000
1621	0.6666650180000033	0.3333350119999992	0.0000000000000000
1622	0.6666650180000033	0.8333350420000016	0.0000000000000000
1623	0.0000000000000000	0.0000000000000000	0.0726099979999972
1624	0.0000000000000000	0.5000000000000000	0.0726099979999972
1625	0.5000000000000000	0.0000000000000000	0.0726099979999972
1626	0.5000000000000000	0.5000000000000000	0.0726099979999972
1627	0.3332639878454131	0.1667360261545809	0.1419733819454123
1628	0.3332706696180807	0.6665296013936697	0.1419744409170178
1629	0.8334704576063316	0.1667293443819133	0.1419744409170178
1630	0.8333352476911884	0.6666648113088129	0.1420391838918675
1631	0.1666749455429297	0.3333250844570728	0.2112713596132210
1632	0.1666415572883935	0.8333133988722281	0.2116682136789336
1633	0.6666866011277719	0.3333584727116090	0.2116682136789336
1634	0.6666835407618379	0.8333164592381621	0.2116645909751327
1635	0.9987853894056045	0.5012146065943952	0.2800487530449516
1636	0.9987960408857575	0.9975643051865006	0.2800385165218344
1637	0.5024356948134994	0.5012039551142422	0.2800385165218344
1638	0.5000044546927569	0.9999955453072431	0.2801793779852133
1639	0.1666650029999985	0.0833349970000015	0.0000000000000000
1640	0.1666650029999985	0.5833349819999967	0.0000000000000000
1641	0.6666650180000033	0.0833349970000015	0.0000000000000000
1642	0.6666650180000033	0.5833349819999967	0.0000000000000000
1643	0.4166649880000008	0.0833349970000015	0.0000000000000000
1644	0.4166649880000008	0.5833349819999967	0.0000000000000000
1645	0.9166649579999984	0.0833349970000015	0.0000000000000000
1646	0.9166649579999984	0.5833349819999967	0.0000000000000000
1647	0.4166649880000008	0.3333350119999992	0.0000000000000000

1648	0.4166649880000008	0.8333350420000016	0.0000000000000000
1649	0.9166649579999984	0.3333350119999992	0.0000000000000000
1650	0.9166649579999984	0.8333350420000016	0.0000000000000000
1651	0.0000000000000000	0.2500000000000000	0.0726099979999972
1652	0.0000000000000000	0.7500000000000000	0.0726099979999972
1653	0.5000000000000000	0.2500000000000000	0.0726099979999972
1654	0.5000000000000000	0.7500000000000000	0.0726099979999972
1655	0.2500000000000000	0.2500000000000000	0.0726099979999972
1656	0.2500000000000000	0.7500000000000000	0.0726099979999972
1657	0.7500000000000000	0.2500000000000000	0.0726099979999972
1658	0.7500000000000000	0.7500000000000000	0.0726099979999972
1659	0.2500000000000000	0.0000000000000000	0.0726099979999972
1660	0.2500000000000000	0.5000000000000000	0.0726099979999972
1661	0.7500000000000000	0.0000000000000000	0.0726099979999972
1662	0.7500000000000000	0.5000000000000000	0.0726099979999972
1663	0.3335179425858001	0.4167614614678925	0.1419614435188734
1664	0.3333074053447618	0.9166497482758516	0.1419647087841227
1665	0.8331695178680434	0.4165893927489321	0.1419509688911162
1666	0.8331546259635871	0.9165661858985743	0.1419444932317120
1667	0.0832410144976947	0.4167589635023035	0.1419635136221657
1668	0.0834066775429605	0.9165622395397151	0.1419485458255494
1669	0.5834377014602836	0.4165933004570377	0.1419485458255494
1670	0.5833448898023832	0.9166550511976155	0.1419607776237015
1671	0.0832385085321121	0.1664820574141999	0.1419614435188734
1672	0.0834105772510725	0.6668304821319566	0.1419509688911162
1673	0.5833502517241484	0.1666925946552382	0.1419647087841227
1674	0.5834338141014257	0.6668453740364129	0.1419444932317120
1675	0.1669281098317796	0.0838161489953393	0.2117150597377346
1676	0.1669378948729019	0.5831003425046362	0.2117200847517822
1677	0.6668093095939369	0.0833935234222025	0.2116236541844572
1678	0.6664859574217559	0.5832455635703937	0.2116284353925124
1679	0.4166032875295045	0.0833966984704944	0.2116241326880299
1680	0.4161897539370827	0.5831029576088227	0.2117144139364058
1681	0.9168970423911773	0.0838102320629162	0.2117144139364058
1682	0.9167604372167162	0.5832395627832838	0.2116326659841050
1683	0.4161838370046596	0.3330719051682181	0.2117150597377346
1684	0.4166064625777963	0.8331906904060631	0.2116236541844572
1685	0.9168996574953638	0.3330621201270958	0.2117200847517822
1686	0.9167544364296063	0.8335140425782441	0.2116284353925124
1687	0.9998282429788716	0.2498975461831847	0.2812232031397386
1688	0.0001535457765556	0.7500753330413232	0.2801641635868251
1689	0.4997571732709361	0.2497113999541867	0.2800879386925246
1690	0.4997697983778124	0.7500327160476701	0.2800877273041138
1691	0.2500979833648884	0.2499020016351139	0.2812236781313260
1692	0.2502802647042870	0.7500396605716517	0.2800914657031228
1693	0.7499602804283541	0.2497197202957153	0.2800914657031228
1694	0.7499308460383958	0.7500690949616100	0.2801622436918052
1695	0.2501024538168153	0.5001717500211242	0.2812232031397386
1696	0.2502886000458133	0.0002428267290639	0.2800879386925246
1697	0.7499246669586768	0.4998464472234403	0.2801641635868251
1698	0.7499672839523299	0.0002302016221876	0.2800877273041138
1699	0.1666730935151648	0.3333269364848377	0.3114365579502447

1700	
1701	NiCu (25% Cu) 111 Facet with Hydrogen supercell 2X2X1 - [Etot = -384.89628749 eV]
1702	0.998485100048875
1703	10.0268001556000002 0.0000000000000000 0.0000000000000000
1704	-5.0134000778000001 8.6834636535000005 0.0000000000000000
1705	0.0000000000000000 0.0000000000000000 28.1868000031000001
1706	Cu Ni H
1707	20 60 1
1708	Direct
1709	0.1666650029999985 0.3333350119999992 0.0000000000000000
1710	0.1666650029999985 0.8333350420000016 0.0000000000000000
1711	0.6666650180000033 0.3333350119999992 0.0000000000000000
1712	0.6666650180000033 0.8333350420000016 0.0000000000000000
1713	0.0000000000000000 0.0000000000000000 0.0726099979999972
1714	0.0000000000000000 0.5000000000000000 0.0726099979999972
1715	0.5000000000000000 0.0000000000000000 0.0726099979999972
1716	0.5000000000000000 0.5000000000000000 0.0726099979999972
1717	0.3333105765030737 0.1666894374969203 0.1456140221127100
1718	0.3333231344815459 0.6666189152926165 0.1456090335055578
1719	0.8333811437073848 0.1666768795184481 0.1456090335055578
1720	0.8333308162382522 0.6666692427617491 0.1457040555273252
1721	0.1666593572402846 0.3333406727597179 0.2174824367266055
1722	0.1665724311383983 0.8332609310511145 0.2171561364583354
1723	0.6667390689488855 0.3334275988616042 0.2171561364583354
1724	0.6667163916429359 0.8332836083570641 0.2171640607083205
1725	0.9994652900400283 0.5005347059599714 0.2927948960501894
1726	0.9994697926158480 0.9989337915095433 0.2927931707191505
1727	0.5010662084904567 0.5005302033841517 0.2927931707191505
1728	0.5000077818701882 0.9999922181298118 0.2928920389614618
1729	0.1666650029999985 0.0833349970000015 0.0000000000000000
1730	0.1666650029999985 0.5833349819999967 0.0000000000000000
1731	0.6666650180000033 0.0833349970000015 0.0000000000000000
1732	0.6666650180000033 0.5833349819999967 0.0000000000000000
1733	0.4166649880000008 0.0833349970000015 0.0000000000000000
1734	0.4166649880000008 0.5833349819999967 0.0000000000000000
1735	0.9166649579999984 0.0833349970000015 0.0000000000000000
1736	0.9166649579999984 0.5833349819999967 0.0000000000000000
1737	0.4166649880000008 0.3333350119999992 0.0000000000000000
1738	0.4166649880000008 0.8333350420000016 0.0000000000000000
1739	0.9166649579999984 0.3333350119999992 0.0000000000000000
1740	0.9166649579999984 0.8333350420000016 0.0000000000000000
1741	0.0000000000000000 0.2500000000000000 0.0726099979999972
1742	0.0000000000000000 0.7500000000000000 0.0726099979999972
1743	0.5000000000000000 0.2500000000000000 0.0726099979999972
1744	0.5000000000000000 0.7500000000000000 0.0726099979999972
1745	0.2500000000000000 0.2500000000000000 0.0726099979999972
1746	0.2500000000000000 0.7500000000000000 0.0726099979999972
1747	0.7500000000000000 0.2500000000000000 0.0726099979999972
1748	0.7500000000000000 0.7500000000000000 0.0726099979999972
1749	0.2500000000000000 0.0000000000000000 0.0726099979999972
1750	0.2500000000000000 0.5000000000000000 0.0726099979999972
1751	0.7500000000000000 0.0000000000000000 0.0726099979999972

1752	0.7500000000000000	0.5000000000000000	0.0726099979999972
1753	0.3336299803663181	0.4168075703957399	0.1453030526238379
1754	0.3336277313407408	0.9168083828906930	0.1451454683873479
1755	0.8335507504304687	0.4167801179657502	0.1451665390131183
1756	0.8335358053024677	0.9167560400938228	0.1451642136069538
1757	0.0831949933844101	0.4168049846155881	0.1453090505600230
1758	0.0832160054467579	0.9167637867353875	0.1451627983097765
1759	0.5832361542646112	0.4167839725532403	0.1451627983097765
1760	0.5831967566072009	0.9168031843927977	0.1451475134953881
1761	0.0831923996042647	0.1663700196336819	0.1453030526238379
1762	0.0832198520342544	0.6664492495695313	0.1451665390131183
1763	0.5831916171093070	0.1663722686592592	0.1451454683873479
1764	0.5832439599061772	0.6664641946975323	0.1451642136069538
1765	0.1658474663464986	0.0829870866989282	0.2184086438597888
1766	0.1658433350039559	0.5828462814723352	0.2184048545338868
1767	0.6656737629700373	0.0828423368906996	0.2182969842190232
1768	0.6655476176741644	0.5827605169523054	0.2184260890547591
1769	0.4171760910860698	0.0828238949139291	0.2182959397558761
1770	0.4169957515375060	0.5828396722498752	0.2184099964446773
1771	0.9171603277501248	0.0830042344624928	0.2184099964446773
1772	0.9172404738882776	0.5827595261117224	0.2184188924452855
1773	0.4170128993010707	0.3341525486534991	0.2184086438597888
1774	0.4171576491092992	0.8343262370299627	0.2182969842190232
1775	0.9171537185276648	0.3341566799960418	0.2184048545338868
1776	0.9172394830476946	0.8344523823258356	0.2184260890547591
1777	0.9983079737992426	0.2491442377544146	0.2903753895728300
1778	0.9997321571174425	0.7498585883848463	0.2891586400653736
1779	0.4993538645963298	0.2494295701898182	0.2889463208112204
1780	0.4993431758980762	0.7499088520806509	0.2889530064421564
1781	0.2508644631395427	0.2491355218604596	0.2903701404162575
1782	0.2505714306498703	0.7499128513158340	0.2889508480605016
1783	0.7500870896841718	0.2494285543501320	0.2889508480605016
1784	0.7501405507288581	0.7498593902711477	0.2891620768015670
1785	0.2508557622455854	0.5016920192007532	0.2903753895728300
1786	0.2505704298101818	0.0006461354036702	0.2889463208112204
1787	0.7501414116151537	0.5002678358825534	0.2891586400653736
1788	0.7500911479193491	0.0006568241019238	0.2889530064421564
1789	0.1666768238361058	0.3333232061638967	0.3213602494994845

1790

1791 NiZn (25% Zn) 111 Facet with Hydrogen supercell 2X2X1 - [Etot = -348.72763126 eV]

1792 1.01038006037737

1793 10.0268001556000002 0.0000000000000000 0.0000000000000000

1794 -5.0134000778000001 8.6834636535000005 0.0000000000000000

1795 0.0000000000000000 0.0000000000000000 28.1868000031000001

1796 Zn Ni H

1797 20 60 1

1798 Direct

1799 0.1666650029999985 0.3333350119999992 0.0000000000000000

1800 0.1666650029999985 0.8333350420000016 0.0000000000000000

1801 0.6666650180000033 0.3333350119999992 0.0000000000000000

1802 0.6666650180000033 0.8333350420000016 0.0000000000000000

1803 0.0000000000000000 0.0000000000000000 0.0726099979999972

1804	0.0000000000000000	0.5000000000000000	0.0726099979999972
1805	0.5000000000000000	0.0000000000000000	0.0726099979999972
1806	0.5000000000000000	0.5000000000000000	0.0726099979999972
1807	0.3332348911438601	0.1667651228561340	0.1454027874876189
1808	0.3332362967914406	0.6664653902690745	0.1454036857226129
1809	0.8335346687309269	0.1667637172085534	0.1454036857226129
1810	0.8333348627560824	0.6666651962439190	0.1454378125422053
1811	0.1666693874681684	0.3333306425318341	0.2171878407534962
1812	0.1664946304815587	0.8332430455072100	0.2161576862551726
1813	0.6667569544927900	0.3335053995184438	0.2161576862551726
1814	0.6667554092989647	0.8332445907010353	0.2161581955298928
1815	0.9998594532101137	0.5001405427898860	0.2938205966171950
1816	0.9998607478266379	0.9997094493442802	0.2938192771689856
1817	0.5002905506557198	0.5001392481733618	0.2938192771689856
1818	0.5000039209114249	0.9999960790885751	0.2940961605235088
1819	0.1666650029999985	0.0833349970000015	0.0000000000000000
1820	0.1666650029999985	0.5833349819999967	0.0000000000000000
1821	0.6666650180000033	0.0833349970000015	0.0000000000000000
1822	0.6666650180000033	0.5833349819999967	0.0000000000000000
1823	0.4166649880000008	0.0833349970000015	0.0000000000000000
1824	0.4166649880000008	0.5833349819999967	0.0000000000000000
1825	0.9166649579999984	0.0833349970000015	0.0000000000000000
1826	0.9166649579999984	0.5833349819999967	0.0000000000000000
1827	0.4166649880000008	0.3333350119999992	0.0000000000000000
1828	0.4166649880000008	0.8333350420000016	0.0000000000000000
1829	0.9166649579999984	0.3333350119999992	0.0000000000000000
1830	0.9166649579999984	0.8333350420000016	0.0000000000000000
1831	0.0000000000000000	0.2500000000000000	0.0726099979999972
1832	0.0000000000000000	0.7500000000000000	0.0726099979999972
1833	0.5000000000000000	0.2500000000000000	0.0726099979999972
1834	0.5000000000000000	0.7500000000000000	0.0726099979999972
1835	0.2500000000000000	0.2500000000000000	0.0726099979999972
1836	0.2500000000000000	0.7500000000000000	0.0726099979999972
1837	0.7500000000000000	0.2500000000000000	0.0726099979999972
1838	0.7500000000000000	0.7500000000000000	0.0726099979999972
1839	0.2500000000000000	0.0000000000000000	0.0726099979999972
1840	0.2500000000000000	0.5000000000000000	0.0726099979999972
1841	0.7500000000000000	0.0000000000000000	0.0726099979999972
1842	0.7500000000000000	0.5000000000000000	0.0726099979999972
1843	0.3333142957139543	0.4166563364331637	0.1449259920229053
1844	0.3335228695596655	0.9167620497845022	0.1446508104879385
1845	0.8336529900553060	0.4166664574406482	0.1446717213438831
1846	0.8336486059224555	0.9169826676868809	0.1446720441718128
1847	0.0833469623301966	0.4166530156698016	0.1449270615798284
1848	0.0833325779898999	0.9169803456319343	0.1446720797828860
1849	0.5830195953680644	0.4166674000100983	0.1446720797828860
1850	0.5832361885389830	0.9167637524610157	0.1446507441551006
1851	0.0833436335668409	0.1666857042860457	0.1449259920229053
1852	0.0833335125593564	0.6663470099446940	0.1446717213438831
1853	0.5832379502154978	0.1664771304403345	0.1446508104879385
1854	0.5830173323131191	0.6663513940775445	0.1446720441718128
1855	0.1647755166197129	0.0824346835306713	0.2177282504470384

1856	0.1647745200126636	0.5823310584927128	0.2177300170448007
1857	0.6645262180191267	0.0822598624366009	0.2174698086131457
1858	0.6642084946874718	0.5821011140974122	0.2175444215417670
1859	0.4177399026930146	0.0822600833069842	0.2174675664506225
1860	0.4175661615379482	0.5823332102031031	0.2177295054585642
1861	0.9176667897968969	0.0824338244620506	0.2177295054585642
1862	0.9178975974500503	0.5821024025499497	0.2175438934050788
1863	0.4175653024693275	0.3352244983802848	0.2177282504470384
1864	0.4177401235633980	0.8354737819808733	0.2174698086131457
1865	0.9176689415072872	0.3352254949873341	0.2177300170448007
1866	0.9178988859025878	0.8357915053125282	0.2175444215417670
1867	0.9985394121035895	0.2492651170926834	0.2894874899805089
1868	0.9993809778024101	0.7496835673924451	0.2875113658056634
1869	0.4987742913200677	0.2488251786509821	0.2872255752951958
1870	0.4987727351882256	0.7499345727795301	0.2872272015814517
1871	0.2507356976764754	0.2492642873235269	0.2894870141697439
1872	0.2511763378019083	0.7499380154731696	0.2872273034085708
1873	0.7500619255268361	0.2488236471980940	0.2872273034085708
1874	0.7503158054047034	0.7496841355953023	0.2875125764940947
1875	0.2507348829073166	0.5014605808964063	0.2894874899805089
1876	0.2511748213490179	0.0012257086799323	0.2872255752951958
1877	0.7503164326075549	0.5006190151975858	0.2875113658056634
1878	0.7500654272204699	0.0012272648117744	0.2872272015814517
1879	0.1666696102703824	0.3333304197296201	0.3196824235584614

1880

1881

1882 Bare- NiSc (25% Sc) 200 Facet supercell 2X2X1 - [Etot = -236.96351133 eV]

1883 1.04735280294076

1884 7.0844001770000000 0.0000000000000000 0.0000000000000000

1885 0.0000000000000000 7.0844001770000000 0.0000000000000000

1886 0.0000000000000000 0.0000000000000000 27.0844993591000005

1887 Sc Ni

1888 12 28

1889 Direct

1890 0.0000000000000000 0.0000000000000000 0.0000000000000000

1891 0.0000000000000000 0.5000000000000000 0.0000000000000000

1892 0.5000000000000000 0.0000000000000000 0.0000000000000000

1893 0.5000000000000000 0.5000000000000000 0.0000000000000000

1894 0.0000000000000000 0.0000000000000000 0.1310425452973263

1895 0.0000000000000000 0.5000000000000000 0.1310425452973263

1896 0.5000000000000000 0.0000000000000000 0.1310425452973263

1897 0.5000000000000000 0.5000000000000000 0.1310425452973263

1898 0.0000000000000000 0.0000000000000000 0.2641528516798530

1899 0.0000000000000000 0.5000000000000000 0.2641528516798530

1900 0.5000000000000000 0.0000000000000000 0.2641528516798530

1901 0.5000000000000000 0.5000000000000000 0.2641528516798530

1902 0.2500000000000000 0.2500000000000000 0.0000000000000000

1903 0.2500000000000000 0.7500000000000000 0.0000000000000000

1904 0.7500000000000000 0.2500000000000000 0.0000000000000000

1905 0.7500000000000000 0.7500000000000000 0.0000000000000000

1906 0.0000000000000000 0.2500000000000000 0.0653899980000006

1907 0.0000000000000000 0.7500000000000000 0.0653899980000006

1908	0.5000000000000000	0.2500000000000000	0.0653899980000006
1909	0.5000000000000000	0.7500000000000000	0.0653899980000006
1910	0.2500000000000000	0.0000000000000000	0.0653899980000006
1911	0.2500000000000000	0.5000000000000000	0.0653899980000006
1912	0.7500000000000000	0.0000000000000000	0.0653899980000006
1913	0.7500000000000000	0.5000000000000000	0.0653899980000006
1914	0.2500000000000000	0.2500000000000000	0.1307262018750777
1915	0.2500000000000000	0.7500000000000000	0.1307262018750777
1916	0.7500000000000000	0.2500000000000000	0.1307262018750777
1917	0.7500000000000000	0.7500000000000000	0.1307262018750777
1918	0.0000000000000000	0.2500000000000000	0.1970729602766639
1919	0.0000000000000000	0.7500000000000000	0.1970729602766639
1920	0.5000000000000000	0.2500000000000000	0.1970729602766639
1921	0.5000000000000000	0.7500000000000000	0.1970729602766639
1922	0.2500000000000000	0.0000000000000000	0.1970729602766639
1923	0.2500000000000000	0.5000000000000000	0.1970729602766639
1924	0.7500000000000000	0.0000000000000000	0.1970729602766639
1925	0.7500000000000000	0.5000000000000000	0.1970729602766639
1926	0.2500000000000000	0.2500000000000000	0.2517333951720957
1927	0.2500000000000000	0.7500000000000000	0.2517333951720957
1928	0.7500000000000000	0.2500000000000000	0.2517333951720957
1929	0.7500000000000000	0.7500000000000000	0.2517333951720957

1930

1931 Bare- NiTi (25% Ti) 200 Facet supercell 2X2X1 - [Etot = -251.89040363 eV]

1932 1.01798110552312

1933	7.0844001770000000	0.0000000000000000	0.0000000000000000
1934	0.0000000000000000	7.0844001770000000	0.0000000000000000
1935	0.0000000000000000	0.0000000000000000	27.0844993591000005

1936 Ti Ni

1937 12 28

1938 Direct

1939	0.0000000000000000	0.0000000000000000	0.0000000000000000
1940	0.0000000000000000	0.5000000000000000	0.0000000000000000
1941	0.5000000000000000	0.0000000000000000	0.0000000000000000
1942	0.5000000000000000	0.5000000000000000	0.0000000000000000
1943	0.0000000000000000	0.0000000000000000	0.1315154384329844
1944	0.0000000000000000	0.5000000000000000	0.1315154384329844
1945	0.5000000000000000	0.0000000000000000	0.1315154384329844
1946	0.5000000000000000	0.5000000000000000	0.1315154384329844
1947	0.0000000000000000	0.0000000000000000	0.2652791379492072
1948	0.0000000000000000	0.5000000000000000	0.2652791379492072
1949	0.5000000000000000	0.0000000000000000	0.2652791379492072
1950	0.5000000000000000	0.5000000000000000	0.2652791379492072
1951	0.2500000000000000	0.2500000000000000	0.0000000000000000
1952	0.2500000000000000	0.7500000000000000	0.0000000000000000
1953	0.7500000000000000	0.2500000000000000	0.0000000000000000
1954	0.7500000000000000	0.7500000000000000	0.0000000000000000
1955	0.0000000000000000	0.2500000000000000	0.0653899980000006
1956	0.0000000000000000	0.7500000000000000	0.0653899980000006
1957	0.5000000000000000	0.2500000000000000	0.0653899980000006
1958	0.5000000000000000	0.7500000000000000	0.0653899980000006
1959	0.2500000000000000	0.0000000000000000	0.0653899980000006

1960	0.2500000000000000	0.5000000000000000	0.0653899980000006
1961	0.7500000000000000	0.0000000000000000	0.0653899980000006
1962	0.7500000000000000	0.5000000000000000	0.0653899980000006
1963	0.2500000000000000	0.2500000000000000	0.1308958383395691
1964	0.2500000000000000	0.7500000000000000	0.1308958383395691
1965	0.7500000000000000	0.2500000000000000	0.1308958383395691
1966	0.7500000000000000	0.7500000000000000	0.1308958383395691
1967	0.0000000000000000	0.2500000000000000	0.1965421368997227
1968	0.0000000000000000	0.7500000000000000	0.1965421368997227
1969	0.5000000000000000	0.2500000000000000	0.1965421368997227
1970	0.5000000000000000	0.7500000000000000	0.1965421368997227
1971	0.2500000000000000	0.0000000000000000	0.1965421368997227
1972	0.2500000000000000	0.5000000000000000	0.1965421368997227
1973	0.7500000000000000	0.0000000000000000	0.1965421368997227
1974	0.7500000000000000	0.5000000000000000	0.1965421368997227
1975	0.2500000000000000	0.2500000000000000	0.2572113090435622
1976	0.2500000000000000	0.7500000000000000	0.2572113090435622
1977	0.7500000000000000	0.2500000000000000	0.2572113090435622
1978	0.7500000000000000	0.7500000000000000	0.2572113090435622

1979
1980 Bare- NiV (25% V) 200 Facet supercell 2X2X1 - [Etot = -251.00618601 eV]
1981 1.00458661266245

1982	7.0844001770000000	0.0000000000000000	0.0000000000000000
1983	0.0000000000000000	7.0844001770000000	0.0000000000000000
1984	0.0000000000000000	0.0000000000000000	27.0844993591000005

1985 V Ni
1986 12 28

1987	Direct		
1988	0.0000000000000000	0.0000000000000000	0.0000000000000000
1989	0.0000000000000000	0.5000000000000000	0.0000000000000000
1990	0.5000000000000000	0.0000000000000000	0.0000000000000000
1991	0.5000000000000000	0.5000000000000000	0.0000000000000000
1992	0.0000000000000000	0.0000000000000000	0.1307616103900031
1993	0.0000000000000000	0.5000000000000000	0.1307616103900031
1994	0.5000000000000000	0.0000000000000000	0.1307616103900031
1995	0.5000000000000000	0.5000000000000000	0.1307616103900031
1996	0.0000000000000000	0.0000000000000000	0.2646446537211702
1997	0.0000000000000000	0.5000000000000000	0.2646446537211702
1998	0.5000000000000000	0.0000000000000000	0.2646446537211702
1999	0.5000000000000000	0.5000000000000000	0.2646446537211702
2000	0.2500000000000000	0.2500000000000000	0.0000000000000000
2001	0.2500000000000000	0.7500000000000000	0.0000000000000000
2002	0.7500000000000000	0.2500000000000000	0.0000000000000000
2003	0.7500000000000000	0.7500000000000000	0.0000000000000000
2004	0.0000000000000000	0.2500000000000000	0.0653899980000006
2005	0.0000000000000000	0.7500000000000000	0.0653899980000006
2006	0.5000000000000000	0.2500000000000000	0.0653899980000006
2007	0.5000000000000000	0.7500000000000000	0.0653899980000006
2008	0.2500000000000000	0.0000000000000000	0.0653899980000006
2009	0.2500000000000000	0.5000000000000000	0.0653899980000006
2010	0.7500000000000000	0.0000000000000000	0.0653899980000006
2011	0.7500000000000000	0.5000000000000000	0.0653899980000006

2012	0.2500000000000000	0.2500000000000000	0.1306105587269855
2013	0.2500000000000000	0.7500000000000000	0.1306105587269855
2014	0.7500000000000000	0.2500000000000000	0.1306105587269855
2015	0.7500000000000000	0.7500000000000000	0.1306105587269855
2016	0.0000000000000000	0.2500000000000000	0.1956455907635402
2017	0.0000000000000000	0.7500000000000000	0.1956455907635402
2018	0.5000000000000000	0.2500000000000000	0.1956455907635402
2019	0.5000000000000000	0.7500000000000000	0.1956455907635402
2020	0.2500000000000000	0.0000000000000000	0.1956455907635402
2021	0.2500000000000000	0.5000000000000000	0.1956455907635402
2022	0.7500000000000000	0.0000000000000000	0.1956455907635402
2023	0.7500000000000000	0.5000000000000000	0.1956455907635402
2024	0.2500000000000000	0.2500000000000000	0.2574233840485647
2025	0.2500000000000000	0.7500000000000000	0.2574233840485647
2026	0.7500000000000000	0.2500000000000000	0.2574233840485647
2027	0.7500000000000000	0.7500000000000000	0.2574233840485647
2028			
2029	Bare- NiCr (25% Cr) 200 Facet supercell 2X2X1 - [Etot = -251.45606664 eV]		
2030	0.995572721824907		
2031	7.0844001770000000	0.0000000000000000	0.0000000000000000
2032	0.0000000000000000	7.0844001770000000	0.0000000000000000
2033	0.0000000000000000	0.0000000000000000	27.0844993591000005
2034	Cr Ni		
2035	12 28		
2036	Direct		
2037	0.0000000000000000	0.0000000000000000	0.0000000000000000
2038	0.0000000000000000	0.5000000000000000	0.0000000000000000
2039	0.5000000000000000	0.0000000000000000	0.0000000000000000
2040	0.5000000000000000	0.5000000000000000	0.0000000000000000
2041	0.0000000000000000	0.0000000000000000	0.1316542368568605
2042	0.0000000000000000	0.5000000000000000	0.1316542368568605
2043	0.5000000000000000	0.0000000000000000	0.1316542368568605
2044	0.5000000000000000	0.5000000000000000	0.1316542368568605
2045	0.0000000000000000	0.0000000000000000	0.2665245603646156
2046	0.0000000000000000	0.5000000000000000	0.2665245603646156
2047	0.5000000000000000	0.0000000000000000	0.2665245603646156
2048	0.5000000000000000	0.5000000000000000	0.2665245603646156
2049	0.2500000000000000	0.2500000000000000	0.0000000000000000
2050	0.2500000000000000	0.7500000000000000	0.0000000000000000
2051	0.7500000000000000	0.2500000000000000	0.0000000000000000
2052	0.7500000000000000	0.7500000000000000	0.0000000000000000
2053	0.0000000000000000	0.2500000000000000	0.0653899980000006
2054	0.0000000000000000	0.7500000000000000	0.0653899980000006
2055	0.5000000000000000	0.2500000000000000	0.0653899980000006
2056	0.5000000000000000	0.7500000000000000	0.0653899980000006
2057	0.2500000000000000	0.0000000000000000	0.0653899980000006
2058	0.2500000000000000	0.5000000000000000	0.0653899980000006
2059	0.7500000000000000	0.0000000000000000	0.0653899980000006
2060	0.7500000000000000	0.5000000000000000	0.0653899980000006
2061	0.2500000000000000	0.2500000000000000	0.1313944603006831
2062	0.2500000000000000	0.7500000000000000	0.1313944603006831
2063	0.7500000000000000	0.2500000000000000	0.1313944603006831

2064	0.7500000000000000	0.7500000000000000	0.1313944603006831
2065	0.0000000000000000	0.2500000000000000	0.1972560321995260
2066	0.0000000000000000	0.7500000000000000	0.1972560321995260
2067	0.5000000000000000	0.2500000000000000	0.1972560321995260
2068	0.5000000000000000	0.7500000000000000	0.1972560321995260
2069	0.2500000000000000	0.0000000000000000	0.1972560321995260
2070	0.2500000000000000	0.5000000000000000	0.1972560321995260
2071	0.7500000000000000	0.0000000000000000	0.1972560321995260
2072	0.7500000000000000	0.5000000000000000	0.1972560321995260
2073	0.2500000000000000	0.2500000000000000	0.2601018645656197
2074	0.2500000000000000	0.7500000000000000	0.2601018645656197
2075	0.7500000000000000	0.2500000000000000	0.2601018645656197
2076	0.7500000000000000	0.7500000000000000	0.2601018645656197
2077			
2078	Bare- NiMn (25% Mn) 200 Facet supercell 2X2X1 - [Etot = -251.85591824 eV]		
2079	0.989317187668226		
2080	7.0844001770000000	0.0000000000000000	0.0000000000000000
2081	0.0000000000000000	7.0844001770000000	0.0000000000000000
2082	0.0000000000000000	0.0000000000000000	27.0844993591000005
2083	Mn	Ni	
2084	12	28	
2085	Direct		
2086	0.0000000000000000	0.0000000000000000	0.0000000000000000
2087	0.0000000000000000	0.5000000000000000	0.0000000000000000
2088	0.5000000000000000	0.0000000000000000	0.0000000000000000
2089	0.5000000000000000	0.5000000000000000	0.0000000000000000
2090	0.0000000000000000	0.0000000000000000	0.1337698263595968
2091	0.0000000000000000	0.5000000000000000	0.1337698263595968
2092	0.5000000000000000	0.0000000000000000	0.1337698263595968
2093	0.5000000000000000	0.5000000000000000	0.1337698263595968
2094	0.0000000000000000	0.0000000000000000	0.2715000394439571
2095	0.0000000000000000	0.5000000000000000	0.2715000394439571
2096	0.5000000000000000	0.0000000000000000	0.2715000394439571
2097	0.5000000000000000	0.5000000000000000	0.2715000394439571
2098	0.2500000000000000	0.2500000000000000	0.0000000000000000
2099	0.2500000000000000	0.7500000000000000	0.0000000000000000
2100	0.7500000000000000	0.2500000000000000	0.0000000000000000
2101	0.7500000000000000	0.7500000000000000	0.0000000000000000
2102	0.0000000000000000	0.2500000000000000	0.0653899980000006
2103	0.0000000000000000	0.7500000000000000	0.0653899980000006
2104	0.5000000000000000	0.2500000000000000	0.0653899980000006
2105	0.5000000000000000	0.7500000000000000	0.0653899980000006
2106	0.2500000000000000	0.0000000000000000	0.0653899980000006
2107	0.2500000000000000	0.5000000000000000	0.0653899980000006
2108	0.7500000000000000	0.0000000000000000	0.0653899980000006
2109	0.7500000000000000	0.5000000000000000	0.0653899980000006
2110	0.2500000000000000	0.2500000000000000	0.1334414099143828
2111	0.2500000000000000	0.7500000000000000	0.1334414099143828
2112	0.7500000000000000	0.2500000000000000	0.1334414099143828
2113	0.7500000000000000	0.7500000000000000	0.1334414099143828
2114	0.0000000000000000	0.2500000000000000	0.2015209686675448
2115	0.0000000000000000	0.7500000000000000	0.2015209686675448

2116	0.5000000000000000	0.2500000000000000	0.2015209686675448
2117	0.5000000000000000	0.7500000000000000	0.2015209686675448
2118	0.2500000000000000	0.0000000000000000	0.2015209686675448
2119	0.2500000000000000	0.5000000000000000	0.2015209686675448
2120	0.7500000000000000	0.0000000000000000	0.2015209686675448
2121	0.7500000000000000	0.5000000000000000	0.2015209686675448
2122	0.2500000000000000	0.2500000000000000	0.2656869777385040
2123	0.2500000000000000	0.7500000000000000	0.2656869777385040
2124	0.7500000000000000	0.2500000000000000	0.2656869777385040
2125	0.7500000000000000	0.7500000000000000	0.2656869777385040
2126			
2127	Bare- NiFe (25% Fe) 200 Facet supercell 2X2X1 - [Etot = -241.93424633 eV]		
2128	1.0000000000000000		
2129	7.0844001770000000	0.0000000000000000	0.0000000000000000
2130	0.0000000000000000	7.0844001770000000	0.0000000000000000
2131	0.0000000000000000	0.0000000000000000	27.0844993591000005
2132	Fe Ni		
2133	12 28		
2134	Direct		
2135	0.0000000000000000	0.0000000000000000	0.0000000000000000
2136	0.0000000000000000	0.5000000000000000	0.0000000000000000
2137	0.5000000000000000	0.0000000000000000	0.0000000000000000
2138	0.5000000000000000	0.5000000000000000	0.0000000000000000
2139	0.0000000000000000	0.0000000000000000	0.1308150637505392
2140	0.0000000000000000	0.5000000000000000	0.1308150637505392
2141	0.5000000000000000	0.0000000000000000	0.1308150637505392
2142	0.5000000000000000	0.5000000000000000	0.1308150637505392
2143	0.0000000000000000	0.0000000000000000	0.2615715394668001
2144	0.0000000000000000	0.5000000000000000	0.2615715394668001
2145	0.5000000000000000	0.0000000000000000	0.2615715394668001
2146	0.5000000000000000	0.5000000000000000	0.2615715394668001
2147	0.2500000000000000	0.2500000000000000	0.0000000000000000
2148	0.2500000000000000	0.7500000000000000	0.0000000000000000
2149	0.7500000000000000	0.2500000000000000	0.0000000000000000
2150	0.7500000000000000	0.7500000000000000	0.0000000000000000
2151	0.0000000000000000	0.2500000000000000	0.0653899980000006
2152	0.0000000000000000	0.7500000000000000	0.0653899980000006
2153	0.5000000000000000	0.2500000000000000	0.0653899980000006
2154	0.5000000000000000	0.7500000000000000	0.0653899980000006
2155	0.2500000000000000	0.0000000000000000	0.0653899980000006
2156	0.2500000000000000	0.5000000000000000	0.0653899980000006
2157	0.7500000000000000	0.0000000000000000	0.0653899980000006
2158	0.7500000000000000	0.5000000000000000	0.0653899980000006
2159	0.2500000000000000	0.2500000000000000	0.1308036703203186
2160	0.2500000000000000	0.7500000000000000	0.1308036703203186
2161	0.7500000000000000	0.2500000000000000	0.1308036703203186
2162	0.7500000000000000	0.7500000000000000	0.1308036703203186
2163	0.0000000000000000	0.2500000000000000	0.1964348914370930
2164	0.0000000000000000	0.7500000000000000	0.1964348914370930
2165	0.5000000000000000	0.2500000000000000	0.1964348914370930
2166	0.5000000000000000	0.7500000000000000	0.1964348914370930
2167	0.2500000000000000	0.0000000000000000	0.1964348914370930

2168	0.2500000000000000	0.5000000000000000	0.1964348914370930
2169	0.7500000000000000	0.0000000000000000	0.1964348914370930
2170	0.7500000000000000	0.5000000000000000	0.1964348914370930
2171	0.2500000000000000	0.2500000000000000	0.2591798791499969
2172	0.2500000000000000	0.7500000000000000	0.2591798791499969
2173	0.7500000000000000	0.2500000000000000	0.2591798791499969
2174	0.7500000000000000	0.7500000000000000	0.2591798791499969
2175			
2176	Bare- NiCo (25% Co) 200 Facet supercell 2X2X1 - [Etot = -222.09981359 eV]		
2177	0.993794164815303		
2178	7.0844001770000000	0.0000000000000000	0.0000000000000000
2179	0.0000000000000000	7.0844001770000000	0.0000000000000000
2180	0.0000000000000000	0.0000000000000000	27.0844993591000005
2181	Co	Ni	
2182	12	28	
2183	Direct		
2184	0.0000000000000000	0.0000000000000000	0.0000000000000000
2185	0.0000000000000000	0.5000000000000000	0.0000000000000000
2186	0.5000000000000000	0.0000000000000000	0.0000000000000000
2187	0.5000000000000000	0.5000000000000000	0.0000000000000000
2188	0.0000000000000000	0.0000000000000000	0.1308311864820837
2189	0.0000000000000000	0.5000000000000000	0.1308311864820837
2190	0.5000000000000000	0.0000000000000000	0.1308311864820837
2191	0.5000000000000000	0.5000000000000000	0.1308311864820837
2192	0.0000000000000000	0.0000000000000000	0.2607322158043175
2193	0.0000000000000000	0.5000000000000000	0.2607322158043175
2194	0.5000000000000000	0.0000000000000000	0.2607322158043175
2195	0.5000000000000000	0.5000000000000000	0.2607322158043175
2196	0.2500000000000000	0.2500000000000000	0.0000000000000000
2197	0.2500000000000000	0.7500000000000000	0.0000000000000000
2198	0.7500000000000000	0.2500000000000000	0.0000000000000000
2199	0.7500000000000000	0.7500000000000000	0.0000000000000000
2200	0.0000000000000000	0.2500000000000000	0.0653899980000006
2201	0.0000000000000000	0.7500000000000000	0.0653899980000006
2202	0.5000000000000000	0.2500000000000000	0.0653899980000006
2203	0.5000000000000000	0.7500000000000000	0.0653899980000006
2204	0.2500000000000000	0.0000000000000000	0.0653899980000006
2205	0.2500000000000000	0.5000000000000000	0.0653899980000006
2206	0.7500000000000000	0.0000000000000000	0.0653899980000006
2207	0.7500000000000000	0.5000000000000000	0.0653899980000006
2208	0.2500000000000000	0.2500000000000000	0.1309176206376250
2209	0.2500000000000000	0.7500000000000000	0.1309176206376250
2210	0.7500000000000000	0.2500000000000000	0.1309176206376250
2211	0.7500000000000000	0.7500000000000000	0.1309176206376250
2212	0.0000000000000000	0.2500000000000000	0.1966978463506166
2213	0.0000000000000000	0.7500000000000000	0.1966978463506166
2214	0.5000000000000000	0.2500000000000000	0.1966978463506166
2215	0.5000000000000000	0.7500000000000000	0.1966978463506166
2216	0.2500000000000000	0.0000000000000000	0.1966978463506166
2217	0.2500000000000000	0.5000000000000000	0.1966978463506166
2218	0.7500000000000000	0.0000000000000000	0.1966978463506166
2219	0.7500000000000000	0.5000000000000000	0.1966978463506166

2220	0.2500000000000000	0.2500000000000000	0.2595134611992549
2221	0.2500000000000000	0.7500000000000000	0.2595134611992549
2222	0.7500000000000000	0.2500000000000000	0.2595134611992549
2223	0.7500000000000000	0.7500000000000000	0.2595134611992549
2224			
2225	Pure-Ni 200 Facet supercell 2X2X1 - [Etot = -203.61032669 eV]		
2226	1.01798110552312		
2227	7.0844001770000000	0.0000000000000000	0.0000000000000000
2228	0.0000000000000000	7.0844001770000000	0.0000000000000000
2229	0.0000000000000000	0.0000000000000000	27.0844993591000005
2230	Ni		
2231	40		
2232	Direct		
2233	0.0000000000000000	0.0000000000000000	0.0000000000000000
2234	0.0000000000000000	0.5000000000000000	0.0000000000000000
2235	0.5000000000000000	0.0000000000000000	0.0000000000000000
2236	0.5000000000000000	0.5000000000000000	0.0000000000000000
2237	0.0000000000000000	0.0000000000000000	0.1273484974330827
2238	0.0000000000000000	0.5000000000000000	0.1273484974330827
2239	0.5000000000000000	0.0000000000000000	0.1273484974330827
2240	0.5000000000000000	0.5000000000000000	0.1273484974330827
2241	0.0000000000000000	0.0000000000000000	0.2492718720670695
2242	0.0000000000000000	0.5000000000000000	0.2492718720670695
2243	0.5000000000000000	0.0000000000000000	0.2492718720670695
2244	0.5000000000000000	0.5000000000000000	0.2492718720670695
2245	0.2500000000000000	0.2500000000000000	0.0000000000000000
2246	0.2500000000000000	0.7500000000000000	0.0000000000000000
2247	0.7500000000000000	0.2500000000000000	0.0000000000000000
2248	0.7500000000000000	0.7500000000000000	0.0000000000000000
2249	0.0000000000000000	0.2500000000000000	0.0653899980000006
2250	0.0000000000000000	0.7500000000000000	0.0653899980000006
2251	0.5000000000000000	0.2500000000000000	0.0653899980000006
2252	0.5000000000000000	0.7500000000000000	0.0653899980000006
2253	0.2500000000000000	0.0000000000000000	0.0653899980000006
2254	0.2500000000000000	0.5000000000000000	0.0653899980000006
2255	0.7500000000000000	0.0000000000000000	0.0653899980000006
2256	0.7500000000000000	0.5000000000000000	0.0653899980000006
2257	0.2500000000000000	0.2500000000000000	0.1273364080441439
2258	0.2500000000000000	0.7500000000000000	0.1273364080441439
2259	0.7500000000000000	0.2500000000000000	0.1273364080441439
2260	0.7500000000000000	0.7500000000000000	0.1273364080441439
2261	0.0000000000000000	0.2500000000000000	0.1899727533166100
2262	0.0000000000000000	0.7500000000000000	0.1899727533166100
2263	0.5000000000000000	0.2500000000000000	0.1899727533166100
2264	0.5000000000000000	0.7500000000000000	0.1899727533166100
2265	0.2500000000000000	0.0000000000000000	0.1899727533166100
2266	0.2500000000000000	0.5000000000000000	0.1899727533166100
2267	0.7500000000000000	0.0000000000000000	0.1899727533166100
2268	0.7500000000000000	0.5000000000000000	0.1899727533166100
2269	0.2500000000000000	0.2500000000000000	0.2492695932662272
2270	0.2500000000000000	0.7500000000000000	0.2492695932662272
2271	0.7500000000000000	0.2500000000000000	0.2492695932662272

2272	0.7500000000000000	0.7500000000000000	0.2492695932662272
2273			
2274	Bare- NiCu (25% Cu) 200 Facet supercell 2X2X1 - [Etot = -184.69603141 eV]		
2275	0.998485100048875		
2276	7.0844001770000000	0.0000000000000000	0.0000000000000000
2277	0.0000000000000000	7.0844001770000000	0.0000000000000000
2278	0.0000000000000000	0.0000000000000000	27.0844993591000005
2279	Cu Ni		
2280	12 28		
2281	Direct		
2282	0.0000000000000000	0.0000000000000000	0.0000000000000000
2283	0.0000000000000000	0.5000000000000000	0.0000000000000000
2284	0.5000000000000000	0.0000000000000000	0.0000000000000000
2285	0.5000000000000000	0.5000000000000000	0.0000000000000000
2286	0.0000000000000000	0.0000000000000000	0.1313946536162192
2287	0.0000000000000000	0.5000000000000000	0.1313946536162192
2288	0.5000000000000000	0.0000000000000000	0.1313946536162192
2289	0.5000000000000000	0.5000000000000000	0.1313946536162192
2290	0.0000000000000000	0.0000000000000000	0.2634817293910956
2291	0.0000000000000000	0.5000000000000000	0.2634817293910956
2292	0.5000000000000000	0.0000000000000000	0.2634817293910956
2293	0.5000000000000000	0.5000000000000000	0.2634817293910956
2294	0.2500000000000000	0.2500000000000000	0.0000000000000000
2295	0.2500000000000000	0.7500000000000000	0.0000000000000000
2296	0.7500000000000000	0.2500000000000000	0.0000000000000000
2297	0.7500000000000000	0.7500000000000000	0.0000000000000000
2298	0.0000000000000000	0.2500000000000000	0.0653899980000006
2299	0.0000000000000000	0.7500000000000000	0.0653899980000006
2300	0.5000000000000000	0.2500000000000000	0.0653899980000006
2301	0.5000000000000000	0.7500000000000000	0.0653899980000006
2302	0.2500000000000000	0.0000000000000000	0.0653899980000006
2303	0.2500000000000000	0.5000000000000000	0.0653899980000006
2304	0.7500000000000000	0.0000000000000000	0.0653899980000006
2305	0.7500000000000000	0.5000000000000000	0.0653899980000006
2306	0.2500000000000000	0.2500000000000000	0.1311315066231558
2307	0.2500000000000000	0.7500000000000000	0.1311315066231558
2308	0.7500000000000000	0.2500000000000000	0.1311315066231558
2309	0.7500000000000000	0.7500000000000000	0.1311315066231558
2310	0.0000000000000000	0.2500000000000000	0.1975016266732936
2311	0.0000000000000000	0.7500000000000000	0.1975016266732936
2312	0.5000000000000000	0.2500000000000000	0.1975016266732936
2313	0.5000000000000000	0.7500000000000000	0.1975016266732936
2314	0.2500000000000000	0.0000000000000000	0.1975016266732936
2315	0.2500000000000000	0.5000000000000000	0.1975016266732936
2316	0.7500000000000000	0.0000000000000000	0.1975016266732936
2317	0.7500000000000000	0.5000000000000000	0.1975016266732936
2318	0.2500000000000000	0.2500000000000000	0.2590786018433775
2319	0.2500000000000000	0.7500000000000000	0.2590786018433775
2320	0.7500000000000000	0.2500000000000000	0.2590786018433775
2321	0.7500000000000000	0.7500000000000000	0.2590786018433775
2322			
2323	Bare- NiZn (25% Zn) 200 Facet supercell 2X2X1 - [Etot = -164.37259736 eV]		

2324	1.01038006037737		
2325	7.0844001770000000	0.0000000000000000	0.0000000000000000
2326	0.0000000000000000	7.0844001770000000	0.0000000000000000
2327	0.0000000000000000	0.0000000000000000	27.0844993591000005
2328	Zn Ni		
2329	12 28		
2330	Direct		
2331	0.0000000000000000	0.0000000000000000	0.0000000000000000
2332	0.0000000000000000	0.5000000000000000	0.0000000000000000
2333	0.5000000000000000	0.0000000000000000	0.0000000000000000
2334	0.5000000000000000	0.5000000000000000	0.0000000000000000
2335	0.0000000000000000	0.0000000000000000	0.1309191281788173
2336	0.0000000000000000	0.5000000000000000	0.1309191281788173
2337	0.5000000000000000	0.0000000000000000	0.1309191281788173
2338	0.5000000000000000	0.5000000000000000	0.1309191281788173
2339	0.0000000000000000	0.0000000000000000	0.2638061277048536
2340	0.0000000000000000	0.5000000000000000	0.2638061277048536
2341	0.5000000000000000	0.0000000000000000	0.2638061277048536
2342	0.5000000000000000	0.5000000000000000	0.2638061277048536
2343	0.2500000000000000	0.2500000000000000	0.0000000000000000
2344	0.2500000000000000	0.7500000000000000	0.0000000000000000
2345	0.7500000000000000	0.2500000000000000	0.0000000000000000
2346	0.7500000000000000	0.7500000000000000	0.0000000000000000
2347	0.0000000000000000	0.2500000000000000	0.0653899980000006
2348	0.0000000000000000	0.7500000000000000	0.0653899980000006
2349	0.5000000000000000	0.2500000000000000	0.0653899980000006
2350	0.5000000000000000	0.7500000000000000	0.0653899980000006
2351	0.2500000000000000	0.0000000000000000	0.0653899980000006
2352	0.2500000000000000	0.5000000000000000	0.0653899980000006
2353	0.7500000000000000	0.0000000000000000	0.0653899980000006
2354	0.7500000000000000	0.5000000000000000	0.0653899980000006
2355	0.2500000000000000	0.2500000000000000	0.1308154385594236
2356	0.2500000000000000	0.7500000000000000	0.1308154385594236
2357	0.7500000000000000	0.2500000000000000	0.1308154385594236
2358	0.7500000000000000	0.7500000000000000	0.1308154385594236
2359	0.0000000000000000	0.2500000000000000	0.1964718969898058
2360	0.0000000000000000	0.7500000000000000	0.1964718969898058
2361	0.5000000000000000	0.2500000000000000	0.1964718969898058
2362	0.5000000000000000	0.7500000000000000	0.1964718969898058
2363	0.2500000000000000	0.0000000000000000	0.1964718969898058
2364	0.2500000000000000	0.5000000000000000	0.1964718969898058
2365	0.7500000000000000	0.0000000000000000	0.1964718969898058
2366	0.7500000000000000	0.5000000000000000	0.1964718969898058
2367	0.2500000000000000	0.2500000000000000	0.2571356678845973
2368	0.2500000000000000	0.7500000000000000	0.2571356678845973
2369	0.7500000000000000	0.2500000000000000	0.2571356678845973
2370	0.7500000000000000	0.7500000000000000	0.2571356678845973
2371			
2372			
2373			
2374	NiSc (25% Sc) 200 Facet with Hydrogen supercell 2X2X1 - [Etot = -240.78858450 eV]		
2375	1.04735280294076		

2376	7.0844001770000000	0.0000000000000000	0.0000000000000000
2377	0.0000000000000000	7.0844001770000000	0.0000000000000000
2378	0.0000000000000000	0.0000000000000000	27.0844993591000005
2379	Sc Ni H		
2380	12 28 1		
2381	Direct		
2382	0.0000000000000000	0.0000000000000000	0.0000000000000000
2383	0.0000000000000000	0.5000000000000000	0.0000000000000000
2384	0.5000000000000000	0.0000000000000000	0.0000000000000000
2385	0.5000000000000000	0.5000000000000000	0.0000000000000000
2386	0.0016091787463424	0.0000000000000000	0.1313379994056305
2387	0.0003376704753961	0.5000000000000000	0.1306523607905135
2388	0.4983908212536576	0.0000000000000000	0.1313379994056305
2389	0.4996623295246039	0.5000000000000000	0.1306523607905135
2390	0.9998088645627732	0.0000000000000000	0.2651101251143402
2391	0.9850692932660365	0.5000000000000000	0.2627544774729529
2392	0.5001911354372268	0.0000000000000000	0.2651101251143402
2393	0.5149307067339635	0.5000000000000000	0.2627544774729529
2394	0.2500000000000000	0.2500000000000000	0.0000000000000000
2395	0.2500000000000000	0.7500000000000000	0.0000000000000000
2396	0.7500000000000000	0.2500000000000000	0.0000000000000000
2397	0.7500000000000000	0.7500000000000000	0.0000000000000000
2398	0.0000000000000000	0.2500000000000000	0.0653899980000006
2399	0.0000000000000000	0.7500000000000000	0.0653899980000006
2400	0.5000000000000000	0.2500000000000000	0.0653899980000006
2401	0.5000000000000000	0.7500000000000000	0.0653899980000006
2402	0.2500000000000000	0.0000000000000000	0.0653899980000006
2403	0.2500000000000000	0.5000000000000000	0.0653899980000006
2404	0.7500000000000000	0.0000000000000000	0.0653899980000006
2405	0.7500000000000000	0.5000000000000000	0.0653899980000006
2406	0.2500000000000000	0.2488108924304200	0.1310670968474668
2407	0.2500000000000000	0.7511891075695800	0.1310670968474668
2408	0.7500000000000000	0.2497644293727248	0.1308376001053659
2409	0.7500000000000000	0.7502355706272752	0.1308376001053659
2410	0.0051308219809627	0.2479422922009675	0.1973433028359750
2411	0.0051308219809627	0.7520577077990325	0.1973433028359750
2412	0.4948691780190373	0.2479422922009675	0.1973433028359750
2413	0.4948691780190373	0.7520577077990325	0.1973433028359750
2414	0.2500000000000000	0.0000000000000000	0.2019067938619656
2415	0.2500000000000000	0.5000000000000000	0.1950251988459044
2416	0.7500000000000000	0.0000000000000000	0.1962600347438723
2417	0.7500000000000000	0.5000000000000000	0.1952727140360793
2418	0.2500000000000000	0.2671492698165849	0.2563177523350220
2419	0.2500000000000000	0.7328507301834151	0.2563177523350220
2420	0.7500000000000000	0.2457166756196898	0.2501497701870363
2421	0.7500000000000000	0.7542833243803031	0.2501497701870363
2422	0.2500000000000000	0.5000000000000000	0.2864900394577319
2423			
2424	NiTi (25% Ti) 200 Facet with Hydrogen supercell 2X2X1 - [Etot = -255.84437464 eV]		
2425	1.01798110552312		
2426	7.0844001770000000	0.0000000000000000	0.0000000000000000
2427	0.0000000000000000	7.0844001770000000	0.0000000000000000

2428	0.0000000000000000	0.0000000000000000	27.0844993591000005
2429	Ti Ni H		
2430	12 28 1		
2431	Direct		
2432	0.0000000000000000	0.0000000000000000	0.0000000000000000
2433	0.0000000000000000	0.5000000000000000	0.0000000000000000
2434	0.5000000000000000	0.0000000000000000	0.0000000000000000
2435	0.5000000000000000	0.5000000000000000	0.0000000000000000
2436	0.0001441113916343	0.0000000000000000	0.1315998410575432
2437	0.0008823657244861	0.5000000000000000	0.1313323039741050
2438	0.4998558886083657	0.0000000000000000	0.1315998410575432
2439	0.4991176342755139	0.5000000000000000	0.1313323039741050
2440	0.9971802769557385	0.0000000000000000	0.2653735189097475
2441	0.9900400970156014	0.5000000000000000	0.2658017118630767
2442	0.5028197230442615	0.0000000000000000	0.2653735189097475
2443	0.5099599029843986	0.5000000000000000	0.2658017118630767
2444	0.2500000000000000	0.2500000000000000	0.0000000000000000
2445	0.2500000000000000	0.7500000000000000	0.0000000000000000
2446	0.7500000000000000	0.2500000000000000	0.0000000000000000
2447	0.7500000000000000	0.7500000000000000	0.0000000000000000
2448	0.0000000000000000	0.2500000000000000	0.0653899980000006
2449	0.0000000000000000	0.7500000000000000	0.0653899980000006
2450	0.5000000000000000	0.2500000000000000	0.0653899980000006
2451	0.5000000000000000	0.7500000000000000	0.0653899980000006
2452	0.2500000000000000	0.0000000000000000	0.0653899980000006
2453	0.2500000000000000	0.5000000000000000	0.0653899980000006
2454	0.7500000000000000	0.0000000000000000	0.0653899980000006
2455	0.7500000000000000	0.5000000000000000	0.0653899980000006
2456	0.2500000000000000	0.2474992812884338	0.1308455381700355
2457	0.2500000000000000	0.7525007187115662	0.1308455381700355
2458	0.7500000000000000	0.2494531016306212	0.1307552263231457
2459	0.7500000000000000	0.7505468983693788	0.1307552263231457
2460	0.0012580143739314	0.2500503922262283	0.1965967146531398
2461	0.0012580143739314	0.7499496077737717	0.1965967146531398
2462	0.4987419856260686	0.2500503922262283	0.1965967146531398
2463	0.4987419856260686	0.7499496077737717	0.1965967146531398
2464	0.2500000000000000	0.0000000000000000	0.1993689385340573
2465	0.2500000000000000	0.5000000000000000	0.1946565508451386
2466	0.7500000000000000	0.0000000000000000	0.1964335518941951
2467	0.7500000000000000	0.5000000000000000	0.1957218101378544
2468	0.2500000000000000	0.2584151963453110	0.2584037982308161
2469	0.2500000000000000	0.7415848036546890	0.2584037982308161
2470	0.7500000000000000	0.2487832182609111	0.2567471768319862
2471	0.7500000000000000	0.7512167817390889	0.2567471768319862
2472	0.2500000000000000	0.5000000000000000	0.2931192133187110
2473			
2474	NiV (25% V) 200 Facet with Hydrogen supercell 2X2X1 - [Etot = -254.93709013 eV]		
2475	1.00458661266245		
2476	7.0844001770000000	0.0000000000000000	0.0000000000000000
2477	0.0000000000000000	7.0844001770000000	0.0000000000000000
2478	0.0000000000000000	0.0000000000000000	27.0844993591000005
2479	V Ni H		

2480	12	28	1
2481	Direct		
2482	0.0000000000000000	0.0000000000000000	0.0000000000000000
2483	0.0000000000000000	0.5000000000000000	0.0000000000000000
2484	0.5000000000000000	0.0000000000000000	0.0000000000000000
2485	0.5000000000000000	0.5000000000000000	0.0000000000000000
2486	0.9998490527311013	0.0000000000000000	0.1311381563295657
2487	0.0010829175454232	0.5000000000000000	0.1303879127343038
2488	0.5001509472688987	0.0000000000000000	0.1311381563295657
2489	0.4989170824545768	0.5000000000000000	0.1303879127343038
2490	0.9988293703108050	0.0000000000000000	0.2665860399788850
2491	0.9882027800577708	0.5000000000000000	0.2632843509380009
2492	0.5011706296891950	0.0000000000000000	0.2665860399788850
2493	0.5117972199422292	0.5000000000000000	0.2632843509380009
2494	0.2500000000000000	0.2500000000000000	0.0000000000000000
2495	0.2500000000000000	0.7500000000000000	0.0000000000000000
2496	0.7500000000000000	0.2500000000000000	0.0000000000000000
2497	0.7500000000000000	0.7500000000000000	0.0000000000000000
2498	0.0000000000000000	0.2500000000000000	0.0653899980000006
2499	0.0000000000000000	0.7500000000000000	0.0653899980000006
2500	0.5000000000000000	0.2500000000000000	0.0653899980000006
2501	0.5000000000000000	0.7500000000000000	0.0653899980000006
2502	0.2500000000000000	0.0000000000000000	0.0653899980000006
2503	0.2500000000000000	0.5000000000000000	0.0653899980000006
2504	0.7500000000000000	0.0000000000000000	0.0653899980000006
2505	0.7500000000000000	0.5000000000000000	0.0653899980000006
2506	0.2500000000000000	0.2474090423402372	0.1307115094433896
2507	0.2500000000000000	0.7525909576597628	0.1307115094433896
2508	0.7500000000000000	0.2500667740410061	0.1304624519540939
2509	0.7500000000000000	0.7499332259589939	0.1304624519540939
2510	0.0009335191450757	0.2511263336308193	0.1958412419630592
2511	0.0009335191450757	0.7488736663691806	0.1958412419630592
2512	0.4990664808549243	0.2511263336308193	0.1958412419630592
2513	0.4990664808549243	0.7488736663691806	0.1958412419630592
2514	0.2500000000000000	0.0000000000000000	0.1981240886681312
2515	0.2500000000000000	0.5000000000000000	0.1935824112348378
2516	0.7500000000000000	0.0000000000000000	0.1956842971509593
2517	0.7500000000000000	0.5000000000000000	0.1947357799873966
2518	0.2500000000000000	0.2646884412482983	0.2590210888074200
2519	0.2500000000000000	0.7353115587517017	0.2590210888074200
2520	0.7500000000000000	0.2540605269208074	0.2571960151590738
2521	0.7500000000000000	0.7459394730791926	0.2571960151590738
2522	0.2500000000000000	0.5000000000000000	0.2903472485069310
2523			
2524	NiCr (25% Cr) 200 Facet with Hydrogen supercell 2X2X1 - [Etot = -255.31348045 eV]		
2525	0.995572721824907		
2526	7.0844001770000000	0.0000000000000000	0.0000000000000000
2527	0.0000000000000000	7.0844001770000000	0.0000000000000000
2528	0.0000000000000000	0.0000000000000000	27.0844993591000005
2529	Cr	Ni	H
2530	12	28	1
2531	Direct		

2532	0.0000000000000000	0.0000000000000000	0.0000000000000000
2533	0.0000000000000000	0.5000000000000000	0.0000000000000000
2534	0.5000000000000000	0.0000000000000000	0.0000000000000000
2535	0.5000000000000000	0.5000000000000000	0.0000000000000000
2536	0.0001715766318071	0.0000000000000000	0.1319319470664766
2537	0.0003421871412357	0.5000000000000000	0.1314664112261568
2538	0.4998284233681929	0.0000000000000000	0.1319319470664766
2539	0.4996578128587643	0.5000000000000000	0.1314664112261568
2540	0.0040976499224783	0.0000000000000000	0.2672723424733974
2541	0.9901252587747251	0.5000000000000000	0.2654401605829335
2542	0.4959023500775217	0.0000000000000000	0.2672723424733974
2543	0.5098747412252749	0.5000000000000000	0.2654401605829335
2544	0.2500000000000000	0.2500000000000000	0.0000000000000000
2545	0.2500000000000000	0.7500000000000000	0.0000000000000000
2546	0.7500000000000000	0.2500000000000000	0.0000000000000000
2547	0.7500000000000000	0.7500000000000000	0.0000000000000000
2548	0.0000000000000000	0.2500000000000000	0.0653899980000006
2549	0.0000000000000000	0.7500000000000000	0.0653899980000006
2550	0.5000000000000000	0.2500000000000000	0.0653899980000006
2551	0.5000000000000000	0.7500000000000000	0.0653899980000006
2552	0.2500000000000000	0.0000000000000000	0.0653899980000006
2553	0.2500000000000000	0.5000000000000000	0.0653899980000006
2554	0.7500000000000000	0.0000000000000000	0.0653899980000006
2555	0.7500000000000000	0.5000000000000000	0.0653899980000006
2556	0.2500000000000000	0.2476631737280712	0.1315409169063386
2557	0.2500000000000000	0.7523368262719288	0.1315409169063386
2558	0.7500000000000000	0.2497411181067548	0.1313397641835223
2559	0.7500000000000000	0.7502588818932452	0.1313397641835223
2560	0.0008899822320032	0.2492856612810996	0.1973705234001102
2561	0.0008899822320032	0.7507143387189004	0.1973705234001102
2562	0.4991100177679968	0.2492856612810996	0.1973705234001102
2563	0.4991100177679968	0.7507143387189004	0.1973705234001102
2564	0.2500000000000000	0.0000000000000000	0.1996168834360788
2565	0.2500000000000000	0.5000000000000000	0.1956202563177953
2566	0.7500000000000000	0.0000000000000000	0.1972810748742901
2567	0.7500000000000000	0.5000000000000000	0.1967321367462418
2568	0.2500000000000000	0.2645518765444379	0.2625883911049698
2569	0.2500000000000000	0.7354481234555621	0.2625883911049698
2570	0.7500000000000000	0.2473382491084593	0.2600929459650203
2571	0.7500000000000000	0.7526617508915407	0.2600929459650203
2572	0.2500000000000000	0.5000000000000000	0.2922267405418069
2573			
2574	NiMn (25% Mn) 200 Facet with Hydrogen supercell 2X2X1 - [Etot = -255.78286619 eV]		
2575	0.989317187668226		
2576	7.0844001770000000	0.0000000000000000	0.0000000000000000
2577	0.0000000000000000	7.0844001770000000	0.0000000000000000
2578	0.0000000000000000	0.0000000000000000	27.0844993591000005
2579	Mn Ni H		
2580	12 28 1		
2581	Direct		
2582	0.0000000000000000	0.0000000000000000	0.0000000000000000
2583	0.0000000000000000	0.5000000000000000	0.0000000000000000

2584	0.5000000000000000	0.0000000000000000	0.0000000000000000
2585	0.5000000000000000	0.5000000000000000	0.0000000000000000
2586	0.0003409153738971	0.0000000000000000	0.1337964123432585
2587	0.9994439969619222	0.5000000000000000	0.1335391377075368
2588	0.4996590846261029	0.0000000000000000	0.1337964123432585
2589	0.5005560030380778	0.5000000000000000	0.1335391377075368
2590	0.0083993978765236	0.0000000000000000	0.2720131993878638
2591	0.9862346758431286	0.5000000000000000	0.2710238020555806
2592	0.4916006021234764	0.0000000000000000	0.2720131993878638
2593	0.5137653241568714	0.5000000000000000	0.2710238020555806
2594	0.2500000000000000	0.2500000000000000	0.0000000000000000
2595	0.2500000000000000	0.7500000000000000	0.0000000000000000
2596	0.7500000000000000	0.2500000000000000	0.0000000000000000
2597	0.7500000000000000	0.7500000000000000	0.0000000000000000
2598	0.0000000000000000	0.2500000000000000	0.0653899980000006
2599	0.0000000000000000	0.7500000000000000	0.0653899980000006
2600	0.5000000000000000	0.2500000000000000	0.0653899980000006
2601	0.5000000000000000	0.7500000000000000	0.0653899980000006
2602	0.2500000000000000	0.0000000000000000	0.0653899980000006
2603	0.2500000000000000	0.5000000000000000	0.0653899980000006
2604	0.7500000000000000	0.0000000000000000	0.0653899980000006
2605	0.7500000000000000	0.5000000000000000	0.0653899980000006
2606	0.2500000000000000	0.2489485287123685	0.1337286942735147
2607	0.2500000000000000	0.7510514712876315	0.1337286942735147
2608	0.7500000000000000	0.2499848175941182	0.1335413867027384
2609	0.7500000000000000	0.7500151824058818	0.1335413867027384
2610	0.0005248659334285	0.2494489225407719	0.2017030444059955
2611	0.0005248659334285	0.7505510774592281	0.2017030444059955
2612	0.4994751340665715	0.2494489225407719	0.2017030444059955
2613	0.4994751340665715	0.7505510774592281	0.2017030444059955
2614	0.2500000000000000	0.0000000000000000	0.2035668392344689
2615	0.2500000000000000	0.5000000000000000	0.1997137574379835
2616	0.7500000000000000	0.0000000000000000	0.2012708590508296
2617	0.7500000000000000	0.5000000000000000	0.2016822831234535
2618	0.2500000000000000	0.2660658602982693	0.2677252757176518
2619	0.2500000000000000	0.7339341397017307	0.2677252757176518
2620	0.7500000000000000	0.2416072234767626	0.2659172790091233
2621	0.7500000000000000	0.7583927765232374	0.2659172790091233
2622	0.2500000000000000	0.5000000000000000	0.2963711632285566

2623

2624 NiFe (25% Fe) 200 Facet with Hydrogen supercell 2X2X1 - [Etot = -245.73437388 eV]

2625 1.0000000000000000

2626	7.0844001770000000	0.0000000000000000	0.0000000000000000
2627	0.0000000000000000	7.0844001770000000	0.0000000000000000
2628	0.0000000000000000	0.0000000000000000	27.0844993591000005

2629 Fe Ni H

2630 12 28 1

2631 Direct

2632	0.0000000000000000	0.0000000000000000	0.0000000000000000
2633	0.0000000000000000	0.5000000000000000	0.0000000000000000
2634	0.5000000000000000	0.0000000000000000	0.0000000000000000
2635	0.5000000000000000	0.5000000000000000	0.0000000000000000

2636	0.9999690309503677	0.0000000000000000	0.1308514166296888
2637	0.0004326928950249	0.5000000000000000	0.1307273921679695
2638	0.5000309690496323	0.0000000000000000	0.1308514166296888
2639	0.4995673071049751	0.5000000000000000	0.1307273921679695
2640	0.0008615474166618	0.0000000000000000	0.2618950269538090
2641	0.9921868605316320	0.5000000000000000	0.2620425289280135
2642	0.4991384525833382	0.0000000000000000	0.2618950269538090
2643	0.5078131394683680	0.5000000000000000	0.2620425289280135
2644	0.2500000000000000	0.2500000000000000	0.0000000000000000
2645	0.2500000000000000	0.7500000000000000	0.0000000000000000
2646	0.7500000000000000	0.2500000000000000	0.0000000000000000
2647	0.7500000000000000	0.7500000000000000	0.0000000000000000
2648	0.0000000000000000	0.2500000000000000	0.0653899980000006
2649	0.0000000000000000	0.7500000000000000	0.0653899980000006
2650	0.5000000000000000	0.2500000000000000	0.0653899980000006
2651	0.5000000000000000	0.7500000000000000	0.0653899980000006
2652	0.2500000000000000	0.0000000000000000	0.0653899980000006
2653	0.2500000000000000	0.5000000000000000	0.0653899980000006
2654	0.7500000000000000	0.0000000000000000	0.0653899980000006
2655	0.7500000000000000	0.5000000000000000	0.0653899980000006
2656	0.2500000000000000	0.2480157250294255	0.1310126058480563
2657	0.2500000000000000	0.7519842749705745	0.1310126058480563
2658	0.7500000000000000	0.2502799401483102	0.1307496903515997
2659	0.7500000000000000	0.7497200598516898	0.1307496903515997
2660	0.0000992817120462	0.2495258346915818	0.1963645940657202
2661	0.0000992817120462	0.7504741653084182	0.1963645940657202
2662	0.4999007182879538	0.2495258346915818	0.1963645940657202
2663	0.4999007182879538	0.7504741653084182	0.1963645940657202
2664	0.2500000000000000	0.0000000000000000	0.1985086963111868
2665	0.2500000000000000	0.5000000000000000	0.1947249800598669
2666	0.7500000000000000	0.0000000000000000	0.1963884492786576
2667	0.7500000000000000	0.5000000000000000	0.1963946454593142
2668	0.2500000000000000	0.2592372883917662	0.2600950967125399
2669	0.2500000000000000	0.7407627116082338	0.2600950967125399
2670	0.7500000000000000	0.2474386332559959	0.2588080259965295
2671	0.7500000000000000	0.7525613667440041	0.2588080259965295
2672	0.2500000000000000	0.5000000000000000	0.2860701421870431

2673

2674 NiCo (25% Co) 200 Facet with Hydrogen supercell 2X2X1 - [Etot = -225.89147144 eV]

2675 0.993794164815303

2676	7.0844001770000000	0.0000000000000000	0.0000000000000000
2677	0.0000000000000000	7.0844001770000000	0.0000000000000000
2678	0.0000000000000000	0.0000000000000000	27.0844993591000005

2679 Co Ni H

2680 12 28 1

2681 Direct

2682	0.0000000000000000	0.0000000000000000	0.0000000000000000
2683	0.0000000000000000	0.5000000000000000	0.0000000000000000
2684	0.5000000000000000	0.0000000000000000	0.0000000000000000
2685	0.5000000000000000	0.5000000000000000	0.0000000000000000
2686	0.0003154867293418	0.0000000000000000	0.1308047203716285
2687	0.9997346727725898	0.5000000000000000	0.1308213465021026

2688	0.4996845132706582	0.0000000000000000	0.1308047203716285
2689	0.5002653272274102	0.5000000000000000	0.1308213465021026
2690	0.9996570629432853	0.0000000000000000	0.2607399767535412
2691	0.9967211359774808	0.5000000000000000	0.2610104871906813
2692	0.5003429370567147	0.0000000000000000	0.2607399767535412
2693	0.5032788640225192	0.5000000000000000	0.2610104871906813
2694	0.2500000000000000	0.2500000000000000	0.0000000000000000
2695	0.2500000000000000	0.7500000000000000	0.0000000000000000
2696	0.7500000000000000	0.2500000000000000	0.0000000000000000
2697	0.7500000000000000	0.7500000000000000	0.0000000000000000
2698	0.0000000000000000	0.2500000000000000	0.0653899980000006
2699	0.0000000000000000	0.7500000000000000	0.0653899980000006
2700	0.5000000000000000	0.2500000000000000	0.0653899980000006
2701	0.5000000000000000	0.7500000000000000	0.0653899980000006
2702	0.2500000000000000	0.0000000000000000	0.0653899980000006
2703	0.2500000000000000	0.5000000000000000	0.0653899980000006
2704	0.7500000000000000	0.0000000000000000	0.0653899980000006
2705	0.7500000000000000	0.5000000000000000	0.0653899980000006
2706	0.2500000000000000	0.2489738538063762	0.1310511167932304
2707	0.2500000000000000	0.7510261461936238	0.1310511167932304
2708	0.7500000000000000	0.2501345160264563	0.1308437257185417
2709	0.7500000000000000	0.7498654839735437	0.1308437257185417
2710	0.9996417240616040	0.2492145784539588	0.1965189195360253
2711	0.9996417240616040	0.7507854215460412	0.1965189195360253
2712	0.5003582759383960	0.2492145784539588	0.1965189195360253
2713	0.5003582759383960	0.7507854215460412	0.1965189195360253
2714	0.2500000000000000	0.0000000000000000	0.1978788255492461
2715	0.2500000000000000	0.5000000000000000	0.1952976516344620
2716	0.7500000000000000	0.0000000000000000	0.1966066065040764
2717	0.7500000000000000	0.5000000000000000	0.1966796562962330
2718	0.2500000000000000	0.2550137526022596	0.2602528810655826
2719	0.2500000000000000	0.7449862473977404	0.2602528810655826
2720	0.7500000000000000	0.2491077141595710	0.2593415682170885
2721	0.7500000000000000	0.7508922858404290	0.2593415682170885
2722	0.2500000000000000	0.5000000000000000	0.2840314618722743

2723
 2724 Pure-Ni 200 Facet with Hydrogen supercell 2X2X1 - [Etot = -207.47182141 eV]
 2725 1.01798110552312

2726	7.0844001770000000	0.0000000000000000	0.0000000000000000
2727	0.0000000000000000	7.0844001770000000	0.0000000000000000
2728	0.0000000000000000	0.0000000000000000	27.0844993591000005

2729 Ni H
 2730 40 1

2731	Direct		
2732	0.0000000000000000	0.0000000000000000	0.0000000000000000
2733	0.0000000000000000	0.5000000000000000	0.0000000000000000
2734	0.5000000000000000	0.0000000000000000	0.0000000000000000
2735	0.5000000000000000	0.5000000000000000	0.0000000000000000
2736	0.0001994065359412	0.0000000000000000	0.1273332544966976
2737	0.9994370797590264	0.5000000000000000	0.1273857577031023
2738	0.4998005934640588	0.0000000000000000	0.1273332544966976
2739	0.5005629202409736	0.5000000000000000	0.1273857577031023

2740	0.9998312736033839	0.0000000000000000	0.2493631321842500
2741	0.0020913230695001	0.5000000000000000	0.2498006864773501
2742	0.5001687263966161	0.0000000000000000	0.2493631321842500
2743	0.4979086769304999	0.5000000000000000	0.2498006864773501
2744	0.2500000000000000	0.2500000000000000	0.0000000000000000
2745	0.2500000000000000	0.7500000000000000	0.0000000000000000
2746	0.7500000000000000	0.2500000000000000	0.0000000000000000
2747	0.7500000000000000	0.7500000000000000	0.0000000000000000
2748	0.0000000000000000	0.2500000000000000	0.0653899980000006
2749	0.0000000000000000	0.7500000000000000	0.0653899980000006
2750	0.5000000000000000	0.2500000000000000	0.0653899980000006
2751	0.5000000000000000	0.7500000000000000	0.0653899980000006
2752	0.2500000000000000	0.0000000000000000	0.0653899980000006
2753	0.2500000000000000	0.5000000000000000	0.0653899980000006
2754	0.7500000000000000	0.0000000000000000	0.0653899980000006
2755	0.7500000000000000	0.5000000000000000	0.0653899980000006
2756	0.2500000000000000	0.2495048766612271	0.1273475614240382
2757	0.2500000000000000	0.7504951233387729	0.1273475614240382
2758	0.7500000000000000	0.2500989833022587	0.1273515230800513
2759	0.7500000000000000	0.7499010166977413	0.1273515230800513
2760	0.9992200599083461	0.2490409550187138	0.1898180742216340
2761	0.9992200599083461	0.7509590449812862	0.1898180742216340
2762	0.5007799400916539	0.2490409550187138	0.1898180742216340
2763	0.5007799400916539	0.7509590449812862	0.1898180742216340
2764	0.2500000000000000	0.0000000000000000	0.1905202706700635
2765	0.2500000000000000	0.5000000000000000	0.1886656489633651
2766	0.7500000000000000	0.0000000000000000	0.1900858123873022
2767	0.7500000000000000	0.5000000000000000	0.1905004123256191
2768	0.2500000000000000	0.2520656948862765	0.2498723702779202
2769	0.2500000000000000	0.7479343051137235	0.2498723702779202
2770	0.7500000000000000	0.2498045618730771	0.2492453276029210
2771	0.7500000000000000	0.7501954381269229	0.2492453276029210
2772	0.2500000000000000	0.5000000000000000	0.2681206669428775
2773			
2774	NiCu (25% Cu) 200 Facet with Hydrogen supercell 2X2X1 - [Etot = -188.52871626 eV]		
2775	0.998485100048875		
2776	7.0844001770000000	0.0000000000000000	0.0000000000000000
2777	0.0000000000000000	7.0844001770000000	0.0000000000000000
2778	0.0000000000000000	0.0000000000000000	27.0844993591000005
2779	Cu Ni H		
2780	12 28 1		
2781	Direct		
2782	0.0000000000000000	0.0000000000000000	0.0000000000000000
2783	0.0000000000000000	0.5000000000000000	0.0000000000000000
2784	0.5000000000000000	0.0000000000000000	0.0000000000000000
2785	0.5000000000000000	0.5000000000000000	0.0000000000000000
2786	0.0005930756671333	0.0000000000000000	0.1314505581818395
2787	0.9992541526533358	0.5000000000000000	0.1313235553635366
2788	0.4994069243328667	0.0000000000000000	0.1314505581818395
2789	0.5007458473466642	0.5000000000000000	0.1313235553635366
2790	0.0062199352298435	0.0000000000000000	0.2634557076304134
2791	0.9922859775202042	0.5000000000000000	0.2643065408250109

2792	0.4937800647701565	0.0000000000000000	0.2634557076304134
2793	0.5077140224797958	0.5000000000000000	0.2643065408250109
2794	0.2500000000000000	0.2500000000000000	0.0000000000000000
2795	0.2500000000000000	0.7500000000000000	0.0000000000000000
2796	0.7500000000000000	0.2500000000000000	0.0000000000000000
2797	0.7500000000000000	0.7500000000000000	0.0000000000000000
2798	0.0000000000000000	0.2500000000000000	0.0653899980000006
2799	0.0000000000000000	0.7500000000000000	0.0653899980000006
2800	0.5000000000000000	0.2500000000000000	0.0653899980000006
2801	0.5000000000000000	0.7500000000000000	0.0653899980000006
2802	0.2500000000000000	0.0000000000000000	0.0653899980000006
2803	0.2500000000000000	0.5000000000000000	0.0653899980000006
2804	0.7500000000000000	0.0000000000000000	0.0653899980000006
2805	0.7500000000000000	0.5000000000000000	0.0653899980000006
2806	0.2500000000000000	0.2492973518341728	0.1311515350055430
2807	0.2500000000000000	0.7507026481658272	0.1311515350055430
2808	0.7500000000000000	0.2499413824171626	0.1311237174759299
2809	0.7500000000000000	0.7500586175828374	0.1311237174759299
2810	0.9993329607583306	0.2495738317086875	0.1973269312481705
2811	0.9993329607583306	0.7504261682913125	0.1973269312481705
2812	0.5006670392416694	0.2495738317086875	0.1973269312481705
2813	0.5006670392416694	0.7504261682913125	0.1973269312481705
2814	0.2500000000000000	0.0000000000000000	0.1983277118368960
2815	0.2500000000000000	0.5000000000000000	0.1957781774549403
2816	0.7500000000000000	0.0000000000000000	0.1972442701336732
2817	0.7500000000000000	0.5000000000000000	0.1979200541390895
2818	0.2500000000000000	0.2611865678164520	0.2600524423727890
2819	0.2500000000000000	0.7388134321835480	0.2600524423727890
2820	0.7500000000000000	0.2437443452131944	0.2589155549142887
2821	0.7500000000000000	0.7562556547868056	0.2589155549142887
2822	0.2500000000000000	0.5000000000000000	0.2828061749508493

2823

2824 NiZn (25% Zn) 200 Facet with Hydrogen supercell 2X2X1 - [Etot = -167.95033235 eV]

2825 1.01038006037737

2826	7.0844001770000000	0.0000000000000000	0.0000000000000000
2827	0.0000000000000000	7.0844001770000000	0.0000000000000000
2828	0.0000000000000000	0.0000000000000000	27.0844993591000005

2829 Zn Ni H

2830 12 28 1

2831 Direct

2832	0.0000000000000000	0.0000000000000000	0.0000000000000000
2833	0.0000000000000000	0.5000000000000000	0.0000000000000000
2834	0.5000000000000000	0.0000000000000000	0.0000000000000000
2835	0.5000000000000000	0.5000000000000000	0.0000000000000000
2836	0.0008317956540225	0.0000000000000000	0.1311716620071408
2837	0.9988435035833021	0.5000000000000000	0.1306818115800823
2838	0.4991682043459775	0.0000000000000000	0.1311716620071408
2839	0.5011564964166979	0.5000000000000000	0.1306818115800823
2840	0.0084788439591463	0.0000000000000000	0.2639284386616509
2841	0.9814738819760080	0.5000000000000000	0.2642212404198077
2842	0.4915211560408537	0.0000000000000000	0.2639284386616509
2843	0.5185261180239920	0.5000000000000000	0.2642212404198077

2844	0.2500000000000000	0.2500000000000000	0.0000000000000000
2845	0.2500000000000000	0.7500000000000000	0.0000000000000000
2846	0.7500000000000000	0.2500000000000000	0.0000000000000000
2847	0.7500000000000000	0.7500000000000000	0.0000000000000000
2848	0.0000000000000000	0.2500000000000000	0.0653899980000006
2849	0.0000000000000000	0.7500000000000000	0.0653899980000006
2850	0.5000000000000000	0.2500000000000000	0.0653899980000006
2851	0.5000000000000000	0.7500000000000000	0.0653899980000006
2852	0.2500000000000000	0.0000000000000000	0.0653899980000006
2853	0.2500000000000000	0.5000000000000000	0.0653899980000006
2854	0.7500000000000000	0.0000000000000000	0.0653899980000006
2855	0.7500000000000000	0.5000000000000000	0.0653899980000006
2856	0.2500000000000000	0.2482663742630820	0.1311060433408500
2857	0.2500000000000000	0.7517336257369180	0.1311060433408500
2858	0.7500000000000000	0.2497164683084776	0.1308855321619120
2859	0.7500000000000000	0.7502835316915224	0.1308855321619120
2860	0.0012671545617380	0.2499289586186038	0.1967063124089847
2861	0.0012671545617380	0.7500710413813962	0.1967063124089847
2862	0.4987328454382620	0.2499289586186038	0.1967063124089847
2863	0.4987328454382620	0.7500710413813962	0.1967063124089847
2864	0.2500000000000000	0.0000000000000000	0.1987774276113328
2865	0.2500000000000000	0.5000000000000000	0.1937358354766161
2866	0.7500000000000000	0.0000000000000000	0.1958664644789891
2867	0.7500000000000000	0.5000000000000000	0.1963385359678682
2868	0.2500000000000000	0.2741800188824186	0.2598735426082328
2869	0.2500000000000000	0.7258199811175885	0.2598735426082328
2870	0.7500000000000000	0.2399339803571792	0.2572786757811869
2871	0.7500000000000000	0.7600660196428208	0.2572786757811869
2872	0.2500000000000000	0.5000000000000000	0.2851581929793667

2873

2874

2875 Bare- NiSc (25% Sc) 220 Facet supercell 2X2X1 - [Etot = -328.56112666 eV]

2876 1.04735280294076

2877 7.090000152600000 0.0000000000000000 0.0000000000000000

2878 0.0000000000000000 10.0268001556000002 0.0000000000000000

2879 0.0000000000000000 0.0000000000000000 27.5200996398999997

2880 Sc Ni

2881 16 40

2882 Direct

2883 0.0000000000000000 0.2500000000000000 0.0000000000000000

2884 0.0000000000000000 0.7500000000000000 0.0000000000000000

2885 0.5000000000000000 0.2500000000000000 0.0000000000000000

2886 0.5000000000000000 0.7500000000000000 0.0000000000000000

2887 0.0000000000000000 0.0000000000000000 0.09109000099999978

2888 0.0000000000000000 0.5000000000000000 0.09109000099999978

2889 0.5000000000000000 0.0000000000000000 0.09109000099999978

2890 0.5000000000000000 0.5000000000000000 0.09109000099999978

2891 0.0000000000000000 0.2500000000000000 0.1802765203686718

2892 0.0000000000000000 0.7500000000000000 0.1802765203686718

2893 0.5000000000000000 0.2500000000000000 0.1802765203686718

2894 0.5000000000000000 0.7500000000000000 0.1802765203686718

2895 0.0000000000000000 0.0000000000000000 0.2729065180152475

2896	0.0000000000000000	0.5000000000000000	0.2729065180152475
2897	0.5000000000000000	0.0000000000000000	0.2729065180152475
2898	0.5000000000000000	0.5000000000000000	0.2729065180152475
2899	0.0000000000000000	0.0000000000000000	0.0000000000000000
2900	0.0000000000000000	0.5000000000000000	0.0000000000000000
2901	0.5000000000000000	0.0000000000000000	0.0000000000000000
2902	0.5000000000000000	0.5000000000000000	0.0000000000000000
2903	0.2500000000000000	0.1250000000000000	0.0455400009999991
2904	0.2500000000000000	0.6250000000000000	0.0455400009999991
2905	0.7500000000000000	0.1250000000000000	0.0455400009999991
2906	0.7500000000000000	0.6250000000000000	0.0455400009999991
2907	0.2500000000000000	0.3750000000000000	0.0455400009999991
2908	0.2500000000000000	0.8750000000000000	0.0455400009999991
2909	0.7500000000000000	0.3750000000000000	0.0455400009999991
2910	0.7500000000000000	0.8750000000000000	0.0455400009999991
2911	0.0000000000000000	0.2500000000000000	0.0889434874281392
2912	0.0000000000000000	0.7500000000000000	0.0889434874281392
2913	0.5000000000000000	0.2500000000000000	0.0889434874281392
2914	0.5000000000000000	0.7500000000000000	0.0889434874281392
2915	0.2500000000000000	0.3759440965842202	0.1365211495551222
2916	0.2500000000000000	0.8759440665842249	0.1365211495551222
2917	0.7500000000000000	0.3759440965842202	0.1365211495551222
2918	0.7500000000000000	0.8759440665842249	0.1365211495551222
2919	0.2500000000000000	0.1240559184157775	0.1365211495551222
2920	0.2500000000000000	0.6240559334157751	0.1365211495551222
2921	0.7500000000000000	0.1240559184157775	0.1365211495551222
2922	0.7500000000000000	0.6240559334157751	0.1365211495551222
2923	0.0000000000000000	0.0000000000000000	0.1839895729184775
2924	0.0000000000000000	0.5000000000000000	0.1839895729184775
2925	0.5000000000000000	0.0000000000000000	0.1839895729184775
2926	0.5000000000000000	0.5000000000000000	0.1839895729184775
2927	0.2500000000000000	0.1234679085232244	0.2294222682762310
2928	0.2500000000000000	0.6234679015232274	0.2294222682762310
2929	0.7500000000000000	0.1234679085232244	0.2294222682762310
2930	0.7500000000000000	0.6234679015232274	0.2294222682762310
2931	0.2500000000000000	0.3765320984767726	0.2294222682762310
2932	0.2500000000000000	0.8765320984767726	0.2294222682762310
2933	0.7500000000000000	0.3765320984767726	0.2294222682762310
2934	0.7500000000000000	0.8765320984767726	0.2294222682762310
2935	0.0000000000000000	0.2500000000000000	0.2661383550878469
2936	0.0000000000000000	0.7500000000000000	0.2661383550878469
2937	0.5000000000000000	0.2500000000000000	0.2661383550878469
2938	0.5000000000000000	0.7500000000000000	0.2661383550878469
2939			
2940	Bare- NiTi (25% Ti) 220 Facet supercell 2X2X1 - [Etot = -348.99973858 eV]		
2941	1.01798110552312		
2942	7.0900001526000000	0.0000000000000000	0.0000000000000000
2943	0.0000000000000000	10.0268001556000002	0.0000000000000000
2944	0.0000000000000000	0.0000000000000000	27.5200996398999997
2945	Ti	Ni	
2946	16	40	
2947	Direct		

2948	0.0000000000000000	0.2500000000000000	0.0000000000000000
2949	0.0000000000000000	0.7500000000000000	0.0000000000000000
2950	0.5000000000000000	0.2500000000000000	0.0000000000000000
2951	0.5000000000000000	0.7500000000000000	0.0000000000000000
2952	0.0000000000000000	0.0000000000000000	0.0910900009999978
2953	0.0000000000000000	0.5000000000000000	0.0910900009999978
2954	0.5000000000000000	0.0000000000000000	0.0910900009999978
2955	0.5000000000000000	0.5000000000000000	0.0910900009999978
2956	0.0000000000000000	0.2500000000000000	0.1831708284496614
2957	0.0000000000000000	0.7500000000000000	0.1831708284496614
2958	0.5000000000000000	0.2500000000000000	0.1831708284496614
2959	0.5000000000000000	0.7500000000000000	0.1831708284496614
2960	0.0000000000000000	0.0000000000000000	0.2697017755456841
2961	0.0000000000000000	0.5000000000000000	0.2697017755456841
2962	0.5000000000000000	0.0000000000000000	0.2697017755456841
2963	0.5000000000000000	0.5000000000000000	0.2697017755456841
2964	0.0000000000000000	0.0000000000000000	0.0000000000000000
2965	0.0000000000000000	0.5000000000000000	0.0000000000000000
2966	0.5000000000000000	0.0000000000000000	0.0000000000000000
2967	0.5000000000000000	0.5000000000000000	0.0000000000000000
2968	0.2500000000000000	0.1250000000000000	0.0455400009999991
2969	0.2500000000000000	0.6250000000000000	0.0455400009999991
2970	0.7500000000000000	0.1250000000000000	0.0455400009999991
2971	0.7500000000000000	0.6250000000000000	0.0455400009999991
2972	0.2500000000000000	0.3750000000000000	0.0455400009999991
2973	0.2500000000000000	0.8750000000000000	0.0455400009999991
2974	0.7500000000000000	0.3750000000000000	0.0455400009999991
2975	0.7500000000000000	0.8750000000000000	0.0455400009999991
2976	0.0000000000000000	0.2500000000000000	0.0903792668438257
2977	0.0000000000000000	0.7500000000000000	0.0903792668438257
2978	0.5000000000000000	0.2500000000000000	0.0903792668438257
2979	0.5000000000000000	0.7500000000000000	0.0903792668438257
2980	0.2500000000000000	0.3748598846929170	0.1374993947505772
2981	0.2500000000000000	0.8748598546929216	0.1374993947505772
2982	0.7500000000000000	0.3748598846929170	0.1374993947505772
2983	0.7500000000000000	0.8748598546929216	0.1374993947505772
2984	0.2500000000000000	0.1251401303070807	0.1374993947505772
2985	0.2500000000000000	0.6251401453070784	0.1374993947505772
2986	0.7500000000000000	0.1251401303070807	0.1374993947505772
2987	0.7500000000000000	0.6251401453070784	0.1374993947505772
2988	0.0000000000000000	0.0000000000000000	0.1837526080311775
2989	0.0000000000000000	0.5000000000000000	0.1837526080311775
2990	0.5000000000000000	0.0000000000000000	0.1837526080311775
2991	0.5000000000000000	0.5000000000000000	0.1837526080311775
2992	0.2500000000000000	0.1228231505927511	0.2307470259288493
2993	0.2500000000000000	0.6228231435927540	0.2307470259288493
2994	0.7500000000000000	0.1228231505927511	0.2307470259288493
2995	0.7500000000000000	0.6228231435927540	0.2307470259288493
2996	0.2500000000000000	0.3771768564072460	0.2307470259288493
2997	0.2500000000000000	0.8771768564072460	0.2307470259288493
2998	0.7500000000000000	0.3771768564072460	0.2307470259288493
2999	0.7500000000000000	0.8771768564072460	0.2307470259288493

3000	0.0000000000000000	0.2500000000000000	0.2685556921147807
3001	0.0000000000000000	0.7500000000000000	0.2685556921147807
3002	0.5000000000000000	0.2500000000000000	0.2685556921147807
3003	0.5000000000000000	0.7500000000000000	0.2685556921147807
3004			
3005	Bare- NiV (25% V) 220 Facet supercell 2X2X1 - [Etot = -349.55862889 eV]		
3006	1.00458661266245		
3007	7.0900001526000000	0.0000000000000000	0.0000000000000000
3008	0.0000000000000000	10.0268001556000002	0.0000000000000000
3009	0.0000000000000000	0.0000000000000000	27.5200996398999997
3010	V	Ni	
3011	16	40	
3012	Direct		
3013	0.0000000000000000	0.2500000000000000	0.0000000000000000
3014	0.0000000000000000	0.7500000000000000	0.0000000000000000
3015	0.5000000000000000	0.2500000000000000	0.0000000000000000
3016	0.5000000000000000	0.7500000000000000	0.0000000000000000
3017	0.0000000000000000	0.0000000000000000	0.0910900009999978
3018	0.0000000000000000	0.5000000000000000	0.0910900009999978
3019	0.5000000000000000	0.0000000000000000	0.0910900009999978
3020	0.5000000000000000	0.5000000000000000	0.0910900009999978
3021	0.0000000000000000	0.2500000000000000	0.1849628740434994
3022	0.0000000000000000	0.7500000000000000	0.1849628740434994
3023	0.5000000000000000	0.2500000000000000	0.1849628740434994
3024	0.5000000000000000	0.7500000000000000	0.1849628740434994
3025	0.0000000000000000	0.0000000000000000	0.2737009002776603
3026	0.0000000000000000	0.5000000000000000	0.2737009002776603
3027	0.5000000000000000	0.0000000000000000	0.2737009002776603
3028	0.5000000000000000	0.5000000000000000	0.2737009002776603
3029	0.0000000000000000	0.0000000000000000	0.0000000000000000
3030	0.0000000000000000	0.5000000000000000	0.0000000000000000
3031	0.5000000000000000	0.0000000000000000	0.0000000000000000
3032	0.5000000000000000	0.5000000000000000	0.0000000000000000
3033	0.2500000000000000	0.1250000000000000	0.0455400009999991
3034	0.2500000000000000	0.6250000000000000	0.0455400009999991
3035	0.7500000000000000	0.1250000000000000	0.0455400009999991
3036	0.7500000000000000	0.6250000000000000	0.0455400009999991
3037	0.2500000000000000	0.3750000000000000	0.0455400009999991
3038	0.2500000000000000	0.8750000000000000	0.0455400009999991
3039	0.7500000000000000	0.3750000000000000	0.0455400009999991
3040	0.7500000000000000	0.8750000000000000	0.0455400009999991
3041	0.0000000000000000	0.2500000000000000	0.0917572987542030
3042	0.0000000000000000	0.7500000000000000	0.0917572987542030
3043	0.5000000000000000	0.2500000000000000	0.0917572987542030
3044	0.5000000000000000	0.7500000000000000	0.0917572987542030
3045	0.2500000000000000	0.3747574008595507	0.1369035818241642
3046	0.2500000000000000	0.8747573708595553	0.1369035818241642
3047	0.7500000000000000	0.3747574008595507	0.1369035818241642
3048	0.7500000000000000	0.8747573708595553	0.1369035818241642
3049	0.2500000000000000	0.1252426141404470	0.1369035818241642
3050	0.2500000000000000	0.6252426291404447	0.1369035818241642
3051	0.7500000000000000	0.1252426141404470	0.1369035818241642

3052	0.7500000000000000	0.6252426291404447	0.1369035818241642
3053	0.0000000000000000	0.0000000000000000	0.1818867909250130
3054	0.0000000000000000	0.5000000000000000	0.1818867909250130
3055	0.5000000000000000	0.0000000000000000	0.1818867909250130
3056	0.5000000000000000	0.5000000000000000	0.1818867909250130
3057	0.2500000000000000	0.1228362047361884	0.2281365363762262
3058	0.2500000000000000	0.6228361977361914	0.2281365363762262
3059	0.7500000000000000	0.1228362047361884	0.2281365363762262
3060	0.7500000000000000	0.6228361977361914	0.2281365363762262
3061	0.2500000000000000	0.3771638022638086	0.2281365363762262
3062	0.2500000000000000	0.8771638022638086	0.2281365363762262
3063	0.7500000000000000	0.3771638022638086	0.2281365363762262
3064	0.7500000000000000	0.8771638022638086	0.2281365363762262
3065	0.0000000000000000	0.2500000000000000	0.2692632341875623
3066	0.0000000000000000	0.7500000000000000	0.2692632341875623
3067	0.5000000000000000	0.2500000000000000	0.2692632341875623
3068	0.5000000000000000	0.7500000000000000	0.2692632341875623
3069			
3070	Bare- NiCr (25% Cr) 220 Facet supercell 2X2X1 - [Etot = -349.74533449 eV]		
3071	0.995572721824907		
3072	7.090000152600000	0.0000000000000000	0.0000000000000000
3073	0.0000000000000000	10.0268001556000002	0.0000000000000000
3074	0.0000000000000000	0.0000000000000000	27.5200996398999997
3075	Cr Ni		
3076	16 40		
3077	Direct		
3078	0.0000000000000000	0.2500000000000000	0.0000000000000000
3079	0.0000000000000000	0.7500000000000000	0.0000000000000000
3080	0.5000000000000000	0.2500000000000000	0.0000000000000000
3081	0.5000000000000000	0.7500000000000000	0.0000000000000000
3082	0.0000000000000000	0.0000000000000000	0.0910900009999978
3083	0.0000000000000000	0.5000000000000000	0.0910900009999978
3084	0.5000000000000000	0.0000000000000000	0.0910900009999978
3085	0.5000000000000000	0.5000000000000000	0.0910900009999978
3086	0.0000000000000000	0.2500000000000000	0.1846507157262849
3087	0.0000000000000000	0.7500000000000000	0.1846507157262849
3088	0.5000000000000000	0.2500000000000000	0.1846507157262849
3089	0.5000000000000000	0.7500000000000000	0.1846507157262849
3090	0.0000000000000000	0.0000000000000000	0.2758805127395618
3091	0.0000000000000000	0.5000000000000000	0.2758805127395618
3092	0.5000000000000000	0.0000000000000000	0.2758805127395618
3093	0.5000000000000000	0.5000000000000000	0.2758805127395618
3094	0.0000000000000000	0.0000000000000000	0.0000000000000000
3095	0.0000000000000000	0.5000000000000000	0.0000000000000000
3096	0.5000000000000000	0.0000000000000000	0.0000000000000000
3097	0.5000000000000000	0.5000000000000000	0.0000000000000000
3098	0.2500000000000000	0.1250000000000000	0.0455400009999991
3099	0.2500000000000000	0.6250000000000000	0.0455400009999991
3100	0.7500000000000000	0.1250000000000000	0.0455400009999991
3101	0.7500000000000000	0.6250000000000000	0.0455400009999991
3102	0.2500000000000000	0.3750000000000000	0.0455400009999991
3103	0.2500000000000000	0.8750000000000000	0.0455400009999991

3104	0.7500000000000000	0.3750000000000000	0.0455400009999991
3105	0.7500000000000000	0.8750000000000000	0.0455400009999991
3106	0.0000000000000000	0.2500000000000000	0.0929699409127238
3107	0.0000000000000000	0.7500000000000000	0.0929699409127238
3108	0.5000000000000000	0.2500000000000000	0.0929699409127238
3109	0.5000000000000000	0.7500000000000000	0.0929699409127238
3110	0.2500000000000000	0.3747388764608175	0.1376758883179932
3111	0.2500000000000000	0.8747388464608221	0.1376758883179932
3112	0.7500000000000000	0.3747388764608175	0.1376758883179932
3113	0.7500000000000000	0.8747388464608221	0.1376758883179932
3114	0.2500000000000000	0.1252611385391802	0.1376758883179932
3115	0.2500000000000000	0.6252611535391779	0.1376758883179932
3116	0.7500000000000000	0.1252611385391802	0.1376758883179932
3117	0.7500000000000000	0.6252611535391779	0.1376758883179932
3118	0.0000000000000000	0.0000000000000000	0.1822185402360219
3119	0.0000000000000000	0.5000000000000000	0.1822185402360219
3120	0.5000000000000000	0.0000000000000000	0.1822185402360219
3121	0.5000000000000000	0.5000000000000000	0.1822185402360219
3122	0.2500000000000000	0.1241268930125798	0.2296760538993894
3123	0.2500000000000000	0.6241268860125828	0.2296760538993894
3124	0.7500000000000000	0.1241268930125798	0.2296760538993894
3125	0.7500000000000000	0.6241268860125828	0.2296760538993894
3126	0.2500000000000000	0.3758731139874172	0.2296760538993894
3127	0.2500000000000000	0.8758731139874172	0.2296760538993894
3128	0.7500000000000000	0.3758731139874172	0.2296760538993894
3129	0.7500000000000000	0.8758731139874172	0.2296760538993894
3130	0.0000000000000000	0.2500000000000000	0.2705993016191357
3131	0.0000000000000000	0.7500000000000000	0.2705993016191357
3132	0.5000000000000000	0.2500000000000000	0.2705993016191357
3133	0.5000000000000000	0.7500000000000000	0.2705993016191357
3134			
3135	Bare- NiMn (25% Mn) 220 Facet supercell 2X2X1 - [Etot = -349.44429759 eV]		
3136	0.989317187668226		
3137	7.090000152600000	0.0000000000000000	0.0000000000000000
3138	0.0000000000000000	10.0268001556000002	0.0000000000000000
3139	0.0000000000000000	0.0000000000000000	27.5200996398999997
3140	Mn Ni		
3141	16 40		
3142	Direct		
3143	0.0000000000000000	0.2500000000000000	0.0000000000000000
3144	0.0000000000000000	0.7500000000000000	0.0000000000000000
3145	0.5000000000000000	0.2500000000000000	0.0000000000000000
3146	0.5000000000000000	0.7500000000000000	0.0000000000000000
3147	0.0000000000000000	0.0000000000000000	0.0910900009999978
3148	0.0000000000000000	0.5000000000000000	0.0910900009999978
3149	0.5000000000000000	0.0000000000000000	0.0910900009999978
3150	0.5000000000000000	0.5000000000000000	0.0910900009999978
3151	0.0000000000000000	0.2500000000000000	0.1859781551164943
3152	0.0000000000000000	0.7500000000000000	0.1859781551164943
3153	0.5000000000000000	0.2500000000000000	0.1859781551164943
3154	0.5000000000000000	0.7500000000000000	0.1859781551164943
3155	0.0000000000000000	0.0000000000000000	0.2807063341992091

3156	0.0000000000000000	0.5000000000000000	0.2807063341992091
3157	0.5000000000000000	0.0000000000000000	0.2807063341992091
3158	0.5000000000000000	0.5000000000000000	0.2807063341992091
3159	0.0000000000000000	0.0000000000000000	0.0000000000000000
3160	0.0000000000000000	0.5000000000000000	0.0000000000000000
3161	0.5000000000000000	0.0000000000000000	0.0000000000000000
3162	0.5000000000000000	0.5000000000000000	0.0000000000000000
3163	0.2500000000000000	0.1250000000000000	0.0455400009999991
3164	0.2500000000000000	0.6250000000000000	0.0455400009999991
3165	0.7500000000000000	0.1250000000000000	0.0455400009999991
3166	0.7500000000000000	0.6250000000000000	0.0455400009999991
3167	0.2500000000000000	0.3750000000000000	0.0455400009999991
3168	0.2500000000000000	0.8750000000000000	0.0455400009999991
3169	0.7500000000000000	0.3750000000000000	0.0455400009999991
3170	0.7500000000000000	0.8750000000000000	0.0455400009999991
3171	0.0000000000000000	0.2500000000000000	0.0928607146838800
3172	0.0000000000000000	0.7500000000000000	0.0928607146838800
3173	0.5000000000000000	0.2500000000000000	0.0928607146838800
3174	0.5000000000000000	0.7500000000000000	0.0928607146838800
3175	0.2500000000000000	0.3754265022537311	0.1393946604531209
3176	0.2500000000000000	0.8754264722537357	0.1393946604531209
3177	0.7500000000000000	0.3754265022537311	0.1393946604531209
3178	0.7500000000000000	0.8754264722537357	0.1393946604531209
3179	0.2500000000000000	0.1245735127462666	0.1393946604531209
3180	0.2500000000000000	0.6245735277462643	0.1393946604531209
3181	0.7500000000000000	0.1245735127462666	0.1393946604531209
3182	0.7500000000000000	0.6245735277462643	0.1393946604531209
3183	0.0000000000000000	0.0000000000000000	0.1862512040510751
3184	0.0000000000000000	0.5000000000000000	0.1862512040510751
3185	0.5000000000000000	0.0000000000000000	0.1862512040510751
3186	0.5000000000000000	0.5000000000000000	0.1862512040510751
3187	0.2500000000000000	0.1245836585341351	0.2340410573981444
3188	0.2500000000000000	0.6245836515341381	0.2340410573981444
3189	0.7500000000000000	0.1245836585341351	0.2340410573981444
3190	0.7500000000000000	0.6245836515341381	0.2340410573981444
3191	0.2500000000000000	0.3754163484658619	0.2340410573981444
3192	0.2500000000000000	0.8754163484658619	0.2340410573981444
3193	0.7500000000000000	0.3754163484658619	0.2340410573981444
3194	0.7500000000000000	0.8754163484658619	0.2340410573981444
3195	0.0000000000000000	0.2500000000000000	0.2757333051301529
3196	0.0000000000000000	0.7500000000000000	0.2757333051301529
3197	0.5000000000000000	0.2500000000000000	0.2757333051301529
3198	0.5000000000000000	0.7500000000000000	0.2757333051301529
3199			
3200	Bare- NiFe (25% Fe) 220 Facet supercell 2X2X1 - [Etot = -335.64641028 eV]		
3201	1.0000000000000000		
3202	7.0900001526000000	0.0000000000000000	0.0000000000000000
3203	0.0000000000000000	10.0268001556000002	0.0000000000000000
3204	0.0000000000000000	0.0000000000000000	27.5200996398999997
3205	Fe Ni		
3206	16 40		
3207	Direct		

3208	0.0000000000000000	0.2500000000000000	0.0000000000000000
3209	0.0000000000000000	0.7500000000000000	0.0000000000000000
3210	0.5000000000000000	0.2500000000000000	0.0000000000000000
3211	0.5000000000000000	0.7500000000000000	0.0000000000000000
3212	0.0000000000000000	0.0000000000000000	0.0910900009999978
3213	0.0000000000000000	0.5000000000000000	0.0910900009999978
3214	0.5000000000000000	0.0000000000000000	0.0910900009999978
3215	0.5000000000000000	0.5000000000000000	0.0910900009999978
3216	0.0000000000000000	0.2500000000000000	0.1824138568842955
3217	0.0000000000000000	0.7500000000000000	0.1824138568842955
3218	0.5000000000000000	0.2500000000000000	0.1824138568842955
3219	0.5000000000000000	0.7500000000000000	0.1824138568842955
3220	0.0000000000000000	0.0000000000000000	0.2698632462982999
3221	0.0000000000000000	0.5000000000000000	0.2698632462982999
3222	0.5000000000000000	0.0000000000000000	0.2698632462982999
3223	0.5000000000000000	0.5000000000000000	0.2698632462982999
3224	0.0000000000000000	0.0000000000000000	0.0000000000000000
3225	0.0000000000000000	0.5000000000000000	0.0000000000000000
3226	0.5000000000000000	0.0000000000000000	0.0000000000000000
3227	0.5000000000000000	0.5000000000000000	0.0000000000000000
3228	0.2500000000000000	0.1250000000000000	0.0455400009999991
3229	0.2500000000000000	0.6250000000000000	0.0455400009999991
3230	0.7500000000000000	0.1250000000000000	0.0455400009999991
3231	0.7500000000000000	0.6250000000000000	0.0455400009999991
3232	0.2500000000000000	0.3750000000000000	0.0455400009999991
3233	0.2500000000000000	0.8750000000000000	0.0455400009999991
3234	0.7500000000000000	0.3750000000000000	0.0455400009999991
3235	0.7500000000000000	0.8750000000000000	0.0455400009999991
3236	0.0000000000000000	0.2500000000000000	0.0900604966333205
3237	0.0000000000000000	0.7500000000000000	0.0900604966333205
3238	0.5000000000000000	0.2500000000000000	0.0900604966333205
3239	0.5000000000000000	0.7500000000000000	0.0900604966333205
3240	0.2500000000000000	0.3749205152567185	0.1370439497211677
3241	0.2500000000000000	0.8749204852567232	0.1370439497211677
3242	0.7500000000000000	0.3749205152567185	0.1370439497211677
3243	0.7500000000000000	0.8749204852567232	0.1370439497211677
3244	0.2500000000000000	0.1250794997432791	0.1370439497211677
3245	0.2500000000000000	0.6250795147432768	0.1370439497211677
3246	0.7500000000000000	0.1250794997432791	0.1370439497211677
3247	0.7500000000000000	0.6250795147432768	0.1370439497211677
3248	0.0000000000000000	0.0000000000000000	0.1827781493552365
3249	0.0000000000000000	0.5000000000000000	0.1827781493552365
3250	0.5000000000000000	0.0000000000000000	0.1827781493552365
3251	0.5000000000000000	0.5000000000000000	0.1827781493552365
3252	0.2500000000000000	0.1243699440501658	0.2301477034749340
3253	0.2500000000000000	0.6243699370501687	0.2301477034749340
3254	0.7500000000000000	0.1243699440501658	0.2301477034749340
3255	0.7500000000000000	0.6243699370501687	0.2301477034749340
3256	0.2500000000000000	0.3756300629498313	0.2301477034749340
3257	0.2500000000000000	0.8756300629498313	0.2301477034749340
3258	0.7500000000000000	0.3756300629498313	0.2301477034749340
3259	0.7500000000000000	0.8756300629498313	0.2301477034749340

3260	0.0000000000000000	0.2500000000000000	0.2695190767121503
3261	0.0000000000000000	0.7500000000000000	0.2695190767121503
3262	0.5000000000000000	0.2500000000000000	0.2695190767121503
3263	0.5000000000000000	0.7500000000000000	0.2695190767121503
3264			
3265	Bare- NiCo (25% Co) 220 Facet supercell 2X2X1 - [Etot = -309.08023845 eV]		
3266	0.993794164815303		
3267	7.0900001526000000	0.0000000000000000	0.0000000000000000
3268	0.0000000000000000	10.0268001556000002	0.0000000000000000
3269	0.0000000000000000	0.0000000000000000	27.5200996398999997
3270	Fe Ni		
3271	16 40		
3272	Direct		
3273	0.0000000000000000	0.2500000000000000	0.0000000000000000
3274	0.0000000000000000	0.7500000000000000	0.0000000000000000
3275	0.5000000000000000	0.2500000000000000	0.0000000000000000
3276	0.5000000000000000	0.7500000000000000	0.0000000000000000
3277	0.0000000000000000	0.0000000000000000	0.0910900009999978
3278	0.0000000000000000	0.5000000000000000	0.0910900009999978
3279	0.5000000000000000	0.0000000000000000	0.0910900009999978
3280	0.5000000000000000	0.5000000000000000	0.0910900009999978
3281	0.0000000000000000	0.2500000000000000	0.1822139803999505
3282	0.0000000000000000	0.7500000000000000	0.1822139803999505
3283	0.5000000000000000	0.2500000000000000	0.1822139803999505
3284	0.5000000000000000	0.7500000000000000	0.1822139803999505
3285	0.0000000000000000	0.0000000000000000	0.2691468443507219
3286	0.0000000000000000	0.5000000000000000	0.2691468443507219
3287	0.5000000000000000	0.0000000000000000	0.2691468443507219
3288	0.5000000000000000	0.5000000000000000	0.2691468443507219
3289	0.0000000000000000	0.0000000000000000	0.0000000000000000
3290	0.0000000000000000	0.5000000000000000	0.0000000000000000
3291	0.5000000000000000	0.0000000000000000	0.0000000000000000
3292	0.5000000000000000	0.5000000000000000	0.0000000000000000
3293	0.2500000000000000	0.1250000000000000	0.0455400009999991
3294	0.2500000000000000	0.6250000000000000	0.0455400009999991
3295	0.7500000000000000	0.1250000000000000	0.0455400009999991
3296	0.7500000000000000	0.6250000000000000	0.0455400009999991
3297	0.2500000000000000	0.3750000000000000	0.0455400009999991
3298	0.2500000000000000	0.8750000000000000	0.0455400009999991
3299	0.7500000000000000	0.3750000000000000	0.0455400009999991
3300	0.7500000000000000	0.8750000000000000	0.0455400009999991
3301	0.0000000000000000	0.2500000000000000	0.0904041628694259
3302	0.0000000000000000	0.7500000000000000	0.0904041628694259
3303	0.5000000000000000	0.2500000000000000	0.0904041628694259
3304	0.5000000000000000	0.7500000000000000	0.0904041628694259
3305	0.2500000000000000	0.3745531558462147	0.1367785304228875
3306	0.2500000000000000	0.8745531258462194	0.1367785304228875
3307	0.7500000000000000	0.3745531558462147	0.1367785304228875
3308	0.7500000000000000	0.8745531258462194	0.1367785304228875
3309	0.2500000000000000	0.1254468591537830	0.1367785304228875
3310	0.2500000000000000	0.6254468741537806	0.1367785304228875
3311	0.7500000000000000	0.1254468591537830	0.1367785304228875

3312	0.7500000000000000	0.6254468741537806	0.1367785304228875
3313	0.0000000000000000	0.0000000000000000	0.1816015195879288
3314	0.0000000000000000	0.5000000000000000	0.1816015195879288
3315	0.5000000000000000	0.0000000000000000	0.1816015195879288
3316	0.5000000000000000	0.5000000000000000	0.1816015195879288
3317	0.2500000000000000	0.1243176538489976	0.2296437448500939
3318	0.2500000000000000	0.6243176468490006	0.2296437448500939
3319	0.7500000000000000	0.1243176538489976	0.2296437448500939
3320	0.7500000000000000	0.6243176468490006	0.2296437448500939
3321	0.2500000000000000	0.3756823531509994	0.2296437448500939
3322	0.2500000000000000	0.8756823531509994	0.2296437448500939
3323	0.7500000000000000	0.3756823531509994	0.2296437448500939
3324	0.7500000000000000	0.8756823531509994	0.2296437448500939
3325	0.0000000000000000	0.2500000000000000	0.2691872348322235
3326	0.0000000000000000	0.7500000000000000	0.2691872348322235
3327	0.5000000000000000	0.2500000000000000	0.2691872348322235
3328	0.5000000000000000	0.7500000000000000	0.2691872348322235
3329			
3330	Pure-Ni 220 Facet supercell 2X2X1 - [Etot = -283.84110616 eV]		
3331	1.01798110552312		
3332	7.0900001526000000	0.0000000000000000	0.0000000000000000
3333	0.0000000000000000	10.0268001556000002	0.0000000000000000
3334	0.0000000000000000	0.0000000000000000	27.5200996398999997
3335	Ni		
3336	56		
3337	Direct		
3338	0.0000000000000000	0.2500000000000000	0.0000000000000000
3339	0.0000000000000000	0.7500000000000000	0.0000000000000000
3340	0.5000000000000000	0.2500000000000000	0.0000000000000000
3341	0.5000000000000000	0.7500000000000000	0.0000000000000000
3342	0.0000000000000000	0.0000000000000000	0.0910900009999978
3343	0.0000000000000000	0.5000000000000000	0.0910900009999978
3344	0.5000000000000000	0.0000000000000000	0.0910900009999978
3345	0.5000000000000000	0.5000000000000000	0.0910900009999978
3346	0.0000000000000000	0.2500000000000000	0.1753785761349178
3347	0.0000000000000000	0.7500000000000000	0.1753785761349178
3348	0.5000000000000000	0.2500000000000000	0.1753785761349178
3349	0.5000000000000000	0.7500000000000000	0.1753785761349178
3350	0.0000000000000000	0.0000000000000000	0.2601367025777961
3351	0.0000000000000000	0.5000000000000000	0.2601367025777961
3352	0.5000000000000000	0.0000000000000000	0.2601367025777961
3353	0.5000000000000000	0.5000000000000000	0.2601367025777961
3354	0.0000000000000000	0.0000000000000000	0.0000000000000000
3355	0.0000000000000000	0.5000000000000000	0.0000000000000000
3356	0.5000000000000000	0.0000000000000000	0.0000000000000000
3357	0.5000000000000000	0.5000000000000000	0.0000000000000000
3358	0.2500000000000000	0.1250000000000000	0.0455400009999991
3359	0.2500000000000000	0.6250000000000000	0.0455400009999991
3360	0.7500000000000000	0.1250000000000000	0.0455400009999991
3361	0.7500000000000000	0.6250000000000000	0.0455400009999991
3362	0.2500000000000000	0.3750000000000000	0.0455400009999991
3363	0.2500000000000000	0.8750000000000000	0.0455400009999991

3364	0.7500000000000000	0.3750000000000000	0.04554000099999991
3365	0.7500000000000000	0.8750000000000000	0.04554000099999991
3366	0.0000000000000000	0.2500000000000000	0.0877372377675272
3367	0.0000000000000000	0.7500000000000000	0.0877372377675272
3368	0.5000000000000000	0.2500000000000000	0.0877372377675272
3369	0.5000000000000000	0.7500000000000000	0.0877372377675272
3370	0.2500000000000000	0.3746298380697368	0.1330617520166797
3371	0.2500000000000000	0.8746298080697414	0.1330617520166797
3372	0.7500000000000000	0.3746298380697368	0.1330617520166797
3373	0.7500000000000000	0.8746298080697414	0.1330617520166797
3374	0.2500000000000000	0.1253701769302609	0.1330617520166797
3375	0.2500000000000000	0.6253701919302586	0.1330617520166797
3376	0.7500000000000000	0.1253701769302609	0.1330617520166797
3377	0.7500000000000000	0.6253701919302586	0.1330617520166797
3378	0.0000000000000000	0.0000000000000000	0.1765021534114410
3379	0.0000000000000000	0.5000000000000000	0.1765021534114410
3380	0.5000000000000000	0.0000000000000000	0.1765021534114410
3381	0.5000000000000000	0.5000000000000000	0.1765021534114410
3382	0.2500000000000000	0.1250227029215694	0.2219691965114237
3383	0.2500000000000000	0.6250226959215723	0.2219691965114237
3384	0.7500000000000000	0.1250227029215694	0.2219691965114237
3385	0.7500000000000000	0.6250226959215723	0.2219691965114237
3386	0.2500000000000000	0.3749773040784277	0.2219691965114237
3387	0.2500000000000000	0.8749773040784277	0.2219691965114237
3388	0.7500000000000000	0.3749773040784277	0.2219691965114237
3389	0.7500000000000000	0.8749773040784277	0.2219691965114237
3390	0.0000000000000000	0.2500000000000000	0.2594914765372778
3391	0.0000000000000000	0.7500000000000000	0.2594914765372778
3392	0.5000000000000000	0.2500000000000000	0.2594914765372778
3393	0.5000000000000000	0.7500000000000000	0.2594914765372778

3394

3395 Bare- NiCu (25% Cu) 220 Facet supercell 2X2X1 - [Etot = -258.56599398 eV]

3396 0.998485100048875

3397	7.0900001526000000	0.0000000000000000	0.0000000000000000
3398	0.0000000000000000	10.0268001556000002	0.0000000000000000
3399	0.0000000000000000	0.0000000000000000	27.5200996398999997

3400 Cu Ni

3401 16 40

3402 Direct

3403	0.0000000000000000	0.2500000000000000	0.0000000000000000
3404	0.0000000000000000	0.7500000000000000	0.0000000000000000
3405	0.5000000000000000	0.2500000000000000	0.0000000000000000
3406	0.5000000000000000	0.7500000000000000	0.0000000000000000
3407	0.0000000000000000	0.0000000000000000	0.09109000099999978
3408	0.0000000000000000	0.5000000000000000	0.09109000099999978
3409	0.5000000000000000	0.0000000000000000	0.09109000099999978
3410	0.5000000000000000	0.5000000000000000	0.09109000099999978
3411	0.0000000000000000	0.2500000000000000	0.1812836558276629
3412	0.0000000000000000	0.7500000000000000	0.1812836558276629
3413	0.5000000000000000	0.2500000000000000	0.1812836558276629
3414	0.5000000000000000	0.7500000000000000	0.1812836558276629
3415	0.0000000000000000	0.0000000000000000	0.2730371062792400

3416	0.0000000000000000	0.5000000000000000	0.2730371062792400
3417	0.5000000000000000	0.0000000000000000	0.2730371062792400
3418	0.5000000000000000	0.5000000000000000	0.2730371062792400
3419	0.0000000000000000	0.0000000000000000	0.0000000000000000
3420	0.0000000000000000	0.5000000000000000	0.0000000000000000
3421	0.5000000000000000	0.0000000000000000	0.0000000000000000
3422	0.5000000000000000	0.5000000000000000	0.0000000000000000
3423	0.2500000000000000	0.1250000000000000	0.0455400009999991
3424	0.2500000000000000	0.6250000000000000	0.0455400009999991
3425	0.7500000000000000	0.1250000000000000	0.0455400009999991
3426	0.7500000000000000	0.6250000000000000	0.0455400009999991
3427	0.2500000000000000	0.3750000000000000	0.0455400009999991
3428	0.2500000000000000	0.8750000000000000	0.0455400009999991
3429	0.7500000000000000	0.3750000000000000	0.0455400009999991
3430	0.7500000000000000	0.8750000000000000	0.0455400009999991
3431	0.0000000000000000	0.2500000000000000	0.0906492756339929
3432	0.0000000000000000	0.7500000000000000	0.0906492756339929
3433	0.5000000000000000	0.2500000000000000	0.0906492756339929
3434	0.5000000000000000	0.7500000000000000	0.0906492756339929
3435	0.2500000000000000	0.3753284903196530	0.1367710371465023
3436	0.2500000000000000	0.8753284603196576	0.1367710371465023
3437	0.7500000000000000	0.3753284903196530	0.1367710371465023
3438	0.7500000000000000	0.8753284603196576	0.1367710371465023
3439	0.2500000000000000	0.1246715246803447	0.1367710371465023
3440	0.2500000000000000	0.6246715396803424	0.1367710371465023
3441	0.7500000000000000	0.1246715246803447	0.1367710371465023
3442	0.7500000000000000	0.6246715396803424	0.1367710371465023
3443	0.0000000000000000	0.0000000000000000	0.1826151505366127
3444	0.0000000000000000	0.5000000000000000	0.1826151505366127
3445	0.5000000000000000	0.0000000000000000	0.1826151505366127
3446	0.5000000000000000	0.5000000000000000	0.1826151505366127
3447	0.2500000000000000	0.1255736346664804	0.2287916037133471
3448	0.2500000000000000	0.6255736276664834	0.2287916037133471
3449	0.7500000000000000	0.1255736346664804	0.2287916037133471
3450	0.7500000000000000	0.6255736276664834	0.2287916037133471
3451	0.2500000000000000	0.3744263723335166	0.2287916037133471
3452	0.2500000000000000	0.8744263723335166	0.2287916037133471
3453	0.7500000000000000	0.3744263723335166	0.2287916037133471
3454	0.7500000000000000	0.8744263723335166	0.2287916037133471
3455	0.0000000000000000	0.2500000000000000	0.2696953807352216
3456	0.0000000000000000	0.7500000000000000	0.2696953807352216
3457	0.5000000000000000	0.2500000000000000	0.2696953807352216
3458	0.5000000000000000	0.7500000000000000	0.2696953807352216
3459			
3460	Bare- NiZn (25% Zn) 220 Facet supercell 2X2X1 - [Etot = -230.77875689 eV]		
3461	1.01038006037737		
3462	7.0900001526000000	0.0000000000000000	0.0000000000000000
3463	0.0000000000000000	10.0268001556000002	0.0000000000000000
3464	0.0000000000000000	0.0000000000000000	27.5200996398999997
3465	Zn	Ni	
3466	16	40	
3467	Direct		

3468	0.0000000000000000	0.2500000000000000	0.0000000000000000
3469	0.0000000000000000	0.7500000000000000	0.0000000000000000
3470	0.5000000000000000	0.2500000000000000	0.0000000000000000
3471	0.5000000000000000	0.7500000000000000	0.0000000000000000
3472	0.0000000000000000	0.0000000000000000	0.0910900009999978
3473	0.0000000000000000	0.5000000000000000	0.0910900009999978
3474	0.5000000000000000	0.0000000000000000	0.0910900009999978
3475	0.5000000000000000	0.5000000000000000	0.0910900009999978
3476	0.0000000000000000	0.2500000000000000	0.1808294241720105
3477	0.0000000000000000	0.7500000000000000	0.1808294241720105
3478	0.5000000000000000	0.2500000000000000	0.1808294241720105
3479	0.5000000000000000	0.7500000000000000	0.1808294241720105
3480	0.0000000000000000	0.0000000000000000	0.2736022190675911
3481	0.0000000000000000	0.5000000000000000	0.2736022190675911
3482	0.5000000000000000	0.0000000000000000	0.2736022190675911
3483	0.5000000000000000	0.5000000000000000	0.2736022190675911
3484	0.0000000000000000	0.0000000000000000	0.0000000000000000
3485	0.0000000000000000	0.5000000000000000	0.0000000000000000
3486	0.5000000000000000	0.0000000000000000	0.0000000000000000
3487	0.5000000000000000	0.5000000000000000	0.0000000000000000
3488	0.2500000000000000	0.1250000000000000	0.0455400009999991
3489	0.2500000000000000	0.6250000000000000	0.0455400009999991
3490	0.7500000000000000	0.1250000000000000	0.0455400009999991
3491	0.7500000000000000	0.6250000000000000	0.0455400009999991
3492	0.2500000000000000	0.3750000000000000	0.0455400009999991
3493	0.2500000000000000	0.8750000000000000	0.0455400009999991
3494	0.7500000000000000	0.3750000000000000	0.0455400009999991
3495	0.7500000000000000	0.8750000000000000	0.0455400009999991
3496	0.0000000000000000	0.2500000000000000	0.0908944302055374
3497	0.0000000000000000	0.7500000000000000	0.0908944302055374
3498	0.5000000000000000	0.2500000000000000	0.0908944302055374
3499	0.5000000000000000	0.7500000000000000	0.0908944302055374
3500	0.2500000000000000	0.3754391005850408	0.1365678346375319
3501	0.2500000000000000	0.8754390705850454	0.1365678346375319
3502	0.7500000000000000	0.3754391005850408	0.1365678346375319
3503	0.7500000000000000	0.8754390705850454	0.1365678346375319
3504	0.2500000000000000	0.1245609144149569	0.1365678346375319
3505	0.2500000000000000	0.6245609294149546	0.1365678346375319
3506	0.7500000000000000	0.1245609144149569	0.1365678346375319
3507	0.7500000000000000	0.6245609294149546	0.1365678346375319
3508	0.0000000000000000	0.0000000000000000	0.1821934700678227
3509	0.0000000000000000	0.5000000000000000	0.1821934700678227
3510	0.5000000000000000	0.0000000000000000	0.1821934700678227
3511	0.5000000000000000	0.5000000000000000	0.1821934700678227
3512	0.2500000000000000	0.1242644364486480	0.2283746263393809
3513	0.2500000000000000	0.6242644294486510	0.2283746263393809
3514	0.7500000000000000	0.1242644364486480	0.2283746263393809
3515	0.7500000000000000	0.6242644294486510	0.2283746263393809
3516	0.2500000000000000	0.3757355705513490	0.2283746263393809
3517	0.2500000000000000	0.8757355705513490	0.2283746263393809
3518	0.7500000000000000	0.3757355705513490	0.2283746263393809
3519	0.7500000000000000	0.8757355705513490	0.2283746263393809

3520	0.0000000000000000	0.2500000000000000	0.2687224200509561
3521	0.0000000000000000	0.7500000000000000	0.2687224200509561
3522	0.5000000000000000	0.2500000000000000	0.2687224200509561
3523	0.5000000000000000	0.7500000000000000	0.2687224200509561
3524			
3525	NiSc (25% Sc) 220 Facet with Hydrogen supercell 2X2X1 - [Etot = -332.62902497 eV]		
3526	1.04735280294076		
3527	7.0900001526000000	0.0000000000000000	0.0000000000000000
3528	0.0000000000000000	10.0268001556000002	0.0000000000000000
3529	0.0000000000000000	0.0000000000000000	27.5200996398999997
3530	Sc Ni H		
3531	16 40 1		
3532	Direct		
3533	0.0000000000000000	0.2500000000000000	0.0000000000000000
3534	0.0000000000000000	0.7500000000000000	0.0000000000000000
3535	0.5000000000000000	0.2500000000000000	0.0000000000000000
3536	0.5000000000000000	0.7500000000000000	0.0000000000000000
3537	0.0000000000000000	0.0000000000000000	0.0910900009999978
3538	0.0000000000000000	0.5000000000000000	0.0910900009999978
3539	0.5000000000000000	0.0000000000000000	0.0910900009999978
3540	0.5000000000000000	0.5000000000000000	0.0910900009999978
3541	0.9986855312968643	0.2501600212666943	0.1801442266706701
3542	0.0008007812609208	0.7501665202296124	0.1801664459620014
3543	0.5013144687031357	0.2501600212666943	0.1801442266706701
3544	0.4991992187390792	0.7501665202296124	0.1801664459620014
3545	0.9970941467093013	0.9983643988987794	0.2729800998638865
3546	0.9971335723470034	0.5022619133891624	0.2729691062451565
3547	0.5029058532906987	0.9983643988987794	0.2729800998638865
3548	0.5028664276529966	0.5022619133891624	0.2729691062451565
3549	0.0000000000000000	0.0000000000000000	0.0000000000000000
3550	0.0000000000000000	0.5000000000000000	0.0000000000000000
3551	0.5000000000000000	0.0000000000000000	0.0000000000000000
3552	0.5000000000000000	0.5000000000000000	0.0000000000000000
3553	0.2500000000000000	0.1250000000000000	0.0455400009999991
3554	0.2500000000000000	0.6250000000000000	0.0455400009999991
3555	0.7500000000000000	0.1250000000000000	0.0455400009999991
3556	0.7500000000000000	0.6250000000000000	0.0455400009999991
3557	0.2500000000000000	0.3750000000000000	0.0455400009999991
3558	0.2500000000000000	0.8750000000000000	0.0455400009999991
3559	0.7500000000000000	0.3750000000000000	0.0455400009999991
3560	0.7500000000000000	0.8750000000000000	0.0455400009999991
3561	0.0002007494946454	0.2500059559462784	0.0889642846576990
3562	0.9998896892322193	0.7500159210075950	0.0888684900409871
3563	0.4997992505053546	0.2500059559462784	0.0889642846576990
3564	0.5001103107677807	0.7500159210075950	0.0888684900409871
3565	0.2500000000000000	0.3759598733961624	0.1367946320147553
3566	0.2500000000000000	0.8758423494745529	0.1362399574779545
3567	0.7500000000000000	0.3762918465052607	0.1364426974620372
3568	0.7500000000000000	0.8758029301971462	0.1364487578254767
3569	0.2500000000000000	0.1243369831626921	0.1367849279595887
3570	0.2500000000000000	0.6244666893099975	0.1361884582357291
3571	0.7500000000000000	0.1237820486061452	0.1364732102209345

3572	0.7500000000000000	0.6242539672159637	0.1364796011749903
3573	0.0006646831218546	0.0004377826423294	0.1840889605136127
3574	0.0007022744216911	0.4999112503835335	0.1840870268760071
3575	0.4993353168781454	0.0004377826423294	0.1840889605136127
3576	0.4992977255783089	0.4999112503835335	0.1840870268760071
3577	0.2500000000000000	0.1220112300377494	0.2298624655508661
3578	0.2500000000000000	0.6236274348847530	0.2296845718739604
3579	0.7500000000000000	0.1237414994925956	0.2296562008518350
3580	0.7500000000000000	0.6239484825229269	0.2290703382828170
3581	0.2500000000000000	0.3785008417558373	0.2298667129760119
3582	0.2500000000000000	0.8768991474934182	0.2296892549899709
3583	0.7500000000000000	0.3768211055748552	0.2296280515451059
3584	0.7500000000000000	0.8766013003298738	0.2290517072702087
3585	0.9985460833491402	0.2503258324013586	0.2662085329802082
3586	0.9991050700257986	0.7503317681748527	0.2660438833173941
3587	0.5014539166508598	0.2503258324013586	0.2662085329802082
3588	0.5008949299742014	0.7503317681748527	0.2660438833173941
3589	0.2500000000000000	0.2501260196077126	0.2686474194003239

3590

3591 NiTi (25% Ti) 220 Facet with Hydrogen supercell 2X2X1 - [Etot = -352.34576879 eV]

3592 1.01798110552312

3593	7.0900001526000000	0.0000000000000000	0.0000000000000000
3594	0.0000000000000000	10.0268001556000002	0.0000000000000000
3595	0.0000000000000000	0.0000000000000000	27.5200996398999997

3596 Ti Ni H

3597 16 40 1

3598 Direct

3599	0.0000000000000000	0.2500000000000000	0.0000000000000000
3600	0.0000000000000000	0.7500000000000000	0.0000000000000000
3601	0.5000000000000000	0.2500000000000000	0.0000000000000000
3602	0.5000000000000000	0.7500000000000000	0.0000000000000000
3603	0.0000000000000000	0.0000000000000000	0.0910900009999978
3604	0.0000000000000000	0.5000000000000000	0.0910900009999978
3605	0.5000000000000000	0.0000000000000000	0.0910900009999978
3606	0.5000000000000000	0.5000000000000000	0.0910900009999978
3607	0.9984608453768615	0.2496959727977526	0.1822788418800130
3608	0.0017367470487883	0.7497042243644927	0.1829760748240545
3609	0.5015391546231385	0.2496959727977526	0.1822788418800130
3610	0.4982632529512117	0.7497042243644927	0.1829760748240545
3611	0.9951681029065611	0.9963438241376750	0.2703619442186707
3612	0.9951828999582517	0.5026752510702792	0.2703897759826432
3613	0.5048318970934389	0.9963438241376750	0.2703619442186707
3614	0.5048171000417483	0.5026752510702792	0.2703897759826432
3615	0.0000000000000000	0.0000000000000000	0.0000000000000000
3616	0.0000000000000000	0.5000000000000000	0.0000000000000000
3617	0.5000000000000000	0.0000000000000000	0.0000000000000000
3618	0.5000000000000000	0.5000000000000000	0.0000000000000000
3619	0.2500000000000000	0.1250000000000000	0.0455400009999991
3620	0.2500000000000000	0.6250000000000000	0.0455400009999991
3621	0.7500000000000000	0.1250000000000000	0.0455400009999991
3622	0.7500000000000000	0.6250000000000000	0.0455400009999991
3623	0.2500000000000000	0.3750000000000000	0.0455400009999991

3624	0.2500000000000000	0.8750000000000000	0.04554000099999991
3625	0.7500000000000000	0.3750000000000000	0.04554000099999991
3626	0.7500000000000000	0.8750000000000000	0.04554000099999991
3627	0.0000146443915554	0.2499597558410755	0.0903597108774719
3628	0.0000034504425415	0.7499006989071972	0.0903829178281015
3629	0.4999853556084446	0.2499597558410755	0.0903597108774719
3630	0.4999965495574585	0.7499006989071972	0.0903829178281015
3631	0.2500000000000000	0.3744090045769752	0.1376535706475792
3632	0.2500000000000000	0.8749219929306449	0.1374704398440514
3633	0.7500000000000000	0.3748914414762581	0.1374167005929081
3634	0.7500000000000000	0.8746763150332484	0.1374696182130677
3635	0.2500000000000000	0.1251596744194856	0.1376585688339418
3636	0.2500000000000000	0.6246584326044271	0.1374879563636711
3637	0.7500000000000000	0.1246904037325294	0.1374288309121354
3638	0.7500000000000000	0.6248588027056527	0.1374998106085101
3639	0.0010367112421719	0.0001018045012557	0.1837195454139575
3640	0.0011007380462615	0.4993095899016780	0.1837732095070450
3641	0.4989632887578281	0.0001018045012557	0.1837195454139575
3642	0.4988992619537385	0.4993095899016780	0.1837732095070450
3643	0.2500000000000000	0.1211690555610758	0.2310452907930696
3644	0.2500000000000000	0.6221682939151307	0.2311325050384809
3645	0.7500000000000000	0.1226649923844079	0.2303372332042102
3646	0.7500000000000000	0.6224643862031556	0.2298942675280600
3647	0.2500000000000000	0.3779300668049643	0.2310731284202987
3648	0.2500000000000000	0.8770848011700920	0.2310648220415104
3649	0.7500000000000000	0.3765439789382867	0.2303273056781237
3650	0.7500000000000000	0.8767911070349896	0.2297975873458782
3651	0.9981901386031495	0.2495198934163128	0.2685993515096854
3652	0.9985116903100462	0.7496306231704395	0.2685617611542526
3653	0.5018098613968505	0.2495198934163128	0.2685993515096854
3654	0.5014883096899538	0.7496306231704395	0.2685617611542526
3655	0.2500000000000000	0.2496935546795882	0.2743030814293022
3656			
3657	NiV (25% V) 220 Facet with Hydrogen supercell 2X2X1 - [Etot = -353.16533057 eV]		
3658	1.00458661266245		
3659	7.0900001526000000	0.0000000000000000	0.0000000000000000
3660	0.0000000000000000	10.0268001556000002	0.0000000000000000
3661	0.0000000000000000	0.0000000000000000	27.5200996398999997
3662	V	Ni	H
3663	16	40	1
3664	Direct		
3665	0.0000000000000000	0.2500000000000000	0.0000000000000000
3666	0.0000000000000000	0.7500000000000000	0.0000000000000000
3667	0.5000000000000000	0.2500000000000000	0.0000000000000000
3668	0.5000000000000000	0.7500000000000000	0.0000000000000000
3669	0.0000000000000000	0.0000000000000000	0.0910900009999978
3670	0.0000000000000000	0.5000000000000000	0.0910900009999978
3671	0.5000000000000000	0.0000000000000000	0.0910900009999978
3672	0.5000000000000000	0.5000000000000000	0.0910900009999978
3673	0.9983061093111445	0.2502693948227517	0.1837560105794580
3674	0.0019499291798439	0.7503011777717532	0.1845929673490758
3675	0.5016938906888555	0.2502693948227517	0.1837560105794580

3676	0.4980500708201561	0.7503011777717532	0.1845929673490758
3677	0.9930543522449256	0.9972175202491016	0.2740976176105505
3678	0.9930939775948460	0.5036991100498085	0.2740455343335881
3679	0.5069456477550744	0.9972175202491016	0.2740976176105505
3680	0.5069060224051540	0.5036991100498085	0.2740455343335881
3681	0.0000000000000000	0.0000000000000000	0.0000000000000000
3682	0.0000000000000000	0.5000000000000000	0.0000000000000000
3683	0.5000000000000000	0.0000000000000000	0.0000000000000000
3684	0.5000000000000000	0.5000000000000000	0.0000000000000000
3685	0.2500000000000000	0.1250000000000000	0.0455400009999991
3686	0.2500000000000000	0.6250000000000000	0.0455400009999991
3687	0.7500000000000000	0.1250000000000000	0.0455400009999991
3688	0.7500000000000000	0.6250000000000000	0.0455400009999991
3689	0.2500000000000000	0.3750000000000000	0.0455400009999991
3690	0.2500000000000000	0.8750000000000000	0.0455400009999991
3691	0.7500000000000000	0.3750000000000000	0.0455400009999991
3692	0.7500000000000000	0.8750000000000000	0.0455400009999991
3693	0.0002468123829473	0.2500916439172514	0.0918084557892058
3694	0.0000930479388686	0.7500765411881218	0.0917352062788837
3695	0.4997531876170527	0.2500916439172514	0.0918084557892058
3696	0.4999069520611314	0.7500765411881218	0.0917352062788837
3697	0.2500000000000000	0.3745481362469505	0.1373100273740846
3698	0.2500000000000000	0.8752174037572971	0.1368910505721885
3699	0.7500000000000000	0.3750086171120586	0.1368346268850260
3700	0.7500000000000000	0.8750740324990005	0.1367476479748504
3701	0.2500000000000000	0.1258058114237599	0.1373367070323539
3702	0.2500000000000000	0.6251245712703550	0.1368721945375455
3703	0.7500000000000000	0.1253775236879804	0.1368395914016105
3704	0.7500000000000000	0.6252770750498655	0.1367127267122257
3705	0.0010163411959425	0.0007411675360132	0.1820183579457293
3706	0.0010239891637980	0.4998306755108288	0.1819729601449893
3707	0.4989836588040575	0.0007411675360132	0.1820183579457293
3708	0.4989760108362020	0.4998306755108288	0.1819729601449893
3709	0.2500000000000000	0.1227759219339504	0.2292913040481324
3710	0.2500000000000000	0.6230196160894295	0.2285838199559578
3711	0.7500000000000000	0.1233000156613997	0.2275517803640952
3712	0.7500000000000000	0.6236377773283692	0.2271392313960803
3713	0.2500000000000000	0.3779374901588994	0.2292151080432063
3714	0.2500000000000000	0.8777806474801508	0.2286206436379246
3715	0.7500000000000000	0.3774708873544057	0.2275623466767556
3716	0.7500000000000000	0.8771747209954199	0.2271863356792565
3717	0.9961251175086048	0.2504558537988686	0.2692095174989504
3718	0.9981028834968626	0.7504733662543899	0.2691536514371791
3719	0.5038748824913952	0.2504558537988686	0.2692095174989504
3720	0.5018971165031374	0.7504733662543899	0.2691536514371791
3721	0.2500000000000000	0.2511843272659746	0.2744812001720334

3722

3723 NiCr (25% Cr) 220 Facet with Hydrogen supercell 2X2X1 - [Etot = -353.54792671 eV]

3724 0.995572721824907

3725	7.0900001526000000	0.0000000000000000	0.0000000000000000
3726	0.0000000000000000	10.0268001556000002	0.0000000000000000
3727	0.0000000000000000	0.0000000000000000	27.5200996398999997

3728	Cr	Ni	H
3729	16	40	1
3730	Direct		
3731	0.0000000000000000	0.2500000000000000	0.0000000000000000
3732	0.0000000000000000	0.7500000000000000	0.0000000000000000
3733	0.5000000000000000	0.2500000000000000	0.0000000000000000
3734	0.5000000000000000	0.7500000000000000	0.0000000000000000
3735	0.0000000000000000	0.0000000000000000	0.0910900009999978
3736	0.0000000000000000	0.5000000000000000	0.0910900009999978
3737	0.5000000000000000	0.0000000000000000	0.0910900009999978
3738	0.5000000000000000	0.5000000000000000	0.0910900009999978
3739	0.9982664619312445	0.2493912146836834	0.1839413454004344
3740	0.0011542918227434	0.7494612031944783	0.1844608397280965
3741	0.5017335380687555	0.2493912146836834	0.1839413454004344
3742	0.4988457081772566	0.7494612031944783	0.1844608397280965
3743	0.9950192580179049	0.9968888395413771	0.2761374198315565
3744	0.9950475264693779	0.5013287010093137	0.2760722468080701
3745	0.5049807419820951	0.9968888395413771	0.2761374198315565
3746	0.5049524735306221	0.5013287010093137	0.2760722468080701
3747	0.0000000000000000	0.0000000000000000	0.0000000000000000
3748	0.0000000000000000	0.5000000000000000	0.0000000000000000
3749	0.5000000000000000	0.0000000000000000	0.0000000000000000
3750	0.5000000000000000	0.5000000000000000	0.0000000000000000
3751	0.2500000000000000	0.1250000000000000	0.0455400009999991
3752	0.2500000000000000	0.6250000000000000	0.0455400009999991
3753	0.7500000000000000	0.1250000000000000	0.0455400009999991
3754	0.7500000000000000	0.6250000000000000	0.0455400009999991
3755	0.2500000000000000	0.3750000000000000	0.0455400009999991
3756	0.2500000000000000	0.8750000000000000	0.0455400009999991
3757	0.7500000000000000	0.3750000000000000	0.0455400009999991
3758	0.7500000000000000	0.8750000000000000	0.0455400009999991
3759	0.0004196207285361	0.2498531985385739	0.0928933144800936
3760	0.0001055792149955	0.7499024578859164	0.0929169054446888
3761	0.4995803792714639	0.2498531985385739	0.0928933144800936
3762	0.4998944207850045	0.7499024578859164	0.0929169054446888
3763	0.2500000000000000	0.3742812628784904	0.1380345077712306
3764	0.2500000000000000	0.8743902043302754	0.1376105719368468
3765	0.7500000000000000	0.3747278400777816	0.1374879188702351
3766	0.7500000000000000	0.8743212054558924	0.1375463588035757
3767	0.2500000000000000	0.1249716959183402	0.1380651190102000
3768	0.2500000000000000	0.6249166155796146	0.1375878478468593
3769	0.7500000000000000	0.1245271877535004	0.1375063646505481
3770	0.7500000000000000	0.6249771882603596	0.1375301122089567
3771	0.0008447424477112	0.9993754801344821	0.1823527529577973
3772	0.0008361841576345	0.4994811602172078	0.1823123356091330
3773	0.4991552575522888	0.9993754801344821	0.1823527529577973
3774	0.4991638158423655	0.4994811602172078	0.1823123356091330
3775	0.2500000000000000	0.1227123394039964	0.2308184495235039
3776	0.2500000000000000	0.6232555126376056	0.2298875358503238
3777	0.7500000000000000	0.1230383190567750	0.2292444184161582
3778	0.7500000000000000	0.6239843348500784	0.2288824774252944
3779	0.2500000000000000	0.3757461727213709	0.2307205401983481

3780	0.2500000000000000	0.8752235687677796	0.2299148946876670
3781	0.7500000000000000	0.3754507006385737	0.2291962921979902
3782	0.7500000000000000	0.8745502878939178	0.2289320494826512
3783	0.9953625230499910	0.2491635775053211	0.2710406637225731
3784	0.9991164805156316	0.7491279351161921	0.2704941199513016
3785	0.5046374769500090	0.2491635775053211	0.2710406637225731
3786	0.5008835194843684	0.7491279351161921	0.2704941199513016
3787	0.2500000000000000	0.2497393901085374	0.2766024808598360
3788			
3789	NiMn (25% Mn) 220 Facet with Hydrogen supercell 2X2X1 -[Etot = -353.29975965 eV]		
3790	0.989317187668226		
3791	7.0900001526000000	0.0000000000000000	0.0000000000000000
3792	0.0000000000000000	10.0268001556000002	0.0000000000000000
3793	0.0000000000000000	0.0000000000000000	27.5200996398999997
3794	Mn Ni H		
3795	16 40 1		
3796	Direct		
3797	0.0000000000000000	0.2500000000000000	0.0000000000000000
3798	0.0000000000000000	0.7500000000000000	0.0000000000000000
3799	0.5000000000000000	0.2500000000000000	0.0000000000000000
3800	0.5000000000000000	0.7500000000000000	0.0000000000000000
3801	0.0000000000000000	0.0000000000000000	0.0910900009999978
3802	0.0000000000000000	0.5000000000000000	0.0910900009999978
3803	0.5000000000000000	0.0000000000000000	0.0910900009999978
3804	0.5000000000000000	0.5000000000000000	0.0910900009999978
3805	0.9997769281276305	0.2488858757320571	0.1856288704301505
3806	0.0012979032857316	0.7488948761406320	0.1858954142318012
3807	0.5002230718723695	0.2488858757320571	0.1856288704301505
3808	0.4987020967142684	0.7488948761406320	0.1858954142318012
3809	0.9949986881772119	0.9971111075541685	0.2806665072463943
3810	0.9946184987879718	0.4996648890288782	0.2806811774802966
3811	0.5050013118227881	0.9971111075541685	0.2806665072463943
3812	0.5053815012120282	0.4996648890288782	0.2806811774802966
3813	0.0000000000000000	0.0000000000000000	0.0000000000000000
3814	0.0000000000000000	0.5000000000000000	0.0000000000000000
3815	0.5000000000000000	0.0000000000000000	0.0000000000000000
3816	0.5000000000000000	0.5000000000000000	0.0000000000000000
3817	0.2500000000000000	0.1250000000000000	0.0455400009999991
3818	0.2500000000000000	0.6250000000000000	0.0455400009999991
3819	0.7500000000000000	0.1250000000000000	0.0455400009999991
3820	0.7500000000000000	0.6250000000000000	0.0455400009999991
3821	0.2500000000000000	0.3750000000000000	0.0455400009999991
3822	0.2500000000000000	0.8750000000000000	0.0455400009999991
3823	0.7500000000000000	0.3750000000000000	0.0455400009999991
3824	0.7500000000000000	0.8750000000000000	0.0455400009999991
3825	0.0001586975240713	0.2498301313801932	0.0927435603549327
3826	0.9999241205486697	0.7498288037800336	0.0928128268193404
3827	0.4998413024759287	0.2498301313801932	0.0927435603549327
3828	0.5000758794513303	0.7498288037800336	0.0928128268193404
3829	0.2500000000000000	0.3747142941186112	0.1395914594284520
3830	0.2500000000000000	0.8747215552997076	0.1392991838266937
3831	0.7500000000000000	0.3749618108833346	0.1391946370579262

3832	0.7500000000000000	0.8746566936684772	0.1393810188260289
3833	0.2500000000000000	0.1239945899270936	0.1396003306908469
3834	0.2500000000000000	0.6239948635697488	0.1393228217722964
3835	0.7500000000000000	0.1237253048108613	0.1392285126629531
3836	0.7500000000000000	0.6240506107571164	0.1393898926883068
3837	0.0012006340343689	0.9988570477526579	0.1861827374346703
3838	0.0012532024572707	0.4989253191990315	0.1861905529797951
3839	0.4987993659656311	0.9988570477526579	0.1861827374346703
3840	0.4987467975427293	0.4989253191990315	0.1861905529797951
3841	0.2500000000000000	0.1222663324388193	0.2351735801421384
3842	0.2500000000000000	0.6231123296937042	0.2346002906890874
3843	0.7500000000000000	0.1227856653031978	0.2331272218565275
3844	0.7500000000000000	0.6238113261481146	0.2333527752184565
3845	0.2500000000000000	0.3748255751297052	0.2352178925750721
3846	0.2500000000000000	0.8740117827755896	0.2345079679552811
3847	0.7500000000000000	0.3743083847366222	0.2330534116640166
3848	0.7500000000000000	0.8734420234607185	0.2333918695270825
3849	0.9940443025904813	0.2484095806748456	0.2759704936710179
3850	0.9985789965340359	0.7483850732989268	0.2757207290220265
3851	0.5059556974095187	0.2484095806748456	0.2759704936710179
3852	0.5014210034659641	0.7483850732989268	0.2757207290220265
3853	0.2500000000000000	0.2480354850354445	0.2809595041827038

3854

3855 NiFe (25% Fe) 220 Facet with Hydrogen supercell 2X2X1 - [Etot = -339.39908880 eV]

3856 1.0000000000000000

3857	7.0900001526000000	0.0000000000000000	0.0000000000000000
3858	0.0000000000000000	10.0268001556000002	0.0000000000000000
3859	0.0000000000000000	0.0000000000000000	27.5200996398999997

3860 Fe Ni H

3861 16 40 1

3862 Direct

3863	0.0000000000000000	0.2500000000000000	0.0000000000000000
3864	0.0000000000000000	0.7500000000000000	0.0000000000000000
3865	0.5000000000000000	0.2500000000000000	0.0000000000000000
3866	0.5000000000000000	0.7500000000000000	0.0000000000000000
3867	0.0000000000000000	0.0000000000000000	0.0910900009999978
3868	0.0000000000000000	0.5000000000000000	0.0910900009999978
3869	0.5000000000000000	0.0000000000000000	0.0910900009999978
3870	0.5000000000000000	0.5000000000000000	0.0910900009999978
3871	0.9995134435069417	0.2498461807133054	0.1819322619557795
3872	0.0012387694882747	0.7498410496805406	0.1821590678111562
3873	0.5004865564930583	0.2498461807133054	0.1819322619557795
3874	0.4987612305117253	0.7498410496805406	0.1821590678111562
3875	0.9957124359950313	0.9975813102300606	0.2699112301345110
3876	0.9957296907276501	0.5019160224694232	0.2698865948804752
3877	0.5042875640049687	0.9975813102300606	0.2699112301345110
3878	0.5042703092723499	0.5019160224694232	0.2698865948804752
3879	0.0000000000000000	0.0000000000000000	0.0000000000000000
3880	0.0000000000000000	0.5000000000000000	0.0000000000000000
3881	0.5000000000000000	0.0000000000000000	0.0000000000000000
3882	0.5000000000000000	0.5000000000000000	0.0000000000000000
3883	0.2500000000000000	0.1250000000000000	0.0455400009999991

3884	0.2500000000000000	0.6250000000000000	0.0455400009999991
3885	0.7500000000000000	0.1250000000000000	0.0455400009999991
3886	0.7500000000000000	0.6250000000000000	0.0455400009999991
3887	0.2500000000000000	0.3750000000000000	0.0455400009999991
3888	0.2500000000000000	0.8750000000000000	0.0455400009999991
3889	0.7500000000000000	0.3750000000000000	0.0455400009999991
3890	0.7500000000000000	0.8750000000000000	0.0455400009999991
3891	0.0001078290072698	0.2500084350070182	0.0900205242004333
3892	0.9999600433185449	0.7499759931281815	0.0899720967803859
3893	0.4998921709927302	0.2500084350070182	0.0900205242004333
3894	0.5000399566814551	0.7499759931281815	0.0899720967803859
3895	0.2500000000000000	0.3745932040235331	0.1373081123486344
3896	0.2500000000000000	0.8749701883417487	0.1369944770608029
3897	0.7500000000000000	0.3749008495558144	0.1370232544821022
3898	0.7500000000000000	0.8748254307526935	0.1369735576567095
3899	0.2500000000000000	0.1252489403875643	0.1373250160251871
3900	0.2500000000000000	0.6248851410558700	0.1369886847933017
3901	0.7500000000000000	0.1249342737544410	0.1370193625363072
3902	0.7500000000000000	0.6250006228616627	0.1369813873375918
3903	0.0009989665083836	0.9999547352037865	0.1828196533545778
3904	0.0010219526369752	0.4997271969726853	0.1828040418098453
3905	0.4990010334916164	0.9999547352037865	0.1828196533545778
3906	0.4989780473630248	0.4997271969726853	0.1828040418098453
3907	0.2500000000000000	0.1230477796836809	0.2313183734001569
3908	0.2500000000000000	0.6238987040970585	0.2305345110168346
3909	0.7500000000000000	0.1240026379063011	0.2296677156523614
3910	0.7500000000000000	0.6243784772298540	0.2295883777911669
3911	0.2500000000000000	0.3764305097988228	0.2313008359996047
3912	0.2500000000000000	0.8756325998810368	0.2305463199239242
3913	0.7500000000000000	0.3755535746690057	0.2296474647022393
3914	0.7500000000000000	0.8752159742969710	0.2295777000725892
3915	0.9963555279485803	0.2497208924386385	0.2696874134232274
3916	0.9988924270542796	0.7497428443627001	0.2693931321799639
3917	0.5036444720514197	0.2497208924386385	0.2696874134232274
3918	0.5011075729457204	0.7497428443627001	0.2693931321799639
3919	0.2500000000000000	0.2494616689196221	0.2767600462054176
3920			

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

3922	0.993794164815303		
3923	7.0900001526000000	0.0000000000000000	0.0000000000000000
3924	0.0000000000000000	10.0268001556000002	0.0000000000000000
3925	0.0000000000000000	0.0000000000000000	27.5200996398999997
3926	Fe Ni H		
3927	16 40 1		
3928	Direct		
3929	0.0000000000000000	0.2500000000000000	0.0000000000000000
3930	0.0000000000000000	0.7500000000000000	0.0000000000000000
3931	0.5000000000000000	0.2500000000000000	0.0000000000000000
3932	0.5000000000000000	0.7500000000000000	0.0000000000000000
3933	0.0000000000000000	0.0000000000000000	0.0910900009999978
3934	0.0000000000000000	0.5000000000000000	0.0910900009999978
3935	0.5000000000000000	0.0000000000000000	0.0910900009999978

3936	0.5000000000000000	0.5000000000000000	0.0910900009999978
3937	0.9995699625617434	0.2496072000249328	0.1818526289782838
3938	0.0010285848919125	0.7496037988165511	0.1820211611135747
3939	0.5004300374382566	0.2496072000249328	0.1818526289782838
3940	0.4989714151080875	0.7496037988165511	0.1820211611135747
3941	0.9956285890604590	0.9971299766101467	0.2693336033956726
3942	0.9956306453330868	0.5016037394544313	0.2693043656213518
3943	0.5043714109395410	0.9971299766101467	0.2693336033956726
3944	0.5043693546669132	0.5016037394544313	0.2693043656213518
3945	0.0000000000000000	0.0000000000000000	0.0000000000000000
3946	0.0000000000000000	0.5000000000000000	0.0000000000000000
3947	0.5000000000000000	0.0000000000000000	0.0000000000000000
3948	0.5000000000000000	0.5000000000000000	0.0000000000000000
3949	0.2500000000000000	0.1250000000000000	0.0455400009999991
3950	0.2500000000000000	0.6250000000000000	0.0455400009999991
3951	0.7500000000000000	0.1250000000000000	0.0455400009999991
3952	0.7500000000000000	0.6250000000000000	0.0455400009999991
3953	0.2500000000000000	0.3750000000000000	0.0455400009999991
3954	0.2500000000000000	0.8750000000000000	0.0455400009999991
3955	0.7500000000000000	0.3750000000000000	0.0455400009999991
3956	0.7500000000000000	0.8750000000000000	0.0455400009999991
3957	0.0000187726282519	0.2499745570888123	0.0904050640911791
3958	0.9997889611852173	0.7499169079668988	0.0903305388875921
3959	0.4999812273717481	0.2499745570888123	0.0904050640911791
3960	0.5002110388147827	0.7499169079668988	0.0903305388875921
3961	0.2500000000000000	0.3741257034155865	0.1370745005004466
3962	0.2500000000000000	0.8746687832388389	0.1366839610943558
3963	0.7500000000000000	0.3744847453241320	0.1368106443502910
3964	0.7500000000000000	0.8743194033791539	0.1366810497122373
3965	0.2500000000000000	0.1254495066534247	0.1370646232226349
3966	0.2500000000000000	0.6249694346554406	0.1366564469589235
3967	0.7500000000000000	0.1250123659805951	0.1367831551988061
3968	0.7500000000000000	0.6251860312127064	0.1367528457013307
3969	0.0013932348660362	0.9996411665075016	0.1816744584331289
3970	0.0014095639985143	0.4995232548079827	0.1816558177557397
3971	0.4986067651339638	0.9996411665075016	0.1816744584331289
3972	0.4985904360014857	0.4995232548079827	0.1816558177557397
3973	0.2500000000000000	0.1223852431414159	0.2307600201222257
3974	0.2500000000000000	0.6236831583020503	0.2298824438625502
3975	0.7500000000000000	0.1236721650771528	0.2290747783130982
3976	0.7500000000000000	0.6240557276823466	0.2290037913342999
3977	0.2500000000000000	0.3763341344163678	0.2308453546761058
3978	0.2500000000000000	0.8752055448864482	0.2299199710663800
3979	0.7500000000000000	0.3753106638900405	0.2291109409751542
3980	0.7500000000000000	0.8749234649075959	0.2289138971971880
3981	0.9963636627068055	0.2493162161380909	0.2694011365407931
3982	0.9988873119571906	0.7494371607125672	0.2690430971953006
3983	0.5036363372931945	0.2493162161380909	0.2694011365407931
3984	0.5011126880428094	0.7494371607125672	0.2690430971953006
3985	0.2500000000000000	0.2489049699003516	0.2773664996741303
3986			
3987	Pure-Ni 220 Facet with Hydrogen supercell 2X2X1 - [Etot = -287.67028384 eV]		

3988	1.01798110552312		
3989	7.0900001526000000	0.0000000000000000	0.0000000000000000
3990	0.0000000000000000	10.0268001556000002	0.0000000000000000
3991	0.0000000000000000	0.0000000000000000	27.5200996398999997
3992	Ni H		
3993	56 1		
3994	Direct		
3995	0.0000000000000000	0.2500000000000000	0.0000000000000000
3996	0.0000000000000000	0.7500000000000000	0.0000000000000000
3997	0.5000000000000000	0.2500000000000000	0.0000000000000000
3998	0.5000000000000000	0.7500000000000000	0.0000000000000000
3999	0.0000000000000000	0.0000000000000000	0.09109000099999978
4000	0.0000000000000000	0.5000000000000000	0.09109000099999978
4001	0.5000000000000000	0.0000000000000000	0.09109000099999978
4002	0.5000000000000000	0.5000000000000000	0.09109000099999978
4003	0.0008991177178714	0.2507991071860403	0.1754344046120906
4004	0.0008872333011567	0.7507967164746034	0.1753952294668366
4005	0.4991008822821286	0.2507991071860403	0.1754344046120906
4006	0.4991127666988433	0.7507967164746034	0.1753952294668366
4007	0.9980049312911703	0.0013191283712075	0.2603704729862812
4008	0.9995473013997227	0.5013820443035470	0.2601017439740616
4009	0.5019950687088297	0.0013191283712075	0.2603704729862812
4010	0.5004526986002773	0.5013820443035470	0.2601017439740616
4011	0.0000000000000000	0.0000000000000000	0.0000000000000000
4012	0.0000000000000000	0.5000000000000000	0.0000000000000000
4013	0.5000000000000000	0.0000000000000000	0.0000000000000000
4014	0.5000000000000000	0.5000000000000000	0.0000000000000000
4015	0.2500000000000000	0.1250000000000000	0.04554000099999991
4016	0.2500000000000000	0.6250000000000000	0.04554000099999991
4017	0.7500000000000000	0.1250000000000000	0.04554000099999991
4018	0.7500000000000000	0.6250000000000000	0.04554000099999991
4019	0.2500000000000000	0.3750000000000000	0.04554000099999991
4020	0.2500000000000000	0.8750000000000000	0.04554000099999991
4021	0.7500000000000000	0.3750000000000000	0.04554000099999991
4022	0.7500000000000000	0.8750000000000000	0.04554000099999991
4023	0.0000409459785686	0.2500640399471550	0.0877854006564078
4024	0.0000315011019651	0.7501648685496392	0.0877728418780990
4025	0.4999590540214314	0.2500640399471550	0.0877854006564078
4026	0.4999684988980349	0.7501648685496392	0.0877728418780990
4027	0.2500000000000000	0.3749341507397617	0.1330885961682924
4028	0.2500000000000000	0.8754609432183429	0.1334055381534540
4029	0.7500000000000000	0.3751046394807602	0.1329866377897986
4030	0.7500000000000000	0.8747898362458386	0.1330942690561656
4031	0.2500000000000000	0.1255276974395159	0.1333830635404922
4032	0.2500000000000000	0.6260325972331344	0.1330369947723469
4033	0.7500000000000000	0.1261299769405184	0.1330781821714595
4034	0.7500000000000000	0.6258179693702814	0.1329737571702339
4035	0.9987908205870255	0.0008452025648111	0.1763348035357808
4036	0.0002043627052544	0.5008322378673142	0.1764483349105319
4037	0.5012091794129745	0.0008452025648111	0.1763348035357808
4038	0.4997956372947456	0.5008322378673142	0.1764483349105319
4039	0.2500000000000000	0.1278361755111845	0.2230633289886796

4040	0.2500000000000000	0.6262780083445634	0.2221362656732069
4041	0.7500000000000000	0.1260697424157797	0.2218353317329402
4042	0.7500000000000000	0.6258900347179903	0.2215874624188956
4043	0.2500000000000000	0.3761284225022195	0.2221858261676175
4044	0.2500000000000000	0.8747250199766299	0.2230564889331887
4045	0.7500000000000000	0.3766241534971186	0.2216234092413600
4046	0.7500000000000000	0.8762516956676407	0.2218687886108768
4047	0.9963295449584919	0.2537806296059699	0.2596080649182539
4048	0.9965337694441061	0.7488695079978953	0.2595724703621087
4049	0.5036704550415081	0.2537806296059699	0.2596080649182539
4050	0.5034662305558939	0.7488695079978953	0.2595724703621087
4051	0.2500000000000000	0.0018803017401936	0.2666742934591113

4052

4053 NiCu (25% Cu) 220 Facet with Hydrogen supercell 2X2X1 - [Etot = -262.44242067 eV]

4054 0.998485100048875

4055	7.0900001526000000	0.0000000000000000	0.0000000000000000
4056	0.0000000000000000	10.0268001556000002	0.0000000000000000
4057	0.0000000000000000	0.0000000000000000	27.5200996398999997

4058	Cu	Ni	H
4059	16	40	1

4060 Direct

4061	0.0000000000000000	0.2500000000000000	0.0000000000000000
4062	0.0000000000000000	0.7500000000000000	0.0000000000000000
4063	0.5000000000000000	0.2500000000000000	0.0000000000000000
4064	0.5000000000000000	0.7500000000000000	0.0000000000000000
4065	0.0000000000000000	0.0000000000000000	0.09109000099999978
4066	0.0000000000000000	0.5000000000000000	0.09109000099999978
4067	0.5000000000000000	0.0000000000000000	0.09109000099999978
4068	0.5000000000000000	0.5000000000000000	0.09109000099999978
4069	0.0005601668974862	0.2499790795158887	0.1812141746891882
4070	0.0005498037900935	0.7499572785851640	0.1810931538614966
4071	0.4994398331025138	0.2499790795158887	0.1812141746891882
4072	0.4994501962099065	0.7499572785851640	0.1810931538614966
4073	0.9952467663673445	0.9988085274751199	0.2730422560834782
4074	0.9954942793702557	0.5010767691635820	0.2730435752126610
4075	0.5047532336326555	0.9988085274751199	0.2730422560834782
4076	0.5045057206297443	0.5010767691635820	0.2730435752126610
4077	0.0000000000000000	0.0000000000000000	0.0000000000000000
4078	0.0000000000000000	0.5000000000000000	0.0000000000000000
4079	0.5000000000000000	0.0000000000000000	0.0000000000000000
4080	0.5000000000000000	0.5000000000000000	0.0000000000000000
4081	0.2500000000000000	0.1250000000000000	0.04554000099999991
4082	0.2500000000000000	0.6250000000000000	0.04554000099999991
4083	0.7500000000000000	0.1250000000000000	0.04554000099999991
4084	0.7500000000000000	0.6250000000000000	0.04554000099999991
4085	0.2500000000000000	0.3750000000000000	0.04554000099999991
4086	0.2500000000000000	0.8750000000000000	0.04554000099999991
4087	0.7500000000000000	0.3750000000000000	0.04554000099999991
4088	0.7500000000000000	0.8750000000000000	0.04554000099999991
4089	0.0001170622223086	0.2500134931016262	0.0905554439745586
4090	0.9999019469203816	0.7499908839658715	0.0904923688397758
4091	0.4998829377776914	0.2500134931016262	0.0905554439745586

4092	0.5000980530796184	0.7499908839658715	0.0904923688397758
4093	0.2500000000000000	0.3752993844733439	0.1369485105878212
4094	0.2500000000000000	0.8751823150231601	0.1366557886368369
4095	0.7500000000000000	0.3754150913853138	0.1366859538395815
4096	0.7500000000000000	0.8754089134167344	0.1366428012583043
4097	0.2500000000000000	0.1246490323278238	0.1369500519386975
4098	0.2500000000000000	0.6246917012366637	0.1366648890222564
4099	0.7500000000000000	0.1246458009332372	0.1366505730662340
4100	0.7500000000000000	0.6246700205274465	0.1366481388646008
4101	0.0014786152491340	0.9998683101714718	0.1824820088054864
4102	0.0013638845698054	0.5000652985376206	0.1825008200934377
4103	0.4985213847508660	0.9998683101714718	0.1824820088054864
4104	0.4986361154301946	0.5000652985376206	0.1825008200934377
4105	0.2500000000000000	0.1242003745486144	0.2301225174738164
4106	0.2500000000000000	0.6255266551585947	0.2290287289865489
4107	0.7500000000000000	0.1249139609684633	0.2278399075827906
4108	0.7500000000000000	0.6258836124865823	0.2282001414667292
4109	0.2500000000000000	0.3756893362927514	0.2300904428474837
4110	0.2500000000000000	0.8744156099539566	0.2290441172242126
4111	0.7500000000000000	0.3749713684390912	0.2279089767128397
4112	0.7500000000000000	0.8740210847947694	0.2281571097804189
4113	0.9941091978528078	0.2499018881870683	0.2700943655502357
4114	0.9990505689725424	0.7499728733103836	0.2695841188470638
4115	0.5058908021471922	0.2499018881870683	0.2700943655502357
4116	0.5009494310274576	0.7499728733103836	0.2695841188470638
4117	0.2500000000000000	0.2500897576940133	0.2749442492994660
4118			

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

4120	1.01038006037737		
4121	7.0900001526000000	0.0000000000000000	0.0000000000000000
4122	0.0000000000000000	10.0268001556000002	0.0000000000000000
4123	0.0000000000000000	0.0000000000000000	27.5200996398999997
4124	Zn Ni H		
4125	16 40 1		
4126	Direct		
4127	0.0000000000000000	0.2500000000000000	0.0000000000000000
4128	0.0000000000000000	0.7500000000000000	0.0000000000000000
4129	0.5000000000000000	0.2500000000000000	0.0000000000000000
4130	0.5000000000000000	0.7500000000000000	0.0000000000000000
4131	0.0000000000000000	0.0000000000000000	0.0910900009999978
4132	0.0000000000000000	0.5000000000000000	0.0910900009999978
4133	0.5000000000000000	0.0000000000000000	0.0910900009999978
4134	0.5000000000000000	0.5000000000000000	0.0910900009999978
4135	0.0011414362837030	0.2491746221190638	0.1809814757180845
4136	0.0002961669669546	0.7491322040834092	0.1806356730141232
4137	0.4988585637162970	0.2491746221190638	0.1809814757180845
4138	0.4997038330330454	0.7491322040834092	0.1806356730141232
4139	0.9961826207250510	0.9974177986355812	0.2734578728747223
4140	0.9964308260096146	0.4995888269453914	0.2734526928970737
4141	0.5038173792749490	0.9974177986355812	0.2734578728747223
4142	0.5035691739903854	0.4995888269453914	0.2734526928970737
4143	0.0000000000000000	0.0000000000000000	0.0000000000000000

4144	0.0000000000000000	0.5000000000000000	0.0000000000000000
4145	0.5000000000000000	0.0000000000000000	0.0000000000000000
4146	0.5000000000000000	0.5000000000000000	0.0000000000000000
4147	0.2500000000000000	0.1250000000000000	0.0455400009999991
4148	0.2500000000000000	0.6250000000000000	0.0455400009999991
4149	0.7500000000000000	0.1250000000000000	0.0455400009999991
4150	0.7500000000000000	0.6250000000000000	0.0455400009999991
4151	0.2500000000000000	0.3750000000000000	0.0455400009999991
4152	0.2500000000000000	0.8750000000000000	0.0455400009999991
4153	0.7500000000000000	0.3750000000000000	0.0455400009999991
4154	0.7500000000000000	0.8750000000000000	0.0455400009999991
4155	0.9999818553892581	0.2498864504379910	0.0909208461749387
4156	0.9997976834624609	0.7498909564137364	0.0907777360590671
4157	0.5000181446107419	0.2498864504379910	0.0909208461749387
4158	0.5002023165375391	0.7498909564137364	0.0907777360590671
4159	0.2500000000000000	0.3749962328761356	0.1367883982900935
4160	0.2500000000000000	0.8749027254900739	0.1364610018954693
4161	0.7500000000000000	0.3747836432560447	0.1365690591953452
4162	0.7500000000000000	0.8751124851373149	0.1363716655234626
4163	0.2500000000000000	0.1239646296146972	0.1368331943556029
4164	0.2500000000000000	0.6241134700410100	0.1364765280787239
4165	0.7500000000000000	0.1242201745669362	0.1365767378403149
4166	0.7500000000000000	0.6239469987608715	0.1364077730813378
4167	0.0012571608287004	0.9990170097217046	0.1820187990127948
4168	0.0012513705563109	0.4991605201882052	0.1820284771642662
4169	0.4987428391712996	0.9990170097217046	0.1820187990127948
4170	0.4987486294436891	0.4991605201882052	0.1820284771642662
4171	0.2500000000000000	0.1215448162650716	0.2299922391003264
4172	0.2500000000000000	0.6232813639345522	0.2283380166196238
4173	0.7500000000000000	0.1220222264653898	0.2275463440487115
4174	0.7500000000000000	0.6233350359229775	0.2276546988009045
4175	0.2500000000000000	0.3757183991158470	0.2299579351762020
4176	0.2500000000000000	0.8741389084760840	0.2283357806315038
4177	0.7500000000000000	0.3753872693380345	0.2276044020375565
4178	0.7500000000000000	0.8740378002908145	0.2276371714741572
4179	0.9938564149627140	0.2484794869604130	0.2689702725658449
4180	0.9988257730730226	0.7485032063356272	0.2685214252010439
4181	0.5061435850372860	0.2484794869604130	0.2689702725658449
4182	0.5011742269269774	0.7485032063356272	0.2685214252010439
4183	0.2500000000000000	0.2484857860653449	0.2724180490908168
4184			
4185	NiCo (25% Co) 111 Facet with OH supercell 2X2X1 - [Etot = -458.05295eV]		
4186	0.993794164815303		
4187	10.0268001556000002	0.0000000000000000	0.0000000000000000
4188	-5.0134000778000001	8.6834636535000005	0.0000000000000000
4189	0.0000000000000000	0.0000000000000000	28.1868000031000001
4190	Co Ni O H		
4191	20 60 1 1		
4192	Direct		
4193	0.1666650029999985	0.3333350119999992	0.0000000000000000
4194	0.1666650029999985	0.8333350420000016	0.0000000000000000
4195	0.6666650180000033	0.3333350119999992	0.0000000000000000

4196	0.6666650180000033	0.8333350420000016	0.0000000000000000
4197	0.0000000000000000	0.0000000000000000	0.0726099979999972
4198	0.0000000000000000	0.5000000000000000	0.0726099979999972
4199	0.5000000000000000	0.0000000000000000	0.0726099979999972
4200	0.5000000000000000	0.5000000000000000	0.0726099979999972
4201	0.3335879071261658	0.1670303600464962	0.1447805994397271
4202	0.3334161797083439	0.6665971105573902	0.1452423986869817
4203	0.8333786486886510	0.1666283961079245	0.1447079377571114
4204	0.8329876557647111	0.6664238869960073	0.1447796141364677
4205	0.1672605113241517	0.3346258950455976	0.2197373562535532
4206	0.1667342572253148	0.8332879057402920	0.2186660245375691
4207	0.6666340964298385	0.3334128168767094	0.2190005550488792
4208	0.6654153173558015	0.8327813017434238	0.2197273979867305
4209	0.9984163415560303	0.4995673932333133	0.2883792485927614
4210	0.0000468401786691	0.0000047127815179	0.2884190499011297
4211	0.5044643741418113	0.4955991357104850	0.2916265735617785
4212	0.5004916842763194	0.0016390542863860	0.2883749528592219
4213	0.1666650029999985	0.0833349970000015	0.0000000000000000
4214	0.1666650029999985	0.5833349819999967	0.0000000000000000
4215	0.6666650180000033	0.0833349970000015	0.0000000000000000
4216	0.6666650180000033	0.5833349819999967	0.0000000000000000
4217	0.4166649880000008	0.0833349970000015	0.0000000000000000
4218	0.4166649880000008	0.5833349819999967	0.0000000000000000
4219	0.9166649579999984	0.0833349970000015	0.0000000000000000
4220	0.9166649579999984	0.5833349819999967	0.0000000000000000
4221	0.4166649880000008	0.3333350119999992	0.0000000000000000
4222	0.4166649880000008	0.8333350420000016	0.0000000000000000
4223	0.9166649579999984	0.3333350119999992	0.0000000000000000
4224	0.9166649579999984	0.8333350420000016	0.0000000000000000
4225	0.0000000000000000	0.2500000000000000	0.0726099979999972
4226	0.0000000000000000	0.7500000000000000	0.0726099979999972
4227	0.5000000000000000	0.2500000000000000	0.0726099979999972
4228	0.5000000000000000	0.7500000000000000	0.0726099979999972
4229	0.2500000000000000	0.2500000000000000	0.0726099979999972
4230	0.2500000000000000	0.7500000000000000	0.0726099979999972
4231	0.7500000000000000	0.2500000000000000	0.0726099979999972
4232	0.7500000000000000	0.7500000000000000	0.0726099979999972
4233	0.2500000000000000	0.0000000000000000	0.0726099979999972
4234	0.2500000000000000	0.5000000000000000	0.0726099979999972
4235	0.7500000000000000	0.0000000000000000	0.0726099979999972
4236	0.7500000000000000	0.5000000000000000	0.0726099979999972
4237	0.3330875818648025	0.4165458152106325	0.1453166880310732
4238	0.3331888633454412	0.9162744616059726	0.1451542400134613
4239	0.8330937784614107	0.4165585359003643	0.1450202109862744
4240	0.8329160687951997	0.9165887614678994	0.1450797710799208
4241	0.0835889294058845	0.4166008968465178	0.1450906480582788
4242	0.0834290865579490	0.9165934674011851	0.1449563550389286
4243	0.5833999779305685	0.4166216702756955	0.1450905729154357
4244	0.5834130600274037	0.9164296876483675	0.1450882315766009
4245	0.0834320582813888	0.1671065860831931	0.1450814589752056
4246	0.0837478130089977	0.6668294035311888	0.1451560104026086
4247	0.5834541572503937	0.1669248377898640	0.1450198682868447

4248	0.5834668289827007	0.6669310256733212	0.1453148687512567
4249	0.1669224963945339	0.0835790333546882	0.2167493049753517
4250	0.1672527935478811	0.5817671771172073	0.2177879659870428
4251	0.6669543712631381	0.0836351860504863	0.2170560600861791
4252	0.6658641435000732	0.5832714414053157	0.2175286158125900
4253	0.4164025792984489	0.0832318068842923	0.2169767477929341
4254	0.4170724300191111	0.5829668457792323	0.2176474962054442
4255	0.9166062499063159	0.0834354143589806	0.2170092009924645
4256	0.9168088860256987	0.5836341529864768	0.2169775119136617
4257	0.4167684575890362	0.3341734789359805	0.2175325164503548
4258	0.4182691540068788	0.8327848348167350	0.2177814726138152
4259	0.9163996524511901	0.3330794906124979	0.2170596194698078
4260	0.9164619980096234	0.8331119078903626	0.2167473554838040
4261	0.9989026970385879	0.2490345380739214	0.2887078370822991
4262	0.0007876982979553	0.7505030609232435	0.2885760507365092
4263	0.5012883636658927	0.2495912116935841	0.2886566010953899
4264	0.5013365653489359	0.7562213548388357	0.2914911045634625
4265	0.2470181731004004	0.2457193317394086	0.2881296028341680
4266	0.2468578145988758	0.7531964152518640	0.2881982506720533
4267	0.7497025375109132	0.2503541781617002	0.2889275208873556
4268	0.7543420803222460	0.7530425156061966	0.2881237077253260
4269	0.2438455743695158	0.4987192626197725	0.2915073965658337
4270	0.2495581305349788	0.9992700251164806	0.2885776035538470
4271	0.7504632186620483	0.4987710278735165	0.2886541268985496
4272	0.7510291216293510	0.0011607386220120	0.2887025948528006
4273	0.4186808833885109	0.5814758039953105	0.3383530814900482
4274	0.4196559890778531	0.5807856531970472	0.3730952250208759
4275			
4276	NiCr (25% Cr) 111 Facet with OH supercell 2X2X1 - [Etot = -506.76655eV]		
4277	0.995572721824907		
4278	10.0268001556000002	0.0000000000000000	0.0000000000000000
4279	-5.0134000778000001	8.6834636535000005	0.0000000000000000
4280	0.0000000000000000	0.0000000000000000	28.1868000031000001
4281	Cr Ni O H		
4282	20 60 1 1		
4283	Direct		
4284	0.1666650029999985	0.3333350119999992	0.0000000000000000
4285	0.1666650029999985	0.8333350420000016	0.0000000000000000
4286	0.6666650180000033	0.3333350119999992	0.0000000000000000
4287	0.6666650180000033	0.8333350420000016	0.0000000000000000
4288	0.0000000000000000	0.0000000000000000	0.0726099979999972
4289	0.0000000000000000	0.5000000000000000	0.0726099979999972
4290	0.5000000000000000	0.0000000000000000	0.0726099979999972
4291	0.5000000000000000	0.5000000000000000	0.0726099979999972
4292	0.3333692873797816	0.1663596557447207	0.1450904693645114
4293	0.3335718615307570	0.6663436559393006	0.1456462499225424
4294	0.8333472406599753	0.1665589825240446	0.1450849261798695
4295	0.8335897010532278	0.6665707063925268	0.1450881022575530
4296	0.1663665569565111	0.3342589718879836	0.2217820030563900
4297	0.1665120964213784	0.8333708568276279	0.2214590073231761
4298	0.6660702379586141	0.3338185900616679	0.2216339647680101
4299	0.6655649565177768	0.8334722620634381	0.2218129762746202

4300	0.9986392502429737	0.4999014708745264	0.2914535133313265
4301	0.9996970014469255	0.0001451370093761	0.2918460539693086
4302	0.5031175960816725	0.4967461208370310	0.2945448402865054
4303	0.4999551389215426	0.0011866154086064	0.2914588698903273
4304	0.1666650029999985	0.0833349970000015	0.0000000000000000
4305	0.1666650029999985	0.5833349819999967	0.0000000000000000
4306	0.6666650180000033	0.0833349970000015	0.0000000000000000
4307	0.6666650180000033	0.5833349819999967	0.0000000000000000
4308	0.4166649880000008	0.0833349970000015	0.0000000000000000
4309	0.4166649880000008	0.5833349819999967	0.0000000000000000
4310	0.9166649579999984	0.0833349970000015	0.0000000000000000
4311	0.9166649579999984	0.5833349819999967	0.0000000000000000
4312	0.4166649880000008	0.3333350119999992	0.0000000000000000
4313	0.4166649880000008	0.8333350420000016	0.0000000000000000
4314	0.9166649579999984	0.3333350119999992	0.0000000000000000
4315	0.9166649579999984	0.8333350420000016	0.0000000000000000
4316	0.0000000000000000	0.2500000000000000	0.0726099979999972
4317	0.0000000000000000	0.7500000000000000	0.0726099979999972
4318	0.5000000000000000	0.2500000000000000	0.0726099979999972
4319	0.5000000000000000	0.7500000000000000	0.0726099979999972
4320	0.2500000000000000	0.2500000000000000	0.0726099979999972
4321	0.2500000000000000	0.7500000000000000	0.0726099979999972
4322	0.7500000000000000	0.2500000000000000	0.0726099979999972
4323	0.7500000000000000	0.7500000000000000	0.0726099979999972
4324	0.2500000000000000	0.0000000000000000	0.0726099979999972
4325	0.2500000000000000	0.5000000000000000	0.0726099979999972
4326	0.7500000000000000	0.0000000000000000	0.0726099979999972
4327	0.7500000000000000	0.5000000000000000	0.0726099979999972
4328	0.3327911831260693	0.4161948532215192	0.1458001224344088
4329	0.3328564256189210	0.9158739803618303	0.1458418459017850
4330	0.8327737616494844	0.4164370964841098	0.1455894650036953
4331	0.8329153920124028	0.9165504337946828	0.1453932858053975
4332	0.0835590506084785	0.4163364831929428	0.1456177303544806
4333	0.0836405406962086	0.9162939715447536	0.1455350878042481
4334	0.5834544077875137	0.4164606322615896	0.1458403765804661
4335	0.5835724938312126	0.9163515993255231	0.1456201941647919
4336	0.0833758600545096	0.1669973967427083	0.1453976458321975
4337	0.0840828655638362	0.6670835713483996	0.1458429086539823
4338	0.5835024125115922	0.1671622053309534	0.1455914046601308
4339	0.5837546087711374	0.6671507419942060	0.1458010099131286
4340	0.1665906105345911	0.0831929058364480	0.2171934379141405
4341	0.1668622439184020	0.5819660760685466	0.2183237037644048
4342	0.6669367560534880	0.0840854881659965	0.2174991163264437
4343	0.6663480846555743	0.5834290942543419	0.2180887299371008
4344	0.4165698001659521	0.0834551926861096	0.2176041057976477
4345	0.4172297974073160	0.5826617612247418	0.2183301847896217
4346	0.9166197730527017	0.0831721851930283	0.2174937755558091
4347	0.9164142678543357	0.5833195271250915	0.2176007858599220
4348	0.4164493427123475	0.3335136727155188	0.2180890810394587
4349	0.4178539487539155	0.8329657733477305	0.2183153456781781
4350	0.9157217303494107	0.3329018548903093	0.2174942730435205
4351	0.9166573167017447	0.8332712393871162	0.2171875127094154

4352	0.9991061528751572	0.2497368114021938	0.2900957022841624
4353	0.0011205329508215	0.7512887042703866	0.2903498005520007
4354	0.5010857045960577	0.2508253375844305	0.2906186910603736
4355	0.5000273418890160	0.7533720900714655	0.2926319673605562
4356	0.2472683533051381	0.2466889969904145	0.2892397089947920
4357	0.2465520351900281	0.7533138623235871	0.2897856953329239
4358	0.7487886431751036	0.2510424490240695	0.2904876885755954
4359	0.7531587729814149	0.7525733195065740	0.2892566491677186
4360	0.2464557953370274	0.4998803110081980	0.2926079826306207
4361	0.2486007385674611	0.9987502815738267	0.2903552832409773
4362	0.7490330810935362	0.4987916293286787	0.2906230621445545
4363	0.7501078576515283	0.0007160849526002	0.2901189153781516
4364	0.4202490712425515	0.5789113618114499	0.3412064539694413
4365	0.4211042016766910	0.5766364017244712	0.3758988680640130
4366			
4367	NiCu (25% Cu) 111 Facet with OH supercell 2X2X1 - [Etot = -391.57869eV]		
4368	0.998485100048875		
4369	10.0268001556000002	0.0000000000000000	0.0000000000000000
4370	-5.0134000778000001	8.6834636535000005	0.0000000000000000
4371	0.0000000000000000	0.0000000000000000	28.1868000031000001
4372	Cu Ni O H		
4373	20 60 1 1		
4374	Direct		
4375	0.1666650029999985	0.3333350119999992	0.0000000000000000
4376	0.1666650029999985	0.8333350420000016	0.0000000000000000
4377	0.6666650180000033	0.3333350119999992	0.0000000000000000
4378	0.6666650180000033	0.8333350420000016	0.0000000000000000
4379	0.0000000000000000	0.0000000000000000	0.0726099979999972
4380	0.0000000000000000	0.5000000000000000	0.0726099979999972
4381	0.5000000000000000	0.0000000000000000	0.0726099979999972
4382	0.5000000000000000	0.5000000000000000	0.0726099979999972
4383	0.3332084363430354	0.1667212787196419	0.1454578270304054
4384	0.3333252530012061	0.6669138278614497	0.1457367121403905
4385	0.8332698227838762	0.1669636235457617	0.1455972018116185
4386	0.8335345220705719	0.6670384877997151	0.1454533598402605
4387	0.1678219901619116	0.3360704895161177	0.2183382006483825
4388	0.1664692553247988	0.8339577516287449	0.2164486033404174
4389	0.6667953502827473	0.3336407028949679	0.2170547608750582
4390	0.6643901889634094	0.8326443769504337	0.2183319286729457
4391	0.9987796079846092	0.4998542353508810	0.2925059327730040
4392	0.0001479131960238	0.0003581122376417	0.2929952535110374
4393	0.5037061732778412	0.4968236210648271	0.2911685592714832
4394	0.5006566243838151	0.0017295142152847	0.2925009725340146
4395	0.1666650029999985	0.0833349970000015	0.0000000000000000
4396	0.1666650029999985	0.5833349819999967	0.0000000000000000
4397	0.6666650180000033	0.0833349970000015	0.0000000000000000
4398	0.6666650180000033	0.5833349819999967	0.0000000000000000
4399	0.4166649880000008	0.0833349970000015	0.0000000000000000
4400	0.4166649880000008	0.5833349819999967	0.0000000000000000
4401	0.9166649579999984	0.0833349970000015	0.0000000000000000
4402	0.9166649579999984	0.5833349819999967	0.0000000000000000
4403	0.4166649880000008	0.3333350119999992	0.0000000000000000

4404	0.4166649880000008	0.8333350420000016	0.0000000000000000
4405	0.9166649579999984	0.3333350119999992	0.0000000000000000
4406	0.9166649579999984	0.8333350420000016	0.0000000000000000
4407	0.0000000000000000	0.2500000000000000	0.0726099979999972
4408	0.0000000000000000	0.7500000000000000	0.0726099979999972
4409	0.5000000000000000	0.2500000000000000	0.0726099979999972
4410	0.5000000000000000	0.7500000000000000	0.0726099979999972
4411	0.2500000000000000	0.2500000000000000	0.0726099979999972
4412	0.2500000000000000	0.7500000000000000	0.0726099979999972
4413	0.7500000000000000	0.2500000000000000	0.0726099979999972
4414	0.7500000000000000	0.7500000000000000	0.0726099979999972
4415	0.2500000000000000	0.0000000000000000	0.0726099979999972
4416	0.2500000000000000	0.5000000000000000	0.0726099979999972
4417	0.7500000000000000	0.0000000000000000	0.0726099979999972
4418	0.7500000000000000	0.5000000000000000	0.0726099979999972
4419	0.3332794326558428	0.4170984091256997	0.1454043191308330
4420	0.3338963316251480	0.9168960024329280	0.1450518086799590
4421	0.8336018316766456	0.4170285241695808	0.1451169117491773
4422	0.8330042673260678	0.9170485166227351	0.1454022698593391
4423	0.0834168472211303	0.4168618880319457	0.1453254659327712
4424	0.0829089100243152	0.9173487017757793	0.1450169037516673
4425	0.5832838095218804	0.4169666594283257	0.1450385041202509
4426	0.5833502484557584	0.9167916778195959	0.1453288229181808
4427	0.0831858206518277	0.1672364881378314	0.1454044934271579
4428	0.0833555700417890	0.6663629778184799	0.1450554175790799
4429	0.5832308860983844	0.1666413199001440	0.1451205238306486
4430	0.5831413316371084	0.6669671281653606	0.1454066999927548
4431	0.1651915180103742	0.0834463407960939	0.2180430237750102
4432	0.1666582810500898	0.5830008688428521	0.2186786948846944
4433	0.6654635161745688	0.0829584321545269	0.2182775671881956
4434	0.6663107200207605	0.5836280117864092	0.2178775018946837
4435	0.4169339068470279	0.0827271828588039	0.2180924328801694
4436	0.4167440923579804	0.5836936897745630	0.2186297726236077
4437	0.9171181580733574	0.0833497124205209	0.2184217093088208
4438	0.9177000870054783	0.5835119975604997	0.2181003726737814
4439	0.4168387958456350	0.3341633767130503	0.2178813101178463
4440	0.4174376642220565	0.8337838464421807	0.2186777866655447
4441	0.9174956861307066	0.3349834136610994	0.2182692522829015
4442	0.9169931946365750	0.8352319329841436	0.2180391179927739
4443	0.9990805455296083	0.2493536256712972	0.2890447703142556
4444	0.9992341034024435	0.7505170825395524	0.2886911852810101
4445	0.5000781697293277	0.2487671011404302	0.2888662188932472
4446	0.5030165677575837	0.7527424335779713	0.2932550403717826
4447	0.2500017203257130	0.2471729411891914	0.2887133392350094
4448	0.2465278054735762	0.7539805977161933	0.2878928840709989
4449	0.7505292686323912	0.2499753999966288	0.2890969273117960
4450	0.7533619188454139	0.7505163044769887	0.2887087129232100
4451	0.2477605927072801	0.4975176613845136	0.2932656502880135
4452	0.2499717550168441	0.0012853714171825	0.2886839071258578
4453	0.7517477646883037	0.5004224725054840	0.2888658556545991
4454	0.7511665900786397	0.0014241317886743	0.2890501946144468
4455	0.3751077801762221	0.6254749383274145	0.3446732444092007

4456	0.3293880388768287	0.6714426979942800	0.3649075433239517
4457			
4458	NiMn (25% Mn) 111 Facet with OH supercell 2X2X1 - [Etot = -504.68025eV]		
4459	1.000000000000000		
4460	9.9196901320999995	0.0000000000000000	0.0000000000000000
4461	-4.9598426818999997	8.5906995225999996	0.0000000000000000
4462	0.0000000000000000	0.0000000000000000	27.8856849669999995
4463	Mn Ni O H		
4464	20 60 1 1		
4465	Direct		
4466	0.1666650029999985	0.3333350119999992	0.0000000000000000
4467	0.1666650029999985	0.8333350420000016	0.0000000000000000
4468	0.6666650180000033	0.3333350119999992	0.0000000000000000
4469	0.6666650180000033	0.8333350420000016	0.0000000000000000
4470	0.0000000000000000	0.0000000000000000	0.0726099979999972
4471	0.0000000000000000	0.5000000000000000	0.0726099979999972
4472	0.5000000000000000	0.0000000000000000	0.0726099979999972
4473	0.5000000000000000	0.5000000000000000	0.0726099979999972
4474	0.3332810206436960	0.1666637144775081	0.1474471141338469
4475	0.3332782666197502	0.6665429695370690	0.1474564110985739
4476	0.8333991997902288	0.1666630366862947	0.1474524703260869
4477	0.8333169859078140	0.6666104628616480	0.1472255818401749
4478	0.1666396354661757	0.3332409293663900	0.2219383829185730
4479	0.1664115269902737	0.8331258781891009	0.2211689376316031
4480	0.6667581820308399	0.3334712644966729	0.2211726145110262
4481	0.6667507436587599	0.8331326955333580	0.2211708905470360
4482	0.5040951514294818	0.5019442543587260	0.2973182429082684
4483	0.4999695617142734	0.9998815024406724	0.2990854455834722
4484	0.9979044127035195	0.5019410457486302	0.2973281966225798
4485	0.9979116131218717	0.9957602303288482	0.2973009453725197
4486	0.1666650029999985	0.0833349970000015	0.0000000000000000
4487	0.1666650029999985	0.5833349819999967	0.0000000000000000
4488	0.6666650180000033	0.0833349970000015	0.0000000000000000
4489	0.6666650180000033	0.5833349819999967	0.0000000000000000
4490	0.0000000000000000	0.2500000000000000	0.0726099979999972
4491	0.0000000000000000	0.7500000000000000	0.0726099979999972
4492	0.5000000000000000	0.2500000000000000	0.0726099979999972
4493	0.5000000000000000	0.7500000000000000	0.0726099979999972
4494	0.4166649880000008	0.0833349970000015	0.0000000000000000
4495	0.4166649880000008	0.5833349819999967	0.0000000000000000
4496	0.9166649579999984	0.0833349970000015	0.0000000000000000
4497	0.9166649579999984	0.5833349819999967	0.0000000000000000
4498	0.2500000000000000	0.2500000000000000	0.0726099979999972
4499	0.2500000000000000	0.7500000000000000	0.0726099979999972
4500	0.7500000000000000	0.2500000000000000	0.0726099979999972
4501	0.7500000000000000	0.7500000000000000	0.0726099979999972
4502	0.4166649880000008	0.3333350119999992	0.0000000000000000
4503	0.4166649880000008	0.8333350420000016	0.0000000000000000
4504	0.9166649579999984	0.3333350119999992	0.0000000000000000
4505	0.9166649579999984	0.8333350420000016	0.0000000000000000
4506	0.2500000000000000	0.0000000000000000	0.0726099979999972
4507	0.2500000000000000	0.5000000000000000	0.0726099979999972

4508	0.7500000000000000	0.0000000000000000	0.0726099979999972
4509	0.7500000000000000	0.5000000000000000	0.0726099979999972
4510	0.3334108377772154	0.4166730952653097	0.1473062413878878
4511	0.3333494980898735	0.9166428056922413	0.1470021299777926
4512	0.8334548862981634	0.4165212761638273	0.1470339150483184
4513	0.8334569389551731	0.9168511049625394	0.1470307656084699
4514	0.1666510557475647	0.0840190760320851	0.2220965249266484
4515	0.1666505135403256	0.5824582678704786	0.2221184010856945
4516	0.6653679530784729	0.0826141340050626	0.2214968883914636
4517	0.6656093812863304	0.5827309504700082	0.2212558542958050
4518	0.5008126771329131	0.2489528602803617	0.2942379645416580
4519	0.5008009708456456	0.7516682040928657	0.2942376734341465
4520	0.9956292995752278	0.2477016271821029	0.2974025750819109
4521	0.9998879002245431	0.7498449037595236	0.2941707800398916
4522	0.0832717760376696	0.4166705373216502	0.1473088122325095
4523	0.0834083609549481	0.9168493009209513	0.1470290554441789
4524	0.5830902210377360	0.4165269950779518	0.1470316377337610
4525	0.5833083640933339	0.9166456976078123	0.1470035214618335
4526	0.4172824936103581	0.0826134437556689	0.2214932071412505
4527	0.4158443639989216	0.5824660809323987	0.2221151681800677
4528	0.9174068816854515	0.0840256872801106	0.2221047493845845
4529	0.9171593671570477	0.5827276202497700	0.2212592656708523
4530	0.2521449206031576	0.2476828308272445	0.2973712860524600
4531	0.2509060901714051	0.7516605521975279	0.2942379267053568
4532	0.7482043216061456	0.2489576968735676	0.2942433705611904
4533	0.7500144986070651	0.7498506585510114	0.2941710927087513
4534	0.0832738124474588	0.1665383624567198	0.1473053679849201
4535	0.0834111977262140	0.6664723346860981	0.1470336363355784
4536	0.5833017854590921	0.1665855039685482	0.1470037061344271
4537	0.5830799163454188	0.6664760505545644	0.1470335416049267
4538	0.4158511571622299	0.3332290052713418	0.2221032670133170
4539	0.4172764875701418	0.8345186520567580	0.2214948168152091
4540	0.9174215951060418	0.3332242109370682	0.2221167835313693
4541	0.9171565089416518	0.8342723849278144	0.2212491400290162
4542	0.2509233316773205	0.9990497722809195	0.2942310868824265
4543	0.2521447659464542	0.5042325909205090	0.2974216210421545
4544	0.7481868669370826	0.9990602113069755	0.2942369721100491
4545	0.7500053974188319	0.4999799288978153	0.2941731223703101
4546	0.1666771834942935	0.3330220186817954	0.3453716488248730
4547	0.1666757037428042	0.3325286048142289	0.3802666621488768
4548			
4549	Pure Ni 111 Facet with OH supercell 2X2X1 - [Etot = -424.99061eV]		
4550	1.01798110552312		
4551	10.0268001556000002	0.0000000000000000	0.0000000000000000
4552	-5.0134000778000001	8.6834636535000005	0.0000000000000000
4553	0.0000000000000000	0.0000000000000000	28.1868000031000001
4554	Ni O H		
4555	80 1 1		
4556	Direct		
4557	0.1666650029999985	0.3333350119999992	0.0000000000000000
4558	0.1666650029999985	0.8333350420000016	0.0000000000000000
4559	0.6666650180000033	0.3333350119999992	0.0000000000000000

4560	0.6666650180000033	0.8333350420000016	0.0000000000000000
4561	0.0000000000000000	0.0000000000000000	0.0726099979999972
4562	0.0000000000000000	0.5000000000000000	0.0726099979999972
4563	0.5000000000000000	0.0000000000000000	0.0726099979999972
4564	0.5000000000000000	0.5000000000000000	0.0726099979999972
4565	0.3331978192353446	0.1668043909385020	0.1420796484226514
4566	0.3331957649151107	0.6663694313217903	0.1420819451841027
4567	0.8336372388023747	0.1668095636335352	0.1420822518903719
4568	0.8333454179321507	0.6666612825324165	0.1419838415992487
4569	0.1666890915227270	0.3333226281427528	0.2118297984514044
4570	0.1665408936304473	0.8332478925045166	0.2114757405024932
4571	0.6667626430043043	0.3334645218721235	0.2114752003967126
4572	0.6667529466151549	0.8332587841524415	0.2114760042963937
4573	0.9968720197625203	0.5031352373767959	0.2795372009096582
4574	0.9968657710158908	0.9936818742259135	0.2795339877202991
4575	0.5063339916988241	0.5031476081172030	0.2795333696346063
4576	0.5000252529250133	0.9999886512241147	0.2803341681946208
4577	0.1666650029999985	0.0833349970000015	0.0000000000000000
4578	0.1666650029999985	0.5833349819999967	0.0000000000000000
4579	0.6666650180000033	0.0833349970000015	0.0000000000000000
4580	0.6666650180000033	0.5833349819999967	0.0000000000000000
4581	0.4166649880000008	0.0833349970000015	0.0000000000000000
4582	0.4166649880000008	0.5833349819999967	0.0000000000000000
4583	0.9166649579999984	0.0833349970000015	0.0000000000000000
4584	0.9166649579999984	0.5833349819999967	0.0000000000000000
4585	0.4166649880000008	0.3333350119999992	0.0000000000000000
4586	0.4166649880000008	0.8333350420000016	0.0000000000000000
4587	0.9166649579999984	0.3333350119999992	0.0000000000000000
4588	0.9166649579999984	0.8333350420000016	0.0000000000000000
4589	0.0000000000000000	0.2500000000000000	0.0726099979999972
4590	0.0000000000000000	0.7500000000000000	0.0726099979999972
4591	0.5000000000000000	0.2500000000000000	0.0726099979999972
4592	0.5000000000000000	0.7500000000000000	0.0726099979999972
4593	0.2500000000000000	0.2500000000000000	0.0726099979999972
4594	0.2500000000000000	0.7500000000000000	0.0726099979999972
4595	0.7500000000000000	0.2500000000000000	0.0726099979999972
4596	0.7500000000000000	0.7500000000000000	0.0726099979999972
4597	0.2500000000000000	0.0000000000000000	0.0726099979999972
4598	0.2500000000000000	0.5000000000000000	0.0726099979999972
4599	0.7500000000000000	0.0000000000000000	0.0726099979999972
4600	0.7500000000000000	0.5000000000000000	0.0726099979999972
4601	0.3336270681535680	0.4168028586862889	0.1422125958657077
4602	0.3333834772816502	0.9166803867426268	0.1419415280847645
4603	0.8332324905799240	0.4164045910411005	0.1419417227104205
4604	0.8332237286750726	0.9168063898835968	0.1419429579639342
4605	0.0832008633000640	0.4168039887684145	0.1422121427498979
4606	0.0835967433714515	0.9168022510227942	0.1419403861178523
4607	0.5832048022710339	0.4164077364812044	0.1419404618711795
4608	0.5833225066952039	0.9166830234013901	0.1419431047841968
4609	0.0832008286192121	0.1663773063715368	0.1422126109650321
4610	0.0836001496502945	0.6667755788932155	0.1419416136531311
4611	0.5833259305271241	0.1666216965488090	0.1419416019911210

4612	0.5832000176716576	0.6667821180875819	0.1419425829468679
4613	0.1678502053668893	0.0850149041216781	0.2122503387177446
4614	0.1678466235648628	0.5827907160101375	0.2122548609236574
4615	0.6665595871003376	0.0832633859975473	0.2115560703233612
4616	0.6662569350511447	0.5831090847205687	0.2111404412869859
4617	0.4167487696595344	0.0832589361385772	0.2115541713124429
4618	0.4149915339639705	0.5827906805215690	0.2122538914797261
4619	0.9172186263293014	0.0850162931658147	0.2122551578183121
4620	0.9169036398496857	0.5831049658987908	0.2111417364869723
4621	0.4149978097377982	0.3321617507591910	0.2122498816623235
4622	0.4167468142190600	0.8334522111505720	0.2115556901165121
4623	0.9172227719207058	0.3321587388678751	0.2122563917858571
4624	0.9168996326247836	0.8337535278682253	0.2111405417208729
4625	0.9937729749984356	0.2468565766252837	0.2828507556583233
4626	0.9998241956158935	0.7498880991619217	0.2799303105706841
4627	0.5015530545299995	0.2493898858394630	0.2801108334008404
4628	0.5015506935694063	0.7521149627239012	0.2801166965261999
4629	0.2531615978364314	0.2468519339022492	0.2828366588008393
4630	0.2506137178680632	0.7521136429155391	0.2801166101732093
4631	0.7479050116553836	0.2493988947637291	0.2801170384785365
4632	0.7501230671593788	0.7498911916486790	0.2799294214378421
4633	0.2531590967669644	0.5062469690684566	0.2828470144063999
4634	0.2506218558863083	0.9984610217889625	0.2801113714383945
4635	0.7501252361770199	0.5001873371686543	0.2799301139355848
4636	0.7479019798082120	0.9984635376210491	0.2801174700170250
4637	0.1667434329099109	0.3333042060946809	0.3271159442361835
4638	0.1668634104475046	0.3332549480976752	0.3610473946072901

4639

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

4641 0.995572721824907

4642 7.0844001770000000 0.0000000000000000 0.0000000000000000

4643 0.0000000000000000 7.0844001770000000 0.0000000000000000

4644 0.0000000000000000 0.0000000000000000 27.0844993591000005

4645 Cr Ni O H

4646 12 28 1 1

4647 Direct

4648 0.0000000000000000 0.0000000000000000 0.0000000000000000

4649 0.0000000000000000 0.5000000000000000 0.0000000000000000

4650 0.5000000000000000 0.0000000000000000 0.0000000000000000

4651 0.5000000000000000 0.5000000000000000 0.0000000000000000

4652 0.0001828165512734 0.9998783065314640 0.1316201145476938

4653 0.0001833835819909 0.5001622154671566 0.1316129572063289

4654 0.4998728500480567 0.0005534001380951 0.1318010605297388

4655 0.4998689691657603 0.4994825384395796 0.1317995020356335

4656 0.9972302843988459 0.9867536898507794 0.2650608272811326

4657 0.9971541660491070 0.5133483560053875 0.2650555765233094

4658 0.4991975895527858 0.0144422195483784 0.2693028837869704

4659 0.4992912912400627 0.4856202229416908 0.2692828924203283

4660 0.2500000000000000 0.2500000000000000 0.0000000000000000

4661 0.2500000000000000 0.7500000000000000 0.0000000000000000

4662 0.7500000000000000 0.2500000000000000 0.0000000000000000

4663 0.7500000000000000 0.7500000000000000 0.0000000000000000

4664	0.0000000000000000	0.2500000000000000	0.0653899980000006
4665	0.0000000000000000	0.7500000000000000	0.0653899980000006
4666	0.5000000000000000	0.2500000000000000	0.0653899980000006
4667	0.5000000000000000	0.7500000000000000	0.0653899980000006
4668	0.2500000000000000	0.0000000000000000	0.0653899980000006
4669	0.2500000000000000	0.5000000000000000	0.0653899980000006
4670	0.7500000000000000	0.0000000000000000	0.0653899980000006
4671	0.7500000000000000	0.5000000000000000	0.0653899980000006
4672	0.2503464097121366	0.2499904747589170	0.1310589496711003
4673	0.2509596482517935	0.7500347781689172	0.1313804202886431
4674	0.7508392084051891	0.249996300421898	0.1311389666624478
4675	0.7486940735175338	0.7500285021448576	0.1314105623349278
4676	0.0033875391605989	0.2500312527027262	0.1961887824940973
4677	0.9994350998555035	0.7500336230445868	0.1967521635464067
4678	0.4996941687011258	0.2499948246349604	0.1968671026602777
4679	0.4990890468890186	0.7500365370339139	0.1980895708644610
4680	0.2506733450338459	0.0005915558835454	0.1973835291337807
4681	0.2506682796890445	0.4994437705474866	0.1973733226183612
4682	0.7484262186339592	0.9993353968342120	0.1971393740282110
4683	0.7483850947220887	0.5006908540692834	0.1971349879413324
4684	0.2251537991329045	0.2500968128520640	0.2625470428510752
4685	0.2576712556382930	0.7499682548108950	0.2601136452228943
4686	0.7684485048637342	0.2499978334007906	0.2586447029322940
4687	0.7386913068537311	0.7500238133867185	0.2606340820502595
4688	0.4366347931735390	0.2501172663532927	0.3124352450957062
4689	0.4063637054860578	0.2502123240385146	0.3477601987674745

4690
4691

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

4693	0.989317187668226		
4694	7.0844001770000000	0.0000000000000000	0.0000000000000000
4695	0.0000000000000000	7.0844001770000000	0.0000000000000000
4696	0.0000000000000000	0.0000000000000000	27.0844993591000005

4697 Mn Ni O H
4698 12 28 1 1

4699	Direct		
4700	0.0000000000000000	0.0000000000000000	0.0000000000000000
4701	0.0000000000000000	0.5000000000000000	0.0000000000000000
4702	0.5000000000000000	0.0000000000000000	0.0000000000000000
4703	0.5000000000000000	0.5000000000000000	0.0000000000000000
4704	0.0000408579614657	0.0011007576853785	0.1338154634203832
4705	0.0000494441706849	0.4989729592890058	0.1338151490248833
4706	0.5000461883464595	0.9989179051630117	0.1336798824875913
4707	0.5000308950181989	0.5011390884454130	0.1336758911378908
4708	0.0001470688123817	0.9961689141690613	0.2711493071149960
4709	0.0001288408319624	0.5039806277288648	0.2711485886456515
4710	0.5001105993836177	0.9961070210383340	0.2719595527474681
4711	0.5001202518483154	0.5040490013375987	0.2719436202238512
4712	0.2500000000000000	0.2500000000000000	0.0000000000000000
4713	0.2500000000000000	0.7500000000000000	0.0000000000000000
4714	0.7500000000000000	0.2500000000000000	0.0000000000000000
4715	0.7500000000000000	0.7500000000000000	0.0000000000000000

4716	0.0000000000000000	0.2500000000000000	0.0653899980000006
4717	0.0000000000000000	0.7500000000000000	0.0653899980000006
4718	0.5000000000000000	0.2500000000000000	0.0653899980000006
4719	0.5000000000000000	0.7500000000000000	0.0653899980000006
4720	0.2500000000000000	0.0000000000000000	0.0653899980000006
4721	0.2500000000000000	0.5000000000000000	0.0653899980000006
4722	0.7500000000000000	0.0000000000000000	0.0653899980000006
4723	0.7500000000000000	0.5000000000000000	0.0653899980000006
4724	0.2501236106280587	0.2500359215735202	0.1336745863240552
4725	0.2497434873648459	0.7500338070608734	0.1335946697820276
4726	0.7499911587233967	0.2500266823977952	0.1336776078612090
4727	0.7503189254691520	0.7500143466522005	0.1335995195174959
4728	0.0000665876478081	0.2500460832569331	0.2032358957062002
4729	0.0000879758879222	0.7500480127292377	0.2013019094926349
4730	0.5000906448365399	0.2500537201875872	0.2006227293429319
4731	0.5000904408294673	0.7500473515125137	0.2020392543428642
4732	0.2505548551632302	0.0008765534619997	0.2016104112159312
4733	0.2505393807300251	0.4992345753420935	0.2016069856844851
4734	0.7496337150323811	0.0008705237510611	0.2016068964579958
4735	0.7496180725113106	0.4992181399656488	0.2016086095366063
4736	0.2454211421248971	0.2500892466440519	0.2678389506011385
4737	0.2495414859168150	0.7500710218822562	0.2654864299198678
4738	0.7548484247927263	0.2500690580183758	0.2678455074496497
4739	0.7506692949083558	0.7500729448331143	0.2654757575806528
4740	0.5006137517739333	0.2501631708363021	0.3147150412044013
4741	0.5010982974341331	0.2502417684439351	0.3511623633369680

4742
4743

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

4745	1.0000000000000000		
4746	7.0844001770000000	0.0000000000000000	0.0000000000000000
4747	0.0000000000000000	7.0844001770000000	0.0000000000000000
4748	0.0000000000000000	0.0000000000000000	27.0844993591000005

4749 Fe Ni O H
4750 12 28 1 1

4751	Direct		
4752	0.0000000000000000	0.0000000000000000	0.0000000000000000
4753	0.0000000000000000	0.5000000000000000	0.0000000000000000
4754	0.5000000000000000	0.0000000000000000	0.0000000000000000
4755	0.5000000000000000	0.5000000000000000	0.0000000000000000
4756	0.9999989127999314	0.0010202053006125	0.1309399142835304
4757	0.0000010055329511	0.4991142046146990	0.1309433230461323
4758	0.5000006868528075	0.0002286663394031	0.1308244875994689
4759	0.4999994903303957	0.4998988516584575	0.1308233233886966
4760	0.0000019076106952	0.9944771772370871	0.2616857678614863
4761	0.9999997908008140	0.5058281664941404	0.2616845126325558
4762	0.4999999268924782	0.9893654357712691	0.2634307780202079
4763	0.5000030281826966	0.5109344470116710	0.2634301361578366
4764	0.2500000000000000	0.2500000000000000	0.0000000000000000
4765	0.2500000000000000	0.7500000000000000	0.0000000000000000
4766	0.7500000000000000	0.2500000000000000	0.0000000000000000
4767	0.7500000000000000	0.7500000000000000	0.0000000000000000

4768	0.0000000000000000	0.2500000000000000	0.0653899980000006
4769	0.0000000000000000	0.7500000000000000	0.0653899980000006
4770	0.5000000000000000	0.2500000000000000	0.0653899980000006
4771	0.5000000000000000	0.7500000000000000	0.0653899980000006
4772	0.2500000000000000	0.0000000000000000	0.0653899980000006
4773	0.2500000000000000	0.5000000000000000	0.0653899980000006
4774	0.7500000000000000	0.0000000000000000	0.0653899980000006
4775	0.7500000000000000	0.5000000000000000	0.0653899980000006
4776	0.2483411369163804	0.2500663815906208	0.1310597117981587
4777	0.2503242941453934	0.7500790572661131	0.1309481710019895
4778	0.7516565905352408	0.2500689121604083	0.1310590876640774
4779	0.7496756520800005	0.7500776876434614	0.1309483979973507
4780	0.9999983724679353	0.2501193602052112	0.1985453326869120
4781	0.9999968144253017	0.7501155515738844	0.1960006499292675
4782	0.4999993154127225	0.2501048412964906	0.1949014761303971
4783	0.5000012756153254	0.7501076202639823	0.1966014127655384
4784	0.2511894342571566	0.0016560759636874	0.1967175913540018
4785	0.2511997105124308	0.4985693035950334	0.1967101297732725
4786	0.7488075683802720	0.0016539389769150	0.1967173516676084
4787	0.7488023629656411	0.4985724784266168	0.1967120526764106
4788	0.2451000532189198	0.2501718387899459	0.2607982185099047
4789	0.2484139293695051	0.7501238173053011	0.2586422755263982
4790	0.7548965229483002	0.2501627781134417	0.2607994236559179
4791	0.7515823150113690	0.7501337348853880	0.2586429928348437
4792	0.4999772036446757	0.2502722215134909	0.3049868694034288
4793	0.4999528068244743	0.2503993374766083	0.3411078489465709

4794

4795

4796 Pure Ni 200 Facet with OH supercell 2X2X1 - [Etot = - 214.75562 eV]

4797 1.01798110552312

4798 7.0844001770000000 0.0000000000000000 0.0000000000000000

4799 0.0000000000000000 7.0844001770000000 0.0000000000000000

4800 0.0000000000000000 0.0000000000000000 27.0844993591000005

4801 Ni O H

4802 40 1 1

4803 Direct

4804 0.0000000000000000 0.0000000000000000 0.0000000000000000

4805 0.0000000000000000 0.5000000000000000 0.0000000000000000

4806 0.5000000000000000 0.0000000000000000 0.0000000000000000

4807 0.5000000000000000 0.5000000000000000 0.0000000000000000

4808 0.9999587924866447 0.0009403294752204 0.1274923391196197

4809 0.9999564036526678 0.4991202147535745 0.1274940949515084

4810 0.4999526877556377 0.9991103570221469 0.1274048404838339

4811 0.4999477529395193 0.5009806822114129 0.1274097761916764

4812 0.9999138832649592 0.9966735038400358 0.2491427480733392

4813 0.9999089734504309 0.5035188173597476 0.2491389262607200

4814 0.4998985283779760 0.9972466887720657 0.2510834867361353

4815 0.4998934022685759 0.5029395874709834 0.2510913596001743

4816 0.2500000000000000 0.2500000000000000 0.0000000000000000

4817 0.2500000000000000 0.7500000000000000 0.0000000000000000

4818 0.7500000000000000 0.2500000000000000 0.0000000000000000

4819 0.7500000000000000 0.7500000000000000 0.0000000000000000

4820	0.0000000000000000	0.2500000000000000	0.0653899980000006
4821	0.0000000000000000	0.7500000000000000	0.0653899980000006
4822	0.5000000000000000	0.2500000000000000	0.0653899980000006
4823	0.5000000000000000	0.7500000000000000	0.0653899980000006
4824	0.2500000000000000	0.0000000000000000	0.0653899980000006
4825	0.2500000000000000	0.5000000000000000	0.0653899980000006
4826	0.7500000000000000	0.0000000000000000	0.0653899980000006
4827	0.7500000000000000	0.5000000000000000	0.0653899980000006
4828	0.2490146842940817	0.2500479555661954	0.1274095935077852
4829	0.2508748968915171	0.7500383697643898	0.1274945325111716
4830	0.7508826811125218	0.2500423773649914	0.1274046321018929
4831	0.7490543903304854	0.7500407399088189	0.1274917977669858
4832	0.9999060583976274	0.2500596416504166	0.1915934672644113
4833	0.9999312186927725	0.7500581268702291	0.1891572277837312
4834	0.4999535572618328	0.2500476277650989	0.1878218470015227
4835	0.4999334476805686	0.7500813533484774	0.1915939832424982
4836	0.2506380115822537	0.0007942548899393	0.1898903653000730
4837	0.2506281307775140	0.4993644441366172	0.1898875289399768
4838	0.7492019260991896	0.0007949295357648	0.1898951296291571
4839	0.7491977805616870	0.4993560243730499	0.1898903156336473
4840	0.2470507355281413	0.2501018116059370	0.2510897900326228
4841	0.2464744620806485	0.7500884988586449	0.2491372011488693
4842	0.7527403578731651	0.2500862833843200	0.2510830826067121
4843	0.7533170696211258	0.7500769296430434	0.2491435493870142
4844	0.4994160727591179	0.2505437994793880	0.2913844924620790
4845	0.4990250050034035	0.2508910694479738	0.3268523504425147

4846
4847

Pure-Ni 220 Facet with OH supercell 2X2X1 - [Etot = - 294.72767 eV]

4849	1.01798110552312		
4850	7.0900001526000000	0.0000000000000000	0.0000000000000000
4851	0.0000000000000000	10.0268001556000002	0.0000000000000000
4852	0.0000000000000000	0.0000000000000000	27.5200996398999997

4853 Ni O H
4854 56 1 1

4855 Direct

4856	0.0000000000000000	0.2500000000000000	0.0000000000000000
4857	0.0000000000000000	0.7500000000000000	0.0000000000000000
4858	0.5000000000000000	0.2500000000000000	0.0000000000000000
4859	0.5000000000000000	0.7500000000000000	0.0000000000000000
4860	0.0000000000000000	0.0000000000000000	0.0910900009999978
4861	0.0000000000000000	0.5000000000000000	0.0910900009999978
4862	0.5000000000000000	0.0000000000000000	0.0910900009999978
4863	0.5000000000000000	0.5000000000000000	0.0910900009999978
4864	0.9991125351668515	0.2500947452853808	0.1769408723561270
4865	0.9989993456667960	0.7500140641999735	0.1751592997426314
4866	0.5008860830838699	0.2500933388623707	0.1769406265504969
4867	0.5009999450826186	0.7500153702779215	0.1751601060238031
4868	0.9984580235094214	0.9965645613502829	0.2596869712100158
4869	0.0000977557714990	0.5028461930059080	0.2597586974881807
4870	0.5015420447978443	0.9965638523959086	0.2596836016282253
4871	0.4999013677369035	0.5028415012490655	0.2597633577674756

4872	0.0000000000000000	0.0000000000000000	0.0000000000000000
4873	0.0000000000000000	0.5000000000000000	0.0000000000000000
4874	0.5000000000000000	0.0000000000000000	0.0000000000000000
4875	0.5000000000000000	0.5000000000000000	0.0000000000000000
4876	0.2500000000000000	0.1250000000000000	0.0455400009999991
4877	0.2500000000000000	0.6250000000000000	0.0455400009999991
4878	0.7500000000000000	0.1250000000000000	0.0455400009999991
4879	0.7500000000000000	0.6250000000000000	0.0455400009999991
4880	0.2500000000000000	0.3750000000000000	0.0455400009999991
4881	0.2500000000000000	0.8750000000000000	0.0455400009999991
4882	0.7500000000000000	0.3750000000000000	0.0455400009999991
4883	0.7500000000000000	0.8750000000000000	0.0455400009999991
4884	0.9988202945637710	0.2499581319486666	0.0879543827421330
4885	0.0005572659437121	0.7499798010882017	0.0876370984200321
4886	0.5011782759217027	0.2499577261598560	0.0879542629362149
4887	0.4994428624481344	0.7499796941262815	0.0876373519384401
4888	0.2500003765595764	0.3738949986536255	0.1322215249025689
4889	0.2500027917335501	0.8750552768610476	0.1330923824815926
4890	0.7500004287440447	0.3741464892318120	0.1339725026075413
4891	0.7500004987599453	0.8744426265579506	0.1327200138017375
4892	0.2499988195475922	0.1261227945365491	0.1324237002221409
4893	0.2500015926289336	0.6250076528334105	0.1330183915324383
4894	0.7500007931595221	0.1258377070737211	0.1338928487599134
4895	0.7499987461490747	0.6255672980591953	0.1327520014218493
4896	0.9981419309639890	0.0000765062925581	0.1762506290308608
4897	0.9977152232985631	0.5000876012400397	0.1763505145077602
4898	0.5018572658680824	0.0000777481868326	0.1762525137152267
4899	0.5022870776710704	0.5000854994851593	0.1763541328197178
4900	0.2500018313043242	0.1183353561237439	0.2186043362754617
4901	0.2500041471269085	0.6270458484206713	0.2216117656331775
4902	0.7499978688080162	0.1288439880820818	0.2241480162098028
4903	0.7499964988530010	0.6240786804443061	0.2217142931646165
4904	0.2500014015687242	0.3818652205086721	0.2181320619603682
4905	0.2500020446595101	0.8732208329621969	0.2218035278644592
4906	0.7499976179296155	0.3702153738169187	0.2245795113980478
4907	0.7499986722847751	0.8754268905524256	0.2215281371733582
4908	0.0275517995477728	0.2504617986036308	0.2636801171770031
4909	0.9986345719912819	0.7500033156969721	0.2593264831654807
4910	0.4724422619599409	0.2504644895099730	0.2636795629464217
4911	0.5013647121217417	0.7500026207932038	0.2593257796188979
4912	0.2500011728370382	0.2470659352220466	0.3059679991537436
4913	0.2500006997262645	0.1624907925790566	0.3224258734121221

4914

4915

4916

Ground state structures-

4917

4918

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

4919

1.04735280294076

4920

5.0134000778000001 0.0000000000000000 0.0000000000000000

4921

-2.5067000389000000 4.3417318267000002 0.0000000000000000

4922

0.0000000000000000 0.0000000000000000 28.1868000031000001

4923

Sc Ni

4924	5	15		
4925	Direct			
4926	0.33333000500000005	0.6666700239999983	0.0000000000000000	
4927	0.0000000000000000	0.0000000000000000	0.0726099979999972	
4928	0.6666877336421848	0.3333122953578140	0.1459873532748972	
4929	0.3333762188998222	0.6666238101001767	0.2164783139378770	
4930	0.0000507295790015	0.9999492704209985	0.2957490578539534	
4931	0.33333000500000005	0.1666699949999995	0.0000000000000000	
4932	0.0000000000000000	0.5000000000000000	0.0726099979999972	
4933	0.8333299760000017	0.1666699949999995	0.0000000000000000	
4934	0.5000000000000000	0.5000000000000000	0.0726099979999972	
4935	0.8333299760000017	0.6666700239999983	0.0000000000000000	
4936	0.5000000000000000	0.0000000000000000	0.0726099979999972	
4937	0.6675867292467075	0.8337580549396435	0.1448025006386402	
4938	0.3244951446298074	0.1621871589671855	0.2184232164346014	
4939	0.9938454426948553	0.4968501859609660	0.2864575781851144	
4940	0.1662386074764086	0.8337613635235925	0.1448029635340617	
4941	0.8378251197993478	0.1621748512006533	0.2184229840010943	
4942	0.5031474713181439	0.4968525286818561	0.2864566601706287	
4943	0.1662419160603577	0.3324132997532843	0.1448025006386402	
4944	0.8378128120328157	0.6755048843701914	0.2184232164346014	
4945	0.5031498140390340	0.0061545573051447	0.2864575781851144	
4946	Bare NiTi (25% Ti) 111 Facet- [Etot = -124.73434036 eV]			
4947	1.01798110552312			
4948	5.0134000778000001	0.0000000000000000	0.0000000000000000	
4949	-2.5067000389000000	4.3417318267000002	0.0000000000000000	
4950	0.0000000000000000	0.0000000000000000	28.1868000031000001	
4951	Ti Ni			
4952	5	15		
4953	Direct			
4954	0.33333000500000005	0.6666700239999983	0.0000000000000000	
4955	0.0000000000000000	0.0000000000000000	0.0726099979999972	
4956	0.6666793069973451	0.3333207220026537	0.1448438379804600	
4957	0.3333729845432885	0.6666270444567104	0.2212717471700429	
4958	0.0000571237841669	0.9999428762158331	0.2885532718654460	
4959	0.33333000500000005	0.1666699949999995	0.0000000000000000	
4960	0.0000000000000000	0.5000000000000000	0.0726099979999972	
4961	0.8333299760000017	0.1666699949999995	0.0000000000000000	
4962	0.5000000000000000	0.5000000000000000	0.0726099979999972	
4963	0.8333299760000017	0.6666700239999983	0.0000000000000000	
4964	0.5000000000000000	0.0000000000000000	0.0726099979999972	
4965	0.6654784271568062	0.8327179325382303	0.1454109468020590	
4966	0.3319878147385182	0.1659368522984224	0.2174517538036937	
4967	0.0019049934663400	0.5008618157720335	0.2894235859865404	
4968	0.1672817315973631	0.8327182394026380	0.1454111960729279	
4969	0.8340467638727063	0.1659532071272949	0.2174508073089640	
4970	0.4991320528685534	0.5008679471314466	0.2894245310976018	
4971	0.1672820384617708	0.3345216018431856	0.1454109468020590	
4972	0.8340631187015788	0.6680122142614806	0.2174517538036937	
4973	0.4991381842279665	0.9980950065336600	0.2894235859865404	
4974				
4975	Bare NiV (25% V) 111 Facet- [Etot = -125.17844066 eV]			

4976	1.00458661266245		
4977	5.0134000778000001	0.0000000000000000	0.0000000000000000
4978	-2.5067000389000000	4.3417318267000002	0.0000000000000000
4979	0.0000000000000000	0.0000000000000000	28.1868000031000001
4980	V Ni		
4981	5 15		
4982	Direct		
4983	0.3333300050000005	0.6666700239999983	0.0000000000000000
4984	0.0000000000000000	0.0000000000000000	0.0726099979999972
4985	0.6666692295599077	0.3333307994400911	0.1445396305549735
4986	0.3333398326731682	0.6666601963268306	0.2234274135847869
4987	0.0000045630584466	0.9999954369415534	0.2898302184578156
4988	0.3333300050000005	0.1666699949999995	0.0000000000000000
4989	0.0000000000000000	0.5000000000000000	0.0726099979999972
4990	0.8333299760000017	0.1666699949999995	0.0000000000000000
4991	0.5000000000000000	0.5000000000000000	0.0726099979999972
4992	0.8333299760000017	0.6666700239999983	0.0000000000000000
4993	0.5000000000000000	0.0000000000000000	0.0726099979999972
4994	0.6650233937483918	0.8325007424903745	0.1452641759619269
4995	0.3319281171412669	0.1659533965168691	0.2165596570391841
4996	0.0015039216987134	0.5007439994255947	0.2895413134284368
4997	0.1674923646062823	0.8325076063937189	0.1452640963818652
4998	0.8340502266249672	0.1659497443750340	0.2165594108217448
4999	0.4992538275403078	0.5007461724596922	0.2895413274732377
5000	0.1674992285096266	0.3349766352516070	0.1452641759619269
5001	0.8340465744831320	0.6680719118587319	0.2165596570391841
5002	0.4992560005744053	0.9984960783012866	0.2895413134284368
5003			
5004	Bare NiCr (25% Cr) 111 Facet- [Etot = -124.07166597 eV]		
5005	0.995572721824907		
5006	5.0134000778000001	0.0000000000000000	0.0000000000000000
5007	-2.5067000389000000	4.3417318267000002	0.0000000000000000
5008	0.0000000000000000	0.0000000000000000	28.1868000031000001
5009	Cr Ni		
5010	5 15		
5011	Direct		
5012	0.3333300050000005	0.6666700239999983	0.0000000000000000
5013	0.0000000000000000	0.0000000000000000	0.0726099979999972
5014	0.6666709300349183	0.3333290989650806	0.1453286339533264
5015	0.3333359851905939	0.6666640438094049	0.2221376565740130
5016	0.0000051748525465	0.9999948251474535	0.2919729278881178
5017	0.3333300050000005	0.1666699949999995	0.0000000000000000
5018	0.0000000000000000	0.5000000000000000	0.0726099979999972
5019	0.8333299760000017	0.1666699949999995	0.0000000000000000
5020	0.5000000000000000	0.5000000000000000	0.0726099979999972
5021	0.8333299760000017	0.6666700239999983	0.0000000000000000
5022	0.5000000000000000	0.0000000000000000	0.0726099979999972
5023	0.6654319020265831	0.8327110100649975	0.1457344032481984
5024	0.3334860648282429	0.1667392342672542	0.2177981924483845
5025	0.0034209591524075	0.5017034910554301	0.2907214994538663
5026	0.1672920494797694	0.8327079215202318	0.1457348632292366
5027	0.8332617556769435	0.1667382153230577	0.2177980522885932

5028	0.4982930932155156	0.5017069067844844	0.2907215316857119
5029	0.1672889609350037	0.3345681269734158	0.1457344032481984
5030	0.8332607367327469	0.6665139641717559	0.2177981924483845
5031	0.4982965089445699	0.9965790408475925	0.2907214994538663
5032			
5033	Bare NiMn (25% Mn) 111 Facet- [Etot = -122.45951645 eV]		
5034	0.989317187668226		
5035	5.0134000778000001	0.0000000000000000	0.0000000000000000
5036	-2.5067000389000000	4.3417318267000002	0.0000000000000000
5037	0.0000000000000000	0.0000000000000000	28.1868000031000001
5038	Mn Ni		
5039	5 15		
5040	Direct		
5041	0.3333300050000005	0.6666700239999983	0.0000000000000000
5042	0.0000000000000000	0.0000000000000000	0.0726099979999972
5043	0.6666754006061311	0.3333246283938678	0.1481797199843697
5044	0.3333499804013016	0.6666500485986973	0.2214280037002112
5045	0.0000127704186212	0.9999872295813788	0.2992758507027204
5046	0.3333300050000005	0.1666699949999995	0.0000000000000000
5047	0.0000000000000000	0.5000000000000000	0.0726099979999972
5048	0.8333299760000017	0.1666699949999995	0.0000000000000000
5049	0.5000000000000000	0.5000000000000000	0.0726099979999972
5050	0.8333299760000017	0.6666700239999983	0.0000000000000000
5051	0.5000000000000000	0.0000000000000000	0.0726099979999972
5052	0.6667130312094329	0.8333429009176569	0.1471516235290693
5053	0.3307414124967210	0.1653475985996664	0.2219501611608408
5054	0.9996680157056232	0.4998104885840107	0.2945941769954104
5055	0.1666561543884768	0.8333438166115243	0.1471518570710799
5056	0.8346494553992443	0.1653505156007569	0.2219501766185275
5057	0.5001869591391355	0.4998130408608645	0.2945949970783062
5058	0.1666570700823442	0.3332869977905659	0.1471516235290693
5059	0.8346523724003347	0.6692586165032779	0.2219501611608408
5060	0.5001895114159893	0.0003319842943768	0.2945941769954104
5061			
5062	Bare NiFe (25% Fe) 111 Facet- [Etot = -119.96372461 eV]		
5063	1.0000000000000000		
5064	5.0134000778000001	0.0000000000000000	0.0000000000000000
5065	-2.5067000389000000	4.3417318267000002	0.0000000000000000
5066	0.0000000000000000	0.0000000000000000	28.1868000031000001
5067	Fe Ni		
5068	5 15		
5069	Direct		
5070	0.3333300050000005	0.6666700239999983	0.0000000000000000
5071	0.0000000000000000	0.0000000000000000	0.0726099979999972
5072	0.6666726360278616	0.3333273929721372	0.1447967649929112
5073	0.3333423114219514	0.6666577175780475	0.2193604419151782
5074	0.0000080976197623	0.9999919023802377	0.2886120754165873
5075	0.3333300050000005	0.1666699949999995	0.0000000000000000
5076	0.0000000000000000	0.5000000000000000	0.0726099979999972
5077	0.8333299760000017	0.1666699949999995	0.0000000000000000
5078	0.5000000000000000	0.5000000000000000	0.0726099979999972
5079	0.8333299760000017	0.6666700239999983	0.0000000000000000

5080	0.5000000000000000	0.0000000000000000	0.0726099979999972
5081	0.6660536756522646	0.8330188069870701	0.1451902134281298
5082	0.3339734451528003	0.1669750504050498	0.2173258326549430
5083	0.0021337141475897	0.5010506557787409	0.2889232790288290
5084	0.1669811099709548	0.8330188610290463	0.1451901262245912
5085	0.8330252113562580	0.1669747596437432	0.2173254096151567
5086	0.4989465874791534	0.5010534125208466	0.2889235431396457
5087	0.1669811640129311	0.3339463533477343	0.1451902134281298
5088	0.8330249205949514	0.6660265838471986	0.2173258326549430
5089	0.4989493442212591	0.9978662858524103	0.2889232790288290
5090			
5091	Bare NiCo (25% Co) 111 Facet- [Etot = -111.83029501 eV]		
5092	0.993794164815303		
5093	5.0134000778000001	0.0000000000000000	0.0000000000000000
5094	-2.5067000389000000	4.3417318267000002	0.0000000000000000
5095	0.0000000000000000	0.0000000000000000	28.1868000031000001
5096	Co Ni		
5097	5 15		
5098	Direct		
5099	0.3333300050000005	0.6666700239999983	0.0000000000000000
5100	0.0000000000000000	0.0000000000000000	0.0726099979999972
5101	0.6666717378888123	0.3333282911111866	0.1448152646550867
5102	0.3333406477954526	0.6666593812045463	0.2192765093165150
5103	0.0000091533811926	0.9999908466188074	0.2886242599373503
5104	0.3333300050000005	0.1666699949999995	0.0000000000000000
5105	0.0000000000000000	0.5000000000000000	0.0726099979999972
5106	0.8333299760000017	0.1666699949999995	0.0000000000000000
5107	0.5000000000000000	0.5000000000000000	0.0726099979999972
5108	0.8333299760000017	0.6666700239999983	0.0000000000000000
5109	0.5000000000000000	0.0000000000000000	0.0726099979999972
5110	0.6661088098468042	0.8330449172864931	0.1451968381070685
5111	0.3338381522038247	0.1669071616841222	0.2173471283767867
5112	0.0018635276826373	0.5009135025436535	0.2889571355090368
5113	0.1669540440549895	0.8330459269450117	0.1451970160117071
5114	0.8330923998837818	0.1669075711162193	0.2173453882124363
5115	0.4990766115369141	0.5009233884630859	0.2889570728616917
5116	0.1669550537135081	0.3338912191531946	0.1451968381070685
5117	0.8330928093158789	0.6661618767961741	0.2173471283767867
5118	0.4990864974563465	0.9981364723173627	0.2889571355090368
5119	Pure Ni 111 Facet- [Etot = -104.25072995 eV]		
5120	0.993602894269297		
5121	5.0134000778000001	0.0000000000000000	0.0000000000000000
5122	-2.5067000389000000	4.3417318267000002	0.0000000000000000
5123	0.0000000000000000	0.0000000000000000	28.1868000031000001
5124	Ni		
5125	20		
5126	Direct		
5127	0.3333300050000005	0.6666700239999983	0.0000000000000000
5128	0.0000000000000000	0.0000000000000000	0.0726099979999972
5129	0.6666854930302293	0.3333145359697767	0.1450032888287893
5130	0.3333782980021738	0.6666217309978251	0.2174623354386966
5131	0.0000573956624237	0.9999426043375763	0.2888105590421830

5132	0.3333300050000005	0.1666699949999995	0.0000000000000000
5133	0.0000000000000000	0.5000000000000000	0.0726099979999972
5134	0.8333299760000017	0.1666699949999995	0.0000000000000000
5135	0.5000000000000000	0.5000000000000000	0.0726099979999972
5136	0.8333299760000017	0.6666700239999983	0.0000000000000000
5137	0.5000000000000000	0.0000000000000000	0.0726099979999972
5138	0.6666691528736379	0.8333057862157176	0.1450053413381767
5139	0.3333688017006651	0.1666220775352656	0.2174469088738320
5140	0.0000512650298816	0.4999366113579811	0.2888165073459277
5141	0.1666936310678437	0.8333063399321574	0.1450058067084257
5142	0.8333782076748193	0.1666217633251819	0.2174453758734813
5143	0.5000620971410044	0.4999379028589956	0.2888178002486796
5144	0.1666941847842836	0.3333308761263538	0.1450053413381767
5145	0.8333778934647356	0.6666312272993338	0.2174469088738320
5146	0.5000633886420189	0.9999487349701184	0.2888165073459277
5147	Bare NiCu (25% Cu) 111 Facet- [Etot = -95.24504276 eV]		
5148	0.998485100048875		
5149	5.0134000778000001	0.0000000000000000	0.0000000000000000
5150	-2.5067000389000000	4.3417318267000002	0.0000000000000000
5151	0.0000000000000000	0.0000000000000000	28.1868000031000001
5152	Cu Ni		
5153	5 15		
5154	Direct		
5155	0.3333300050000005	0.6666700239999983	0.0000000000000000
5156	0.0000000000000000	0.0000000000000000	0.0726099979999972
5157	0.6666691638760867	0.3333308651239122	0.1456779528850873
5158	0.3333325519903738	0.6666674770096250	0.2172014328735301
5159	0.0000001887715442	0.9999998112284558	0.2930262779943646
5160	0.3333300050000005	0.1666699949999995	0.0000000000000000
5161	0.0000000000000000	0.5000000000000000	0.0726099979999972
5162	0.8333299760000017	0.1666699949999995	0.0000000000000000
5163	0.5000000000000000	0.5000000000000000	0.0726099979999972
5164	0.8333299760000017	0.6666700239999983	0.0000000000000000
5165	0.5000000000000000	0.0000000000000000	0.0726099979999972
5166	0.6672051723242802	0.8335887699879834	0.1451784090771540
5167	0.3311497404969685	0.1655638979590535	0.2184795188845925
5168	0.9990556861101467	0.4995178636112811	0.2891432952507174
5169	0.1663998098371167	0.8336001611628845	0.1451792441383688
5170	0.8344272803847019	0.1655726906152992	0.2184822265445661
5171	0.5004884278843917	0.4995115721156083	0.2891240811401374
5172	0.1664112010120178	0.3327948566757186	0.1451784090771540
5173	0.8344360730409477	0.6688502885030303	0.2184795188845925
5174	0.5004821363887189	0.0009443138898533	0.2891432952507174
5175			
5176	Bare NiZn (25% Zn) 111 Facet- [Etot = -85.99800042 eV]		
5177	1.01038006037737		
5178	5.0134000778000001	0.0000000000000000	0.0000000000000000
5179	-2.5067000389000000	4.3417318267000002	0.0000000000000000
5180	0.0000000000000000	0.0000000000000000	28.1868000031000001
5181	Zn Ni		
5182	5 15		
5183	Direct		

5184	0.3333300050000005	0.6666700239999983	0.0000000000000000
5185	0.0000000000000000	0.0000000000000000	0.0726099979999972
5186	0.6666812614782387	0.3333187675217602	0.1451053471859396
5187	0.3333871518183003	0.6666128771816986	0.2163052420120053
5188	0.0000778136012300	0.9999221863987700	0.2937604876721309
5189	0.3333300050000005	0.1666699949999995	0.0000000000000000
5190	0.0000000000000000	0.5000000000000000	0.0726099979999972
5191	0.8333299760000017	0.1666699949999995	0.0000000000000000
5192	0.5000000000000000	0.5000000000000000	0.0726099979999972
5193	0.8333299760000017	0.6666700239999983	0.0000000000000000
5194	0.5000000000000000	0.0000000000000000	0.0726099979999972
5195	0.6671208666371911	0.8335339273661830	0.1448729569854308
5196	0.3294418968447985	0.1646459398167082	0.2175054318884833
5197	0.9982571378226694	0.4990254376866190	0.2875059296465636
5198	0.1664642246813202	0.8335357463186810	0.1448762549205611
5199	0.8353669829719763	0.1646329880280248	0.2174974874269395
5200	0.5009480523458691	0.4990519476541309	0.2875099961894492
5201	0.1664660436338181	0.3328791623628007	0.1448729569854308
5202	0.8353540311832930	0.6705581321552003	0.2175054318884833
5203	0.5009745623133810	0.0017428621773306	0.2875059296465636

5204
5205

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

5207	1.04735280294076		
5208	5.0134000778000001	0.0000000000000000	0.0000000000000000
5209	-2.5067000389000000	4.3417318267000002	0.0000000000000000
5210	0.0000000000000000	0.0000000000000000	28.1868000031000001

5211 Sc Ni H
5212 5 15 4

5213	Direct		
5214	0.3333300050000005	0.6666700239999983	0.0000000000000000
5215	0.0000000000000000	0.0000000000000000	0.0726099979999972
5216	0.6665211837770002	0.3332157935581179	0.1450435113597237
5217	0.3330955227570769	0.6664580150351682	0.2169453801214445
5218	0.9996758633902658	0.9997260733370226	0.2896387922934878
5219	0.3333300050000005	0.1666699949999995	0.0000000000000000
5220	0.0000000000000000	0.5000000000000000	0.0726099979999972
5221	0.8333299760000017	0.1666699949999995	0.0000000000000000
5222	0.5000000000000000	0.5000000000000000	0.0726099979999972
5223	0.8333299760000017	0.6666700239999983	0.0000000000000000
5224	0.5000000000000000	0.0000000000000000	0.0726099979999972
5225	0.6675838938586054	0.8337414503520790	0.1451635749965163
5226	0.3320526062732370	0.1659394660855469	0.2183667090120593
5227	0.9920372080620652	0.4959036922275786	0.2917688658009610
5228	0.1659921184902160	0.8337387523564459	0.1451649932477252
5229	0.8336058372007997	0.1659438160110085	0.2183686320391303
5230	0.5034885871077606	0.4959083622924680	0.2917728336684462
5231	0.1659859734106846	0.3321405098810573	0.1451652337096405
5232	0.8336083331955564	0.6674925186855418	0.2183684492837017
5233	0.5034729285087991	0.0073309140493620	0.2917745114139905
5234	0.6663285496073286	0.3330396516644143	0.3206444901658259
5235	0.5974963868901213	0.7986211875452227	0.3215653591710179

5236	0.2007333972425371	0.7986131629954656	0.3215634936747875
5237	0.2007477137855886	0.4018924255246148	0.3215607227309363
5238			
5239	NiTi (25% Ti) 111 Facet with Hydrogen- [Etot = -140.22047452 eV]		
5240	1.01798110552312		
5241	5.0134000778000001	0.0000000000000000	0.0000000000000000
5242	-2.5067000389000000	4.3417318267000002	0.0000000000000000
5243	0.0000000000000000	0.0000000000000000	28.1868000031000001
5244	Ti Ni H		
5245	5 15 4		
5246	Direct		
5247	0.3333300050000005	0.6666700239999983	0.0000000000000000
5248	0.0000000000000000	0.0000000000000000	0.0726099979999972
5249	0.6665886887733876	0.3332729434318864	0.1432204078588768
5250	0.3331363018879472	0.6664863363295623	0.2201972145199349
5251	0.9997777346533283	0.9998011001463141	0.2861974412704882
5252	0.3333300050000005	0.1666699949999995	0.0000000000000000
5253	0.0000000000000000	0.5000000000000000	0.0726099979999972
5254	0.8333299760000017	0.1666699949999995	0.0000000000000000
5255	0.5000000000000000	0.5000000000000000	0.0726099979999972
5256	0.8333299760000017	0.6666700239999983	0.0000000000000000
5257	0.5000000000000000	0.0000000000000000	0.0726099979999972
5258	0.6645780350819592	0.8322549112579196	0.1463508368927577
5259	0.3357853388051808	0.1678262327901834	0.2178941756626642
5260	0.9953063661863126	0.4975716941988040	0.2933692036781750
5261	0.1675627376513518	0.8322409824555521	0.1463530713662706
5262	0.8318271704116142	0.1678167463976763	0.2178925558355544
5263	0.5019972378000759	0.4975565437455174	0.2933721612016029
5264	0.1675722148390761	0.3352610899925139	0.1463546282540520
5265	0.8318394827977187	0.6638669400733050	0.2178927631290222
5266	0.5020008354907617	0.0042511724366179	0.2933746277521365
5267	0.6664361861074255	0.3331239005185225	0.3247246107676958
5268	0.6336724828422930	0.8167346576290697	0.3243729080684687
5269	0.1828052054275346	0.8167380834548936	0.3243718663105994
5270	0.1828136529975666	0.3658890508247481	0.3243719698050427
5271			
5272	NiV (25% V) 111 Facet with Hydrogen- [Etot = -140.30623781 eV]		
5273	1.00458661266245		
5274	5.0134000778000001	0.0000000000000000	0.0000000000000000
5275	-2.5067000389000000	4.3417318267000002	0.0000000000000000
5276	0.0000000000000000	0.0000000000000000	28.1868000031000001
5277	V Ni H		
5278	5 15 4		
5279	Direct		
5280	0.3333300050000005	0.6666700239999983	0.0000000000000000
5281	0.0000000000000000	0.0000000000000000	0.0726099979999972
5282	0.6664405050046653	0.3331399587529091	0.1444546098310013
5283	0.3329706424403724	0.6663686004402862	0.2211238704689862
5284	0.9994331937250465	0.9995077151966711	0.2875598299293003
5285	0.3333300050000005	0.1666699949999995	0.0000000000000000
5286	0.0000000000000000	0.5000000000000000	0.0726099979999972
5287	0.8333299760000017	0.1666699949999995	0.0000000000000000

5288	0.5000000000000000	0.5000000000000000	0.0726099979999972
5289	0.8333299760000017	0.6666700239999983	0.0000000000000000
5290	0.5000000000000000	0.0000000000000000	0.0726099979999972
5291	0.6648279534639698	0.8323431844312950	0.1458592167489385
5292	0.3341049369926239	0.1669524132137994	0.2172806206386610
5293	0.9959574317812354	0.4978362406656203	0.2932752631742730
5294	0.1672761464885824	0.8323462914203006	0.1458585830384962
5295	0.8324754251040360	0.1669405969001119	0.2172721865846441
5296	0.5011927099232807	0.4977835095674408	0.2932752142236765
5297	0.1672811578620923	0.3347924495205774	0.1458589475238057
5298	0.8324820648622904	0.6653308955909267	0.2172716866224462
5299	0.5011369289523557	0.0030276594308276	0.2932745124363976
5300	0.6660773103403912	0.3328663668511780	0.3257221306171303
5301	0.6453264694106267	0.8224775224042773	0.3246639143898378
5302	0.1764607173631632	0.8224655523157764	0.3246532674870011
5303	0.1764718368872096	0.3536401809623371	0.3246535588788291
5304			
5305			
5306	NiCr (25% Cr) 111 Facet with Hydrogen- [Etot = -139.70832220 eV]		
5307	0.995572721824907		
5308	5.0134000778000001	0.0000000000000000	0.0000000000000000
5309	-2.5067000389000000	4.3417318267000002	0.0000000000000000
5310	0.0000000000000000	0.0000000000000000	28.1868000031000001
5311	Cr Ni H		
5312	5 15 4		
5313	Direct		
5314	0.3333300050000005	0.6666700239999983	0.0000000000000000
5315	0.0000000000000000	0.0000000000000000	0.0726099979999972
5316	0.6665057957647278	0.3332042942078388	0.1447094167208363
5317	0.3329894996935963	0.6663803194318660	0.2201983316030294
5318	0.9994868450642755	0.9995717544679366	0.2904975480174272
5319	0.3333300050000005	0.1666699949999995	0.0000000000000000
5320	0.0000000000000000	0.5000000000000000	0.0726099979999972
5321	0.8333299760000017	0.1666699949999995	0.0000000000000000
5322	0.5000000000000000	0.5000000000000000	0.0726099979999972
5323	0.8333299760000017	0.6666700239999983	0.0000000000000000
5324	0.5000000000000000	0.0000000000000000	0.0726099979999972
5325	0.6661144293465142	0.8330025688381753	0.1458093720430469
5326	0.3349347404919314	0.1673586488320424	0.2185466941693903
5327	0.9958397026910006	0.4977672706881648	0.2944880970203982
5328	0.1666979021180239	0.8330005975307628	0.1458096171367060
5329	0.8320211129352018	0.1673656145736899	0.2185440970754797
5330	0.5013202332026552	0.4977904079919924	0.2944895657317090
5331	0.1666935843709965	0.3335774994935932	0.1458084716318169
5332	0.8320284032702929	0.6644510312916978	0.2185429027649590
5333	0.5012998007540901	0.0031801445492476	0.2944913668617204
5334	0.6661180866442749	0.3328759090636311	0.3272120375744123
5335	0.6439878640301302	0.8218112055512137	0.3264908972491511
5336	0.1771884794149940	0.8217941854675956	0.3264877784184108
5337	0.1772017634296859	0.3550529305170826	0.3264870345175481
5338			
5339	NiMn (25% Mn) 111 Facet with Hydrogen- [Etot = -139.17664835 eV]		

5340	0.989317187668226		
5341	5.0134000778000001	0.0000000000000000	0.0000000000000000
5342	-2.5067000389000000	4.3417318267000002	0.0000000000000000
5343	0.0000000000000000	0.0000000000000000	28.1868000031000001
5344	Mn Ni H		
5345	5 15 4		
5346	Direct		
5347	0.3333300050000005	0.6666700239999983	0.0000000000000000
5348	0.0000000000000000	0.0000000000000000	0.0726099979999972
5349	0.6664816028378411	0.3331734672289528	0.1467584417558072
5350	0.3328892482036707	0.6662711763302696	0.2224131334905479
5351	0.9994083569845813	0.9994917117569386	0.2941701139517718
5352	0.3333300050000005	0.1666699949999995	0.0000000000000000
5353	0.0000000000000000	0.5000000000000000	0.0726099979999972
5354	0.8333299760000017	0.1666699949999995	0.0000000000000000
5355	0.5000000000000000	0.5000000000000000	0.0726099979999972
5356	0.8333299760000017	0.6666700239999983	0.0000000000000000
5357	0.5000000000000000	0.0000000000000000	0.0726099979999972
5358	0.6664237560577604	0.8331148315022077	0.1472516356529141
5359	0.3347150886301336	0.1671986742976586	0.2216587028895063
5360	0.9975331289614289	0.4985522252363594	0.2981997891982360
5361	0.1664579819136520	0.8331184231156428	0.1472531815539568
5362	0.8320202789556035	0.1671976655457712	0.2216551159962776
5363	0.5003458941583787	0.4985385534834776	0.2982034743173116
5364	0.1664716690242827	0.3331591680943049	0.1472532709978935
5365	0.8320412351286137	0.6645272035418230	0.2216529894198871
5366	0.5003459234035645	0.0013612527476923	0.2982051450107335
5367	0.6660579718969473	0.3327991185170944	0.3300147611266695
5368	0.6458936681803422	0.8227080974651670	0.3302791283271560
5369	0.1761233598814087	0.8227024309599997	0.3302745270411691
5370	0.1761278575058611	0.3529745162184383	0.3302710612194772
5371			
5372	NiFe (25% Fe) 111 Facet with Hydrogen- [Etot = -135.21095788 eV]		
5373	1.0000000000000000		
5374	5.0134000778000001	0.0000000000000000	0.0000000000000000
5375	-2.5067000389000000	4.3417318267000002	0.0000000000000000
5376	0.0000000000000000	0.0000000000000000	28.1868000031000001
5377	Fe Ni H		
5378	5 15 4		
5379	Direct		
5380	0.3333300050000005	0.6666700239999983	0.0000000000000000
5381	0.0000000000000000	0.0000000000000000	0.0726099979999972
5382	0.6662828763873208	0.3330235014170100	0.1447311138440668
5383	0.3327231973685159	0.6661829303083664	0.2177619708974845
5384	0.9991927560594149	0.9993184186496649	0.2886579181628193
5385	0.3333300050000005	0.1666699949999995	0.0000000000000000
5386	0.0000000000000000	0.5000000000000000	0.0726099979999972
5387	0.8333299760000017	0.1666699949999995	0.0000000000000000
5388	0.5000000000000000	0.5000000000000000	0.0726099979999972
5389	0.8333299760000017	0.6666700239999983	0.0000000000000000
5390	0.5000000000000000	0.0000000000000000	0.0726099979999972
5391	0.6661210868015957	0.8329479620283919	0.1453801238364392

5392	0.3324523708088520	0.1660421566173227	0.2176519850724006
5393	0.9987301075191723	0.4991022366432531	0.2916035467694869
5394	0.1663816620648362	0.8329449420730910	0.1453809034130060
5395	0.8328791697473150	0.1660456819429328	0.2176503514642860
5396	0.4994275638290020	0.4991017308609074	0.2915997318325552
5397	0.1663776527502492	0.3332144498479508	0.1453817915961011
5398	0.8328748786328575	0.6664674635172929	0.2176487809767167
5399	0.4994480053002519	0.9998018203794885	0.2916006667510587
5400	0.665835888629223	0.3326384178016468	0.3222131573983802
5401	0.6501206759460700	0.8247834612875096	0.3223958586999132
5402	0.1737083350049815	0.8247921736975812	0.3223926994141593
5403	0.1736878244908695	0.3483404851620904	0.3223881491305676

5404

5405 NiCo (25% Co) 111 Facet with Hydrogen- [Etot = -127.17202572 eV]

5406 0.993794164815303

5407 5.0134000778000001 0.0000000000000000 0.0000000000000000

5408 -2.5067000389000000 4.3417318267000002 0.0000000000000000

5409 0.0000000000000000 0.0000000000000000 28.1868000031000001

5410 Co Ni H

5411 5 15 4

5412 Direct

5413 0.3333300050000005 0.6666700239999983 0.0000000000000000

5414 0.0000000000000000 0.0000000000000000 0.0726099979999972

5415 0.6664509065868529 0.3331470285872626 0.1455569304960562

5416 0.3328838536997765 0.6662885924160733 0.2182646706096492

5417 0.9991828333305222 0.9993560239047028 0.2894908644645042

5418 0.3333300050000005 0.1666699949999995 0.0000000000000000

5419 0.0000000000000000 0.5000000000000000 0.0726099979999972

5420 0.8333299760000017 0.1666699949999995 0.0000000000000000

5421 0.5000000000000000 0.5000000000000000 0.0726099979999972

5422 0.8333299760000017 0.6666700239999983 0.0000000000000000

5423 0.5000000000000000 0.0000000000000000 0.0726099979999972

5424 0.6665422253828197 0.8331940018247153 0.1451464456016609

5425 0.3324625712476035 0.1660740811147150 0.2173674754383867

5426 0.9983036350110837 0.4988759029581473 0.2916189651640764

5427 0.1664297071023597 0.8331891184786073 0.1451468819401498

5428 0.8330504602905435 0.1660756290318233 0.2173701755539952

5429 0.4995541794590608 0.4988876721814961 0.2916179578271638

5430 0.1664306594817617 0.3330947399576729 0.1451465485786727

5431 0.8330487718090254 0.6666538731670215 0.2173725991651168

5432 0.4994959982047575 0.0001049264441519 0.2916097662221233

5433 0.6658409291943812 0.3326507899467117 0.3226898938395379

5434 0.6686929380935140 0.8340926570365639 0.3220070308102834

5435 0.1644057143732098 0.8340573066844001 0.3220190428317053

5436 0.1644329838595269 0.3298411151418605 0.3220196652433884

5437

5438 Pure Ni 111 Facet with Hydrogen- [Etot = -119.88927303 eV]

5439 0.993602894269297

5440 5.0134000778000001 0.0000000000000000 0.0000000000000000

5441 -2.5067000389000000 4.3417318267000002 0.0000000000000000

5442 0.0000000000000000 0.0000000000000000 28.1868000031000001

5443 Ni H

5444	20	4		
5445	Direct			
5446	0.33333000500000005	0.6666700239999983	0.0000000000000000	
5447	0.0000000000000000	0.0000000000000000	0.0726099979999972	
5448	0.6666208622973642	0.3332971810225587	0.1447034909988005	
5449	0.3331436905877894	0.6664968355097969	0.2172928857295702	
5450	0.9996043162200721	0.9996576830244805	0.2909376149045144	
5451	0.33333000500000005	0.1666699949999995	0.0000000000000000	
5452	0.0000000000000000	0.5000000000000000	0.0726099979999972	
5453	0.8333299760000017	0.1666699949999995	0.0000000000000000	
5454	0.5000000000000000	0.5000000000000000	0.0726099979999972	
5455	0.8333299760000017	0.6666700239999983	0.0000000000000000	
5456	0.5000000000000000	0.0000000000000000	0.0726099979999972	
5457	0.6665973775892340	0.8332794472477758	0.1447586648177079	
5458	0.3332273208333660	0.1665387361151076	0.2172300408248802	
5459	0.9995610167718638	0.4996303378062592	0.2910084048294124	
5460	0.1666172577705751	0.8332725549696391	0.1447561486094031	
5461	0.8330938726272450	0.1665330491718251	0.2172356930721975	
5462	0.4996478067441501	0.4996083718177076	0.2910069419982193	
5463	0.1666193479634117	0.3333114927210516	0.1447551000173632	
5464	0.8330911909203493	0.6664060103010101	0.2172382548398843	
5465	0.4996497913759796	0.9997545894704274	0.2910071872704236	
5466	0.6662830919158154	0.3330046133606643	0.3215130235367738	
5467	0.6665897818466462	0.8331538324765688	0.3214095782127870	
5468	0.1661518285414303	0.8331968354946682	0.3214132773072507	
5469	0.1661478991905696	0.3326677660822028	0.3214158444132380	
5470				
5471	NiCu (25% Cu) 111 Facet with Hydrogen- [Etot = -110.72417251 eV]			
5472	0.998485100048875			
5473	5.0134000778000001	0.0000000000000000	0.0000000000000000	
5474	-2.5067000389000000	4.3417318267000002	0.0000000000000000	
5475	0.0000000000000000	0.0000000000000000	28.1868000031000001	
5476	Cu Ni H			
5477	5 15 4			
5478	Direct			
5479	0.33333000500000005	0.6666700239999983	0.0000000000000000	
5480	0.0000000000000000	0.0000000000000000	0.0726099979999972	
5481	0.6664517347050065	0.3331599770790845	0.1456153219306415	
5482	0.3329174736570195	0.6663192941991269	0.2176978360136559	
5483	0.9993370259116077	0.9994630440118115	0.2939016243843966	
5484	0.33333000500000005	0.1666699949999995	0.0000000000000000	
5485	0.0000000000000000	0.5000000000000000	0.0726099979999972	
5486	0.8333299760000017	0.1666699949999995	0.0000000000000000	
5487	0.5000000000000000	0.5000000000000000	0.0726099979999972	
5488	0.8333299760000017	0.6666700239999983	0.0000000000000000	
5489	0.5000000000000000	0.0000000000000000	0.0726099979999972	
5490	0.6666986443899887	0.8332760722964991	0.1448516968942428	
5491	0.3304230350210204	0.1650815876276610	0.2178670999307926	
5492	0.9998771938100788	0.4997405750080119	0.291449359195304	
5493	0.1663526842725815	0.8332667268250091	0.1448520245316161	
5494	0.8341511409224864	0.1651081646733417	0.2178757173438655	
5495	0.4992175629840929	0.4997949620170559	0.2914494712974829	

5496	0.1663625432440696	0.3329706385620526	0.1448516381694702
5497	0.8341418725824852	0.6687592152532815	0.2178791384339718
5498	0.4992244058331252	0.9990446150064543	0.2914493226960175
5499	0.6660740255735718	0.3328460666529125	0.3209286673490084
5500	0.6391268737773927	0.8193626416441049	0.3229180678013819
5501	0.1795241766552351	0.8193986265271107	0.3229211612605383
5502	0.1795035607552435	0.3597054939093951	0.3229207532906528
5503			
5504	NiZn (25% Zn) 111 Facet with Hydrogen- [Etot = -101.48473710 eV]		
5505	1.01038006037737		
5506	5.0134000778000001	0.0000000000000000	0.0000000000000000
5507	-2.5067000389000000	4.3417318267000002	0.0000000000000000
5508	0.0000000000000000	0.0000000000000000	28.1868000031000001
5509	Zn Ni H		
5510	5 15 4		
5511	Direct		
5512	0.33333000500000005	0.66667002399999983	0.00000000000000000
5513	0.00000000000000000	0.00000000000000000	0.07260999799999972
5514	0.6665112169105143	0.3332228912293900	0.1453121807534288
5515	0.3329752147847316	0.6663679056071743	0.2174056230466093
5516	0.9995744657170746	0.9996297098943572	0.2907585762757279
5517	0.33333000500000005	0.16666999499999995	0.00000000000000000
5518	0.00000000000000000	0.50000000000000000	0.07260999799999972
5519	0.8333299760000017	0.16666999499999995	0.00000000000000000
5520	0.50000000000000000	0.50000000000000000	0.07260999799999972
5521	0.8333299760000017	0.66667002399999983	0.00000000000000000
5522	0.50000000000000000	0.00000000000000000	0.07260999799999972
5523	0.6657456658664813	0.8328126719616904	0.1447571551476230
5524	0.3326569671536959	0.1662181924857720	0.2172112927635936
5525	0.0015234963119966	0.5006388164551794	0.2913906555288648
5526	0.1669351426730756	0.8328521677456990	0.1447597019669615
5527	0.8332082477984528	0.1661986593163007	0.2172170527759718
5528	0.4986832686427931	0.5006473095651032	0.2913934134931679
5529	0.1669461006573343	0.3339870994302530	0.1447566950928092
5530	0.8332083241538655	0.6667932527634832	0.2172125801249010
5531	0.4986716927588546	0.9977427611548464	0.2913953306519019
5532	0.6663009849460337	0.3330125628800715	0.3191221450760864
5533	0.6194891486179657	0.8096093056399880	0.3232250080973813
5534	0.1896746214357279	0.8096318438448051	0.3232290211557682
5535	0.1896656652726563	0.3797521076237871	0.3232285239802337
5536			
5537	Bare NiSc (30% Sc) 200 Facet - [Etot = -59.26045307 eV]		
5538	1.04735280294076		
5539	3.5422000885000000	0.0000000000000000	0.0000000000000000
5540	0.0000000000000000	3.5422000885000000	0.0000000000000000
5541	0.0000000000000000	0.0000000000000000	27.0844993591000005
5542	Sc Ni		
5543	3 7		
5544	Direct		
5545	0.00000000000000000	0.00000000000000000	0.00000000000000000
5546	0.00000000000000000	0.00000000000000000	0.1312859042261749
5547	0.00000000000000000	0.00000000000000000	0.2652545561185349

5548	0.5000000000000000	0.5000000000000000	0.0000000000000000
5549	0.0000000000000000	0.5000000000000000	0.0653899980000006
5550	0.5000000000000000	0.0000000000000000	0.0653899980000006
5551	0.5000000000000000	0.5000000000000000	0.1310034635120658
5552	0.0000000000000000	0.5000000000000000	0.1976849372197407
5553	0.5000000000000000	0.0000000000000000	0.1976849372197407
5554	0.5000000000000000	0.5000000000000000	0.2516505255088433
5555			
5556	Bare NiTi (30% Ti) 200 Facet - [Etot = -63.02218105 eV]		
5557	1.01798110552312		
5558	3.542200885000000	0.0000000000000000	0.0000000000000000
5559	0.0000000000000000	3.542200885000000	0.0000000000000000
5560	0.0000000000000000	0.0000000000000000	27.0844993591000005
5561	Ti Ni		
5562	3 7		
5563	Direct		
5564	0.0000000000000000	0.0000000000000000	0.0000000000000000
5565	-0.0000000000000000	0.0000000000000000	0.1312426529275885
5566	-0.0000000000000000	-0.0000000000000000	0.2648892700000515
5567	0.5000000000000000	0.5000000000000000	0.0000000000000000
5568	0.0000000000000000	0.5000000000000000	0.0653899980000006
5569	0.5000000000000000	0.0000000000000000	0.0653899980000006
5570	0.5000000000000000	0.5000000000000000	0.1309601012622824
5571	-0.0000000000000000	0.5000000000000000	0.1966007751060960
5572	0.5000000000000000	-0.0000000000000000	0.1966007751060960
5573	0.5000000000000000	0.5000000000000000	0.2572003691964161
5574			
5575	Bare NiV (25% V) 200 Facet - [Etot = -62.75957795 eV]		
5576	1.00458661266245		
5577	3.542200885000000	0.0000000000000000	0.0000000000000000
5578	0.0000000000000000	3.542200885000000	0.0000000000000000
5579	0.0000000000000000	0.0000000000000000	27.0844993591000005
5580	V Ni		
5581	3 7		
5582	Direct		
5583	0.0000000000000000	0.0000000000000000	0.0000000000000000
5584	0.0000000000000000	0.0000000000000000	0.1313102592749544
5585	0.0000000000000000	0.0000000000000000	0.2649128679249202
5586	0.5000000000000000	0.5000000000000000	0.0000000000000000
5587	0.0000000000000000	0.5000000000000000	0.0653899980000006
5588	0.5000000000000000	0.0000000000000000	0.0653899980000006
5589	0.5000000000000000	0.5000000000000000	0.1307333918986089
5590	0.0000000000000000	0.5000000000000000	0.1959074836131549
5591	0.5000000000000000	0.0000000000000000	0.1959074836131549
5592	0.5000000000000000	0.5000000000000000	0.2581471483085878
5593			
5594	Bare NiCr (30% Cr) 200 Facet - [Etot = -62.87764789 eV]		
5595	0.995572721824907		
5596	3.542200885000000	0.0000000000000000	0.0000000000000000
5597	0.0000000000000000	3.542200885000000	0.0000000000000000
5598	0.0000000000000000	0.0000000000000000	27.0844993591000005
5599	Cr Ni		

5600	3	7			
5601	Direct				
5602	0.0000000000000000	0.0000000000000000	0.0000000000000000		
5603	0.0000000000000000	0.0000000000000000	0.1317328421960511		
5604	0.0000000000000000	0.0000000000000000	0.2671042513257831		
5605	0.5000000000000000	0.5000000000000000	0.0000000000000000		
5606	0.0000000000000000	0.5000000000000000	0.0653899980000006		
5607	0.5000000000000000	0.0000000000000000	0.0653899980000006		
5608	0.5000000000000000	0.5000000000000000	0.1315838659237869		
5609	0.0000000000000000	0.5000000000000000	0.1975189857674522		
5610	0.5000000000000000	0.0000000000000000	0.1975189857674522		
5611	0.5000000000000000	0.5000000000000000	0.2604284135161024		
5612					
5613	Bare NiMn (25% Mn) 200 Facet - [Etot = -62.92430140 eV]				
5614	0.989317187668226				
5615	3.5422000885000000	0.0000000000000000	0.0000000000000000		
5616	0.0000000000000000	3.5422000885000000	0.0000000000000000		
5617	0.0000000000000000	0.0000000000000000	27.0844993591000005		
5618	Mn	Ni			
5619	3	7			
5620	Direct				
5621	0.0000000000000000	0.0000000000000000	0.0000000000000000		
5622	0.0000000000000000	0.0000000000000000	0.1337845967442135		
5623	0.0000000000000000	0.0000000000000000	0.2720593563633571		
5624	0.5000000000000000	0.5000000000000000	0.0000000000000000		
5625	0.0000000000000000	0.5000000000000000	0.0653899980000006		
5626	0.5000000000000000	0.0000000000000000	0.0653899980000006		
5627	0.5000000000000000	0.5000000000000000	0.1334605811899010		
5628	0.0000000000000000	0.5000000000000000	0.2015201312150339		
5629	0.5000000000000000	0.0000000000000000	0.2015201312150339		
5630	0.5000000000000000	0.5000000000000000	0.2655143964691931		
5631					
5632	Bare NiFe (30% Fe) 200 Facet - [Etot = -60.48459440 eV]				
5633	1.0000000000000000				
5634	3.5422000885000000	0.0000000000000000	0.0000000000000000		
5635	0.0000000000000000	3.5422000885000000	0.0000000000000000		
5636	0.0000000000000000	0.0000000000000000	27.0844993591000005		
5637	Fe	Ni			
5638	3	7			
5639	Direct				
5640	0.0000000000000000	0.0000000000000000	0.0000000000000000		
5641	0.0000000000000000	0.0000000000000000	0.1310262016318333		
5642	0.0000000000000000	0.0000000000000000	0.2623047982847879		
5643	0.5000000000000000	0.5000000000000000	0.0000000000000000		
5644	0.0000000000000000	0.5000000000000000	0.0653899980000006		
5645	0.5000000000000000	0.0000000000000000	0.0653899980000006		
5646	0.5000000000000000	0.5000000000000000	0.1309871519793404		
5647	0.0000000000000000	0.5000000000000000	0.1967624143260949		
5648	0.5000000000000000	0.0000000000000000	0.1967624143260949		
5649	0.5000000000000000	0.5000000000000000	0.2594996221837036		
5650					
5651	Bare NiCo (30% Co) 200 Facet - [Etot = -55.55706988 eV]				

5652	0.993794164815303		
5653	3.5422000885000000	0.0000000000000000	0.0000000000000000
5654	0.0000000000000000	3.5422000885000000	0.0000000000000000
5655	0.0000000000000000	0.0000000000000000	27.0844993591000005
5656	Co Ni		
5657	3 7		
5658	Direct		
5659	0.0000000000000000	0.0000000000000000	0.0000000000000000
5660	0.0000000000000000	0.0000000000000000	0.1310206751132910
5661	0.0000000000000000	0.0000000000000000	0.2612143230630863
5662	0.5000000000000000	0.5000000000000000	0.0000000000000000
5663	0.0000000000000000	0.5000000000000000	0.0653899980000006
5664	0.5000000000000000	0.0000000000000000	0.0653899980000006
5665	0.5000000000000000	0.5000000000000000	0.1310844068296859
5666	0.0000000000000000	0.5000000000000000	0.1970354134184120
5667	0.5000000000000000	0.0000000000000000	0.1970354134184120
5668	0.5000000000000000	0.5000000000000000	0.2602208148552378
5669			
5670	Pure Ni 200 Facet - [Etot = -50.89616180 eV]		
5671	1.01798110552312		
5672	3.5422000885000000	0.0000000000000000	0.0000000000000000
5673	0.0000000000000000	3.5422000885000000	0.0000000000000000
5674	0.0000000000000000	0.0000000000000000	27.0844993591000005
5675	Ni		
5676	10		
5677	Direct		
5678	0.0000000000000000	0.0000000000000000	0.0000000000000000
5679	0.0000000000000000	0.0000000000000000	0.1273596480353731
5680	0.0000000000000000	0.0000000000000000	0.2494919539913170
5681	0.5000000000000000	0.5000000000000000	0.0000000000000000
5682	0.0000000000000000	0.5000000000000000	0.0653899980000006
5683	0.5000000000000000	0.0000000000000000	0.0653899980000006
5684	0.5000000000000000	0.5000000000000000	0.1273483065571952
5685	0.0000000000000000	0.5000000000000000	0.1900511076671521
5686	0.5000000000000000	0.0000000000000000	0.1900511076671521
5687	0.5000000000000000	0.5000000000000000	0.2495026632962265
5688			
5689	Bare NiCu (30% Cu) 200 Facet - [Etot = -46.17902883 eV]		
5690	0.998485100048875		
5691	3.5422000885000000	0.0000000000000000	0.0000000000000000
5692	0.0000000000000000	3.5422000885000000	0.0000000000000000
5693	0.0000000000000000	0.0000000000000000	27.0844993591000005
5694	Cu Ni		
5695	3 7		
5696	Direct		
5697	0.0000000000000000	0.0000000000000000	0.0000000000000000
5698	0.0000000000000000	0.0000000000000000	0.1313632986931665
5699	0.0000000000000000	0.0000000000000000	0.2633617604973750
5700	0.5000000000000000	0.5000000000000000	0.0000000000000000
5701	0.0000000000000000	0.5000000000000000	0.0653899980000006
5702	0.5000000000000000	0.0000000000000000	0.0653899980000006
5703	0.5000000000000000	0.5000000000000000	0.1311633260883127

5704	0.0000000000000000	0.5000000000000000	0.1973624566677401
5705	0.5000000000000000	0.0000000000000000	0.1973624566677401
5706	0.5000000000000000	0.5000000000000000	0.2592972507347255
5707			
5708	Bare NiZn (30% Zn) 200 Facet - [Etot = -41.11663348 eV]		
5709	1.01038006037737		
5710	3.5422000885000000	0.0000000000000000	0.0000000000000000
5711	0.0000000000000000	3.5422000885000000	0.0000000000000000
5712	0.0000000000000000	0.0000000000000000	27.0844993591000005
5713	Zn Ni		
5714	3 7		
5715	Direct		
5716	0.0000000000000000	0.0000000000000000	0.0000000000000000
5717	0.0000000000000000	0.0000000000000000	0.1314133226571528
5718	0.0000000000000000	0.0000000000000000	0.2652804859278888
5719	0.5000000000000000	0.5000000000000000	0.0000000000000000
5720	0.0000000000000000	0.5000000000000000	0.0653899980000006
5721	0.5000000000000000	0.0000000000000000	0.0653899980000006
5722	0.5000000000000000	0.5000000000000000	0.1311807051115821
5723	0.0000000000000000	0.5000000000000000	0.1973788415422959
5724	0.5000000000000000	0.0000000000000000	0.1973788415422959
5725	0.5000000000000000	0.5000000000000000	0.2579351728787103
5726			
5727			
5728	NiSc (30% Sc) 200 Facet with Hydrogen- [Etot = -67.03527104 eV]		
5729	1.04735280294076		
5730	3.5422000885000000	0.0000000000000000	0.0000000000000000
5731	0.0000000000000000	3.5422000885000000	0.0000000000000000
5732	0.0000000000000000	0.0000000000000000	27.0844993591000005
5733	Sc Ni H		
5734	3 7 2		
5735	Direct		
5736	0.0000000000000000	0.0000000000000000	0.0000000000000000
5737	0.0000517642777567	0.0001076935102020	0.1312756564973228
5738	0.0001540908572224	0.0000173334462445	0.2662601816194226
5739	0.5000000000000000	0.5000000000000000	0.0000000000000000
5740	0.0000000000000000	0.5000000000000000	0.0653899980000006
5741	0.5000000000000000	0.0000000000000000	0.0653899980000006
5742	0.5000372546099925	0.5000937613436278	0.1308769681616866
5743	0.0000580093529905	0.5001344838060930	0.1987846428183886
5744	0.5001388356236873	0.0001089271383066	0.1972875155083216
5745	0.5001518299279581	0.4999642795064219	0.2565432901606144
5746	0.7542064239182480	0.5001187646399572	0.2986957229746992
5747	0.2465146217720431	0.4994482165003262	0.2987382819841073
5748			
5749	NiTi (30% Ti) 200 Facet with Hydrogen- [Etot = -70.35968884 eV]		
5750	1.01798110552312		
5751	3.5422000885000000	0.0000000000000000	0.0000000000000000
5752	0.0000000000000000	3.5422000885000000	0.0000000000000000
5753	0.0000000000000000	0.0000000000000000	27.0844993591000005
5754	Ti Ni H		
5755	3 7 2		

5756	Direct			
5757	0.0000000000000000	0.0000000000000000	0.0000000000000000	
5758	0.0000407950432617	0.0000185822378853	0.1311559569658769	
5759	0.0000577550735912	0.9999783822625616	0.2633925300940518	
5760	0.5000000000000000	0.5000000000000000	0.0000000000000000	
5761	0.0000000000000000	0.5000000000000000	0.0653899980000006	
5762	0.5000000000000000	0.0000000000000000	0.0653899980000006	
5763	0.5000343944288446	0.5000236870681718	0.1309098578560324	
5764	0.0000661415424972	0.5000286613433644	0.1963468885494493	
5765	0.5000578416998991	0.0000295409504076	0.1963571798055526	
5766	0.5000647652736916	0.5000044507151955	0.2596071578579782	
5767	0.6995089695718946	0.6972678772666541	0.3031421193651056	
5768	0.3006164132269475	0.3026715770286614	0.3031361338455412	
5769				
5770	NiV (30% V) 200 Facet with Hydrogen- [Etot = -70.48830245 eV]			
5771	1.00458661266245			
5772	3.5422000885000000	0.0000000000000000	0.0000000000000000	
5773	0.0000000000000000	3.5422000885000000	0.0000000000000000	
5774	0.0000000000000000	0.0000000000000000	27.0844993591000005	
5775	V Ni H			
5776	3 7 2			
5777	Direct			
5778	0.0000000000000000	0.0000000000000000	0.0000000000000000	
5779	0.0001646146820491	0.9998911400705168	0.1322127633544099	
5780	0.0006540084180671	0.9996718519031731	0.2656140809625924	
5781	0.5000000000000000	0.5000000000000000	0.0000000000000000	
5782	0.0000000000000000	0.5000000000000000	0.0653899980000006	
5783	0.5000000000000000	0.0000000000000000	0.0653899980000006	
5784	0.5001054402758243	0.4999328110211252	0.1302693240673776	
5785	0.0001253327637230	0.4999158335989691	0.1952501153034234	
5786	0.5001697954210087	0.9999404548861293	0.1952497886494911	
5787	0.5001541401233922	0.5000159507093613	0.2628201369126302	
5788	0.5008128722048610	0.9986967131592692	0.2894330383783768	
5789	0.0020808836916117	0.4995637554556751	0.2894307157568647	
5790				
5791	NiCr (30% Cr) 200 Facet with Hydrogen- [Etot = -70.69361570 eV]			
5792	0.995572721824907			
5793	3.5422000885000000	0.0000000000000000	0.0000000000000000	
5794	0.0000000000000000	3.5422000885000000	0.0000000000000000	
5795	0.0000000000000000	0.0000000000000000	27.0844993591000005	
5796	Cr Ni H			
5797	3 7 2			
5798	Direct			
5799	0.0000000000000000	0.0000000000000000	0.0000000000000000	
5800	0.0001127060387986	0.9999070388309477	0.1315446257106174	
5801	0.0004406733756497	0.9996922995738302	0.2657877565467217	
5802	0.5000000000000000	0.5000000000000000	0.0000000000000000	
5803	0.0000000000000000	0.5000000000000000	0.0653899980000006	
5804	0.5000000000000000	0.0000000000000000	0.0653899980000006	
5805	0.5001015913228670	0.4999543733385465	0.1314379698166945	
5806	0.0002026670038902	0.4998749192674055	0.1977589336876520	
5807	0.5002506630393739	0.9998358889145962	0.1977588444135918	

5808	0.5003994124556712	0.4997531899952747	0.2680138491720854
5809	0.5005756581370164	0.9992265851946627	0.2915923980874879
5810	0.0013032068978163	0.4996527847697436	0.2915901763759194
5811			
5812	NiMn (30% Mn) 200 Facet with Hydrogen- [Etot = -70.68252715 eV]		
5813	0.989317187668226		
5814	3.5422000885000000	0.0000000000000000	0.0000000000000000
5815	0.0000000000000000	3.5422000885000000	0.0000000000000000
5816	0.0000000000000000	0.0000000000000000	27.0844993591000005
5817	Mn Ni H		
5818	3 7 2		
5819	Direct		
5820	0.0000000000000000	0.0000000000000000	0.0000000000000000
5821	0.0001836385068970	0.9999170523314689	0.1337435197797632
5822	0.0004730655001097	0.9997410415264198	0.2715774266753215
5823	0.5000000000000000	0.5000000000000000	0.0000000000000000
5824	0.0000000000000000	0.5000000000000000	0.0653899980000006
5825	0.5000000000000000	0.0000000000000000	0.0653899980000006
5826	0.5001842032488000	0.4999035711441735	0.1343632002431221
5827	0.0002762977896964	0.4998464828861486	0.2022446587750011
5828	0.5002934814986517	0.9998603736401890	0.2022429474637448
5829	0.5004289264169728	0.4997911203137448	0.2717082868419922
5830	0.5005321777287008	0.9993895158493302	0.2958970725193026
5831	0.0009997011536313	0.4996740243047952	0.2958967202145288
5832			
5833	NiFe (30% Fe) 200 Facet with Hydrogen- [Etot = -64.31742027 eV]		
5834	1.0000000000000000		
5835	3.5422000885000000	0.0000000000000000	0.0000000000000000
5836	0.0000000000000000	3.5422000885000000	0.0000000000000000
5837	0.0000000000000000	0.0000000000000000	27.0844993591000005
5838	Fe Ni H		
5839	3 7 2		
5840	Direct		
5841	0.0000000000000000	0.0000000000000000	0.0000000000000000
5842	0.0006907491286031	0.9997258110894944	0.1303186326476950
5843	0.0013652580979092	0.9990569964874932	0.2626581305521456
5844	0.5000000000000000	0.5000000000000000	0.0000000000000000
5845	0.0000000000000000	0.5000000000000000	0.0653899980000006
5846	0.5000000000000000	0.0000000000000000	0.0653899980000006
5847	0.5007342091677482	0.4996618160056331	0.1314489825240394
5848	0.0010717460937783	0.4993391868699448	0.1963529672235798
5849	0.5011382742240513	0.9993262071561976	0.1963641260749912
5850	0.5013010413536825	0.4992311793354717	0.2639345393209585
5851	0.5015885550649007	0.9988492452206363	0.2838743503153899
5852	0.0019130523435243	0.4991432475134888	0.2838820249225652
5853			
5854	NiCo (30% Co) 200 Facet with Hydrogen- [Etot = -63.33402605 eV]		
5855	0.993794164815303		
5856	3.5422000885000000	0.0000000000000000	0.0000000000000000
5857	0.0000000000000000	3.5422000885000000	0.0000000000000000
5858	0.0000000000000000	0.0000000000000000	27.0844993591000005
5859	Co Ni H		

5860	3	7	2
5861	Direct		
5862	0.0000000000000000	0.0000000000000000	0.0000000000000000
5863	0.0002569082904245	0.9998379049835577	0.1314167072751644
5864	0.0006148345969095	0.9996334983620301	0.2632815133692503
5865	0.5000000000000000	0.5000000000000000	0.0000000000000000
5866	0.0000000000000000	0.5000000000000000	0.0653899980000006
5867	0.5000000000000000	0.0000000000000000	0.0653899980000006
5868	0.5002612504532067	0.4998568974363522	0.1313249638275806
5869	0.0004440903827287	0.4997498360635149	0.1964041040849764
5870	0.5004270155483965	0.9997295336240555	0.1964038407410413
5871	0.5006230143338328	0.4996300131835056	0.2635938551959214
5872	0.5007405011364270	0.9996506497489577	0.2812594986706500
5873	0.0007097765832142	0.4996023179219549	0.2812573656913600
5874			
5875	Pure Ni 200 Facet with Hydrogen- [Etot = -58.01666781 eV]		
5876	1.01798110552312		
5877	3.5422000885000000	0.0000000000000000	0.0000000000000000
5878	0.0000000000000000	3.5422000885000000	0.0000000000000000
5879	0.0000000000000000	0.0000000000000000	27.0844993591000005
5880	Ni H		
5881	10	2	
5882	Direct		
5883	0.0000000000000000	0.0000000000000000	0.0000000000000000
5884	0.0000331273925909	0.9999737049389807	0.1275634442078228
5885	0.0000676394244579	0.9999296566902984	0.2485699110005726
5886	0.5000000000000000	0.5000000000000000	0.0000000000000000
5887	0.0000000000000000	0.5000000000000000	0.0653899980000006
5888	0.5000000000000000	0.0000000000000000	0.0653899980000006
5889	0.5000289063123162	0.4999813833875848	0.1268402821457428
5890	0.0000676849283181	0.4999432724318709	0.1896360106868045
5891	0.5000651046115863	0.9999540934593369	0.1896322954618981
5892	0.5000664984250278	0.4999247888854512	0.2526911626051103
5893	0.5879024323548094	0.5861695052393117	0.3079721527077837
5894	0.4122199999215113	0.4138576833145464	0.3079768214322129
5895			
5896	NiCu (30% Cu) 200 Facet with Hydrogen- [Etot = -53.77002599 eV]		
5897	0.998485100048875		
5898	3.5422000885000000	0.0000000000000000	0.0000000000000000
5899	0.0000000000000000	3.5422000885000000	0.0000000000000000
5900	0.0000000000000000	0.0000000000000000	27.0844993591000005
5901	Cu Ni H		
5902	3	7	2
5903	Direct		
5904	0.0000000000000000	0.0000000000000000	0.0000000000000000
5905	0.0004750546013668	0.9996894528271199	0.1314202166295644
5906	0.0011957462777730	0.9992821758343382	0.2661845044205364
5907	0.5000000000000000	0.5000000000000000	0.0000000000000000
5908	0.0000000000000000	0.5000000000000000	0.0653899980000006
5909	0.5000000000000000	0.0000000000000000	0.0653899980000006
5910	0.5004739234317555	0.4997330704985501	0.1315848105200601
5911	0.0008384116497453	0.4995230820232592	0.1968234985293549

5912	0.5008125355304145	0.9994851655604009	0.1968238507762905
5913	0.5011268276712073	0.4993304598247263	0.2655097765972201
5914	0.5013440898142605	0.9991142878898032	0.2818169470759955
5915	0.0015048429765514	0.4991980545378780	0.2818205938126681

5916

5917 NiZn (30% Zn) 200 Facet with Hydrogen- [Etot = -48.26799493 eV]

5918 1.01038006037737

5919 3.5422000885000000 0.0000000000000000 0.0000000000000000

5920 0.0000000000000000 3.5422000885000000 0.0000000000000000

5921 0.0000000000000000 0.0000000000000000 27.0844993591000005

5922 Zn Ni H

5923 3 7 2

5924 Direct

5925 0.0000000000000000 0.0000000000000000 0.0000000000000000

5926 -0.0001000990030342 0.0003806786205839 0.1312847376188165

5927 -0.0001953917743792 0.0003451177264793 0.2621722241881438

5928 0.5000000000000000 0.5000000000000000 0.0000000000000000

5929 0.0000000000000000 0.5000000000000000 0.0653899980000006

5930 0.5000000000000000 0.0000000000000000 0.0653899980000006

5931 0.4999768877092408 0.5004000331043875 0.1311246958887670

5932 -0.0000956458499871 0.5004789064502541 0.1969041008951693

5933 0.4997291529015526 0.0002966051735593 0.1968895917328777

5934 0.4999010504543327 0.5002938249053722 0.2641710190135788

5935 0.5880727494360842 0.5850200771673191 0.3208355948047200

5936 0.4127291958212252 0.4142228057435987 0.3208103028303055

5937

5938

5939

5940 Bare NiSc (28.57% Sc) 220 Facet - [Etot = -82.19892257 eV]

5941 1.04735280294076

5942 3.5450000763000000 0.0000000000000000 0.0000000000000000

5943 0.0000000000000000 5.0134000778000001 0.0000000000000000

5944 0.0000000000000000 0.0000000000000000 27.5200996398999997

5945 Ti Ni

5946 4 10

5947 Direct

5948 0.0000000000000000 0.5000000000000000 0.0000000000000000

5949 0.0000000000000000 0.0000000000000000 0.0910900009999978

5950 0.0000000000000000 0.5000000000000000 0.1814129549948973

5951 0.0000000000000000 0.0000000000000000 0.2737207834881445

5952 0.0000000000000000 0.0000000000000000 0.0000000000000000

5953 0.5000000000000000 0.2500000000000000 0.0455400009999991

5954 0.5000000000000000 0.7500000000000000 0.0455400009999991

5955 0.0000000000000000 0.5000000000000000 0.0910900009999978

5956 0.5000000000000000 0.7520103422324809 0.1370254515899845

5957 0.5000000000000000 0.2479896577675191 0.1370254515899845

5958 0.0000000000000000 0.0000000000000000 0.1845186708041098

5959 0.5000000000000000 0.2461441991371771 0.2301315707850335

5960 0.5000000000000000 0.7538558008628229 0.2301315707850335

5961 0.0000000000000000 0.5000000000000000 0.2667671605914421

5962

5963 Bare NiTi (28.57% Ti) 220 Facet - [Etot = -87.22227187 eV]

5964	1.01798110552312		
5965	3.5450000763000000	0.0000000000000000	0.0000000000000000
5966	0.0000000000000000	5.0134000778000001	0.0000000000000000
5967	0.0000000000000000	0.0000000000000000	27.5200996398999997
5968	Ti Ni		
5969	4 10		
5970	Direct		
5971	0.0000000000000000	0.5000000000000000	0.0000000000000000
5972	0.0000000000000000	0.0000000000000000	0.0910900009999978
5973	0.0000000000000000	0.5000000000000000	0.1833059258352989
5974	0.0000000000000000	0.0000000000000000	0.2696591452685482
5975	0.0000000000000000	0.0000000000000000	0.0000000000000000
5976	0.5000000000000000	0.2500000000000000	0.0455400009999991
5977	0.5000000000000000	0.7500000000000000	0.0455400009999991
5978	0.0000000000000000	0.5000000000000000	0.0910900009999978
5979	0.5000000000000000	0.7499617181842524	0.1375903862375409
5980	0.5000000000000000	0.2500382818157476	0.1375903862375409
5981	0.0000000000000000	0.0000000000000000	0.1838549078102503
5982	0.5000000000000000	0.2454038667961100	0.2307959998963938
5983	0.5000000000000000	0.7545961332038900	0.2307959998963938
5984	0.0000000000000000	0.5000000000000000	0.2685540049113442
5985			
5986	Bare NiV (28.57% V) 220 Facet - [Etot = -87.15577727 eV]		
5987	1.01798110552312		
5988	3.5450000763000000	0.0000000000000000	0.0000000000000000
5989	0.0000000000000000	5.0134000778000001	0.0000000000000000
5990	0.0000000000000000	0.0000000000000000	27.5200996398999997
5991	Ti Ni		
5992	4 10		
5993	Direct		
5994	0.0000000000000000	0.5000000000000000	0.0000000000000000
5995	0.0000000000000000	0.0000000000000000	0.0910900009999978
5996	0.0000000000000000	0.5000000000000000	0.1817785925848625
5997	0.0000000000000000	0.0000000000000000	0.2680857924438840
5998	0.0000000000000000	0.0000000000000000	0.0000000000000000
5999	0.5000000000000000	0.2500000000000000	0.0455400009999991
6000	0.5000000000000000	0.7500000000000000	0.0455400009999991
6001	0.0000000000000000	0.5000000000000000	0.0910900009999978
6002	0.5000000000000000	0.7494768084158636	0.1352267940461829
6003	0.5000000000000000	0.2505231915841364	0.1352267940461829
6004	0.0000000000000000	0.0000000000000000	0.1792037315087782
6005	0.5000000000000000	0.2445923261349066	0.2251595608406518
6006	0.5000000000000000	0.7554076738650934	0.2251595608406518
6007	0.0000000000000000	0.5000000000000000	0.2641561484325621
6008			
6009	Bare NiCr (28.57% Cr) 220 Facet - [Etot = -87.39538807 eV]		
6010	0.995572721824907		
6011	3.5450000763000000	0.0000000000000000	0.0000000000000000
6012	0.0000000000000000	5.0134000778000001	0.0000000000000000
6013	0.0000000000000000	0.0000000000000000	27.5200996398999997
6014	Cr Ni		
6015	4 10		

6016	Direct			
6017		0.0000000000000000	0.5000000000000000	0.0000000000000000
6018		0.0000000000000000	0.0000000000000000	0.0910900009999978
6019		0.0000000000000000	0.5000000000000000	0.1841174964431147
6020		0.0000000000000000	0.0000000000000000	0.2755097899507106
6021		0.0000000000000000	0.0000000000000000	0.0000000000000000
6022		0.5000000000000000	0.2500000000000000	0.0455400009999991
6023		0.5000000000000000	0.7500000000000000	0.0455400009999991
6024		0.0000000000000000	0.5000000000000000	0.0910900009999978
6025		0.5000000000000000	0.7491851831162890	0.1371621917744363
6026		0.5000000000000000	0.2508148168837110	0.1371621917744363
6027		0.0000000000000000	0.0000000000000000	0.1818701758089034
6028		0.5000000000000000	0.2485455198952877	0.2291487382866109
6029		0.5000000000000000	0.7514544801047123	0.2291487382866109
6030		0.0000000000000000	0.5000000000000000	0.2703211703465271
6031				
6032	Bare NiMn (28.57% Mn) 220 Facet - [Etot = -87.18222007 eV]			
6033		1.01798110552312		
6034		3.5450000763000000	0.0000000000000000	0.0000000000000000
6035		0.0000000000000000	5.0134000778000001	0.0000000000000000
6036		0.0000000000000000	0.0000000000000000	27.5200996398999997
6037	Ti Ni			
6038	4 10			
6039	Direct			
6040		0.0000000000000000	0.5000000000000000	0.0000000000000000
6041		0.0000000000000000	0.0000000000000000	0.0910900009999978
6042		0.0000000000000000	0.5000000000000000	0.1796695249021951
6043		0.0000000000000000	0.0000000000000000	0.2691625721429673
6044		0.0000000000000000	0.0000000000000000	0.0000000000000000
6045		0.5000000000000000	0.2500000000000000	0.0455400009999991
6046		0.5000000000000000	0.7500000000000000	0.0455400009999991
6047		0.0000000000000000	0.5000000000000000	0.0910900009999978
6048		0.5000000000000000	0.7502404582143285	0.1355969428589532
6049		0.5000000000000000	0.2497595417856715	0.1355969428589532
6050		0.0000000000000000	0.0000000000000000	0.1803489673500636
6051		0.5000000000000000	0.2496042979322937	0.2260279615156833
6052		0.5000000000000000	0.7503957020677063	0.2260279615156833
6053		0.0000000000000000	0.5000000000000000	0.2648725973890151
6054				
6055	Bare NiFe (28.57% Fe) 220 Facet - [Etot = -83.94041813 eV]			
6056		1.0000000000000000		
6057		3.5450000763000000	0.0000000000000000	0.0000000000000000
6058		0.0000000000000000	5.0134000778000001	0.0000000000000000
6059		0.0000000000000000	0.0000000000000000	27.5200996398999997
6060	Fe Ni			
6061	4 10			
6062	Direct			
6063		0.0000000000000000	0.5000000000000000	0.0000000000000000
6064		0.0000000000000000	0.0000000000000000	0.0910900009999978
6065		0.0000000000000000	0.5000000000000000	0.1827931444331625
6066		0.0000000000000000	0.0000000000000000	0.2701758164477894
6067		0.0000000000000000	0.0000000000000000	0.0000000000000000

6068	0.5000000000000000	0.2500000000000000	0.0455400009999991
6069	0.5000000000000000	0.7500000000000000	0.0455400009999991
6070	0.0000000000000000	0.5000000000000000	0.0910900009999978
6071	0.5000000000000000	0.7500119520163935	0.1372950642117701
6072	0.5000000000000000	0.2499880479836065	0.1372950642117701
6073	0.0000000000000000	0.0000000000000000	0.1830476252628443
6074	0.5000000000000000	0.2486959908710560	0.2304854736194244
6075	0.5000000000000000	0.7513040091289440	0.2304854736194244
6076	0.0000000000000000	0.5000000000000000	0.2697993978265814
6077			
6078	Bare NiCo (28.57% Co) 220 Facet - [Etot = -77.30883532 eV]		
6079	0.993794164815303		
6080	3.5450000763000000	0.0000000000000000	0.0000000000000000
6081	0.0000000000000000	5.0134000778000001	0.0000000000000000
6082	0.0000000000000000	0.0000000000000000	27.5200996398999997
6083	Co Ni		
6084	4 10		
6085	Direct		
6086	0.0000000000000000	0.5000000000000000	0.0000000000000000
6087	0.0000000000000000	0.0000000000000000	0.0910900009999978
6088	0.0000000000000000	0.5000000000000000	0.1826907547229766
6089	0.0000000000000000	0.0000000000000000	0.2696660201127727
6090	0.0000000000000000	0.0000000000000000	0.0000000000000000
6091	0.5000000000000000	0.2500000000000000	0.0455400009999991
6092	0.5000000000000000	0.7500000000000000	0.0455400009999991
6093	0.0000000000000000	0.5000000000000000	0.0910900009999978
6094	0.5000000000000000	0.7493507901032075	0.1370025999022246
6095	0.5000000000000000	0.2506492098967925	0.1370025999022246
6096	0.0000000000000000	0.0000000000000000	0.1819664213974974
6097	0.5000000000000000	0.2487151031307917	0.2299591562094037
6098	0.5000000000000000	0.7512848968692083	0.2299591562094037
6099	0.0000000000000000	0.5000000000000000	0.2697273579343289
6100			
6101	Bare Pure-Ni 220 Facet - [Etot = -70.95118829 eV]		
6102	1.01798110552312		
6103	3.5450000763000000	0.0000000000000000	0.0000000000000000
6104	0.0000000000000000	5.0134000778000001	0.0000000000000000
6105	0.0000000000000000	0.0000000000000000	27.5200996398999997
6106	Ni		
6107	14		
6108	Direct		
6109	0.0000000000000000	0.5000000000000000	0.0000000000000000
6110	0.0000000000000000	0.0000000000000000	0.0910900009999978
6111	0.0000000000000000	0.5000000000000000	0.1770422364030537
6112	0.0000000000000000	0.0000000000000000	0.2608398138929076
6113	0.0000000000000000	0.0000000000000000	0.0000000000000000
6114	0.5000000000000000	0.2500000000000000	0.0455400009999991
6115	0.5000000000000000	0.7500000000000000	0.0455400009999991
6116	0.0000000000000000	0.5000000000000000	0.0910900009999978
6117	0.5000000000000000	0.7499626033605793	0.1338818603876248
6118	0.5000000000000000	0.2500373966394207	0.1338818603876248
6119	0.0000000000000000	0.0000000000000000	0.1770081288543039

6120	0.5000000000000000	0.2500232954063648	0.2230343063240099
6121	0.5000000000000000	0.7499767045936352	0.2230343063240099
6122	0.0000000000000000	0.5000000000000000	0.2608656262583082
6123			
6124			
6125	Bare NiCu (28.57% Cu) 220 Facet - [Etot = -64.65470018 eV]		
6126	0.998485100048875		
6127	3.5450000763000000	0.0000000000000000	0.0000000000000000
6128	0.0000000000000000	5.0134000778000001	0.0000000000000000
6129	0.0000000000000000	0.0000000000000000	27.5200996398999997
6130	Cu Ni		
6131	4 10		
6132	Direct		
6133	0.0000000000000000	0.5000000000000000	0.0000000000000000
6134	0.0000000000000000	0.0000000000000000	0.0910900009999978
6135	0.0000000000000000	0.5000000000000000	0.1814407851904036
6136	0.0000000000000000	0.0000000000000000	0.2732427264603103
6137	0.0000000000000000	0.0000000000000000	0.0000000000000000
6138	0.5000000000000000	0.2500000000000000	0.0455400009999991
6139	0.5000000000000000	0.7500000000000000	0.0455400009999991
6140	0.0000000000000000	0.5000000000000000	0.0910900009999978
6141	0.5000000000000000	0.7508344608217214	0.1368888301452316
6142	0.5000000000000000	0.2491655391782786	0.1368888301452316
6143	0.0000000000000000	0.0000000000000000	0.1827482707795909
6144	0.5000000000000000	0.2512558193052570	0.2289303671017677
6145	0.5000000000000000	0.7487441806947430	0.2289303671017677
6146	0.0000000000000000	0.5000000000000000	0.2698793109472390
6147			
6148	Bare NiZn (28.57% Zn) 220 Facet - [Etot = -57.70415899 eV]		
6149	1.01038006037737		
6150	3.5450000763000000	0.0000000000000000	0.0000000000000000
6151	0.0000000000000000	5.0134000778000001	0.0000000000000000
6152	0.0000000000000000	0.0000000000000000	27.5200996398999997
6153	Zn Ni		
6154	4 10		
6155	Direct		
6156	0.0000000000000000	0.5000000000000000	0.0000000000000000
6157	0.0000000000000000	0.0000000000000000	0.0910900009999978
6158	0.0000000000000000	0.5000000000000000	0.1811932639445004
6159	0.0000000000000000	0.0000000000000000	0.2738217275372961
6160	0.0000000000000000	0.0000000000000000	0.0000000000000000
6161	0.5000000000000000	0.2500000000000000	0.0455400009999991
6162	0.5000000000000000	0.7500000000000000	0.0455400009999991
6163	0.0000000000000000	0.5000000000000000	0.0910900009999978
6164	0.5000000000000000	0.7506666104335764	0.1366888405304465
6165	0.5000000000000000	0.2493333895664236	0.1366888405304465
6166	0.0000000000000000	0.0000000000000000	0.1823815719361903
6167	0.5000000000000000	0.2480670550393498	0.2285578138307471
6168	0.5000000000000000	0.7519329449606502	0.2285578138307471
6169	0.0000000000000000	0.5000000000000000	0.2689292886038714
6170			
6171	NiSc (28.57% Sc) 220 Facet with Hydrogen- [Etot = -86.22694515 eV]		

6172	1.04735280294076		
6173	3.5450000763000000	0.0000000000000000	0.0000000000000000
6174	0.0000000000000000	5.0134000778000001	0.0000000000000000
6175	0.0000000000000000	0.0000000000000000	27.5200996398999997
6176	Ti Ni H		
6177	4 10 1		
6178	Direct		
6179	0.0000000000000000	0.5000000000000000	0.0000000000000000
6180	0.0000000000000000	0.0000000000000000	0.09109000099999978
6181	0.0000000000000000	0.5006156562202335	0.1803074518768426
6182	0.0000000000000000	0.0009265686610220	0.2742702427132144
6183	0.0000000000000000	0.0000000000000000	0.0000000000000000
6184	0.5000000000000000	0.2500000000000000	0.04554000099999991
6185	0.5000000000000000	0.7500000000000000	0.04554000099999991
6186	0.0000000000000000	0.5000000000000000	0.09109000099999978
6187	0.5000000000000000	0.7528116475667588	0.1372439226789055
6188	0.5000000000000000	0.2479268130705492	0.1372286140753332
6189	0.0000000000000000	0.0006665742537706	0.1854128314653565
6190	0.5000000000000000	0.2435312571991517	0.2312203995928144
6191	0.5000000000000000	0.7581292775655086	0.2312147036036976
6192	0.0000000000000000	0.5009368390732050	0.2670653684875290
6193	0.5000000000000000	0.5009052849659454	0.2693518237170878
6194			
6195	NiTi (28.57% Ti) 220 Facet with Hydrogen- [Etot = -90.56844229 eV]		
6196	1.01798110552312		
6197	3.5450000763000000	0.0000000000000000	0.0000000000000000
6198	0.0000000000000000	5.0134000778000001	0.0000000000000000
6199	0.0000000000000000	0.0000000000000000	27.5200996398999997
6200	Ti Ni H		
6201	4 10 1		
6202	Direct		
6203	0.0000000000000000	0.5000000000000000	0.0000000000000000
6204	0.0000000000000000	0.0000000000000000	0.09109000099999978
6205	0.0000000000000000	0.5004396523593755	0.1817389398222886
6206	0.0000000000000000	0.0007568305826595	0.2732976233555036
6207	0.0000000000000000	0.0000000000000000	0.0000000000000000
6208	0.5000000000000000	0.2500000000000000	0.04554000099999991
6209	0.5000000000000000	0.7500000000000000	0.04554000099999991
6210	0.0000000000000000	0.5000000000000000	0.09109000099999978
6211	0.5000000000000000	0.7508216659517828	0.1377733946018935
6212	0.5000000000000000	0.2497908856160436	0.1377809712270235
6213	0.0000000000000000	0.0005875996001237	0.1841498514523821
6214	0.5000000000000000	0.2435361570216088	0.2303341756020316
6215	0.5000000000000000	0.7578697427998051	0.2303266964048092
6216	0.0000000000000000	0.5007865941741230	0.2694182615203005
6217	0.5000000000000000	0.5010060690450189	0.2741360535429820
6218			
6219	NiV (28.57% V) 220 Facet with Hydrogen- [Etot = -90.73268590 eV]		
6220	1.01798110552312		
6221	3.5450000763000000	0.0000000000000000	0.0000000000000000
6222	0.0000000000000000	5.0134000778000001	0.0000000000000000
6223	0.0000000000000000	0.0000000000000000	27.5200996398999997

6224	Ti	Ni	H
6225	4	10	1
6226	Direct		
6227	0.0000000000000000	0.5000000000000000	0.0000000000000000
6228	0.0000000000000000	0.0000000000000000	0.0910900009999978
6229	0.0000000000000000	0.5004155288131500	0.1794392912242273
6230	0.0000000000000000	0.0007952116385681	0.2697318379972273
6231	0.0000000000000000	0.0000000000000000	0.0000000000000000
6232	0.5000000000000000	0.2500000000000000	0.0455400009999991
6233	0.5000000000000000	0.7500000000000000	0.0455400009999991
6234	0.0000000000000000	0.5000000000000000	0.0910900009999978
6235	0.5000000000000000	0.7503244523076162	0.1354391602529290
6236	0.5000000000000000	0.2502223371901451	0.1354378216511662
6237	0.0000000000000000	0.0005089078136606	0.1799285628230862
6238	0.5000000000000000	0.2449585502163458	0.2255441182003892
6239	0.5000000000000000	0.7565045005275621	0.2255334014921999
6240	0.0000000000000000	0.5008092505014403	0.2642344246699224
6241	0.5000000000000000	0.5011428366572801	0.2690981329499493
6242			
6243	NiCr (28.57% Cr) 220 Facet with Hydrogen- [Etot = -91.18828281 eV]		
6244	0.995572721824907		
6245	3.5450000763000000	0.0000000000000000	0.0000000000000000
6246	0.0000000000000000	5.0134000778000001	0.0000000000000000
6247	0.0000000000000000	0.0000000000000000	27.5200996398999997
6248	Cr	Ni	H
6249	4	10	1
6250	Direct		
6251	0.0000000000000000	0.5000000000000000	0.0000000000000000
6252	0.0000000000000000	0.0000000000000000	0.0910900009999978
6253	0.0000000000000000	0.5005928459111786	0.1824263349284365
6254	0.0000000000000000	0.0009469068285171	0.2768359428721681
6255	0.0000000000000000	0.0000000000000000	0.0000000000000000
6256	0.5000000000000000	0.2500000000000000	0.0455400009999991
6257	0.5000000000000000	0.7500000000000000	0.0455400009999991
6258	0.0000000000000000	0.5000000000000000	0.0910900009999978
6259	0.5000000000000000	0.7500256209979668	0.1373861175386324
6260	0.5000000000000000	0.2506499651781340	0.1373824745066869
6261	0.0000000000000000	0.0005928537548172	0.1824483648522204
6262	0.5000000000000000	0.2484367574184319	0.2295967273708541
6263	0.5000000000000000	0.7533358554561218	0.2296021261864709
6264	0.0000000000000000	0.5008913799408177	0.2709969933303213
6265	0.5000000000000000	0.5017140655950101	0.2762917420319368
6266			
6267	NiMn (28.57% Mn) 220 Facet with Hydrogen- [Etot = -91.11217186 eV]		
6268	1.01798110552312		
6269	3.5450000763000000	0.0000000000000000	0.0000000000000000
6270	0.0000000000000000	5.0134000778000001	0.0000000000000000
6271	0.0000000000000000	0.0000000000000000	27.5200996398999997
6272	Ti	Ni	H
6273	4	10	1
6274	Direct		
6275	0.0000000000000000	0.5000000000000000	0.0000000000000000

6276	0.0000000000000000	0.0000000000000000	0.0910900009999978
6277	0.0000000000000000	0.5005859063218310	0.1791657418979469
6278	0.0000000000000000	0.0008774712756363	0.2698645286406247
6279	0.0000000000000000	0.0000000000000000	0.0000000000000000
6280	0.5000000000000000	0.2500000000000000	0.0455400009999991
6281	0.5000000000000000	0.7500000000000000	0.0455400009999991
6282	0.0000000000000000	0.5000000000000000	0.0910900009999978
6283	0.5000000000000000	0.7507004521380196	0.1357621244219303
6284	0.5000000000000000	0.2499908442078365	0.1357575024005939
6285	0.0000000000000000	0.0006701567114220	0.1805834788524479
6286	0.5000000000000000	0.2480935047717452	0.2269381325686837
6287	0.5000000000000000	0.7536901421922479	0.2269436923782138
6288	0.0000000000000000	0.5009391619907078	0.2654099180810263
6289	0.5000000000000000	0.5009993740461525	0.2698124332647041

6290

6291 NiFe (28.57% Fe) 220 Facet with Hydrogen- [Etot = -87.68000922 eV]

6292 1.0000000000000000

6293 3.5450000763000000 0.0000000000000000 0.0000000000000000

6294 0.0000000000000000 5.0134000778000001 0.0000000000000000

6295 0.0000000000000000 0.0000000000000000 27.5200996398999997

6296 Fe Ni H

6297 4 10 1

6298 Direct

6299 0.0000000000000000 0.5000000000000000 0.0000000000000000

6300 0.0000000000000000 0.0000000000000000 0.0910900009999978

6301 0.0000000000000000 0.5006674538188065 0.1816213631462489

6302 0.0000000000000000 0.0011434869506814 0.2705856558411242

6303 0.0000000000000000 0.0000000000000000 0.0000000000000000

6304 0.5000000000000000 0.2500000000000000 0.0455400009999991

6305 0.5000000000000000 0.7500000000000000 0.0455400009999991

6306 0.0000000000000000 0.5000000000000000 0.0910900009999978

6307 0.5000000000000000 0.7500813655165572 0.1375012094126262

6308 0.5000000000000000 0.2502176953858779 0.1375169688247766

6309 0.0000000000000000 0.0009090184406588 0.1834368880791004

6310 0.5000000000000000 0.2474551700604763 0.2312548558982925

6311 0.5000000000000000 0.7549227083700103 0.2311636349134503

6312 0.0000000000000000 0.5014226833279380 0.2704856048295099

6313 0.5000000000000000 0.5021489462762219 0.2773796174304124

6314

6315 NiCo (28.57% Co) 220 Facet with Hydrogen- [Etot = -81.06656270 eV]

6316 0.993794164815303

6317 3.5450000763000000 0.0000000000000000 0.0000000000000000

6318 0.0000000000000000 5.0134000778000001 0.0000000000000000

6319 0.0000000000000000 0.0000000000000000 27.5200996398999997

6320 Co Ni H

6321 4 10 1

6322 Direct

6323 0.0000000000000000 0.5000000000000000 0.0000000000000000

6324 0.0000000000000000 0.0000000000000000 0.0910900009999978

6325 0.0000000000000000 0.5006076576684748 0.1817539678007449

6326 0.0000000000000000 0.0010080352707078 0.2702541568500294

6327 0.0000000000000000 0.0000000000000000 0.0000000000000000

6328	0.5000000000000000	0.2500000000000000	0.0455400009999991
6329	0.5000000000000000	0.7500000000000000	0.0455400009999991
6330	0.0000000000000000	0.5000000000000000	0.0910900009999978
6331	0.5000000000000000	0.7497053031272642	0.1371837000970970
6332	0.5000000000000000	0.2509801844542423	0.1371856544743224
6333	0.0000000000000000	0.0006244354208533	0.1821400377001510
6334	0.5000000000000000	0.2467803464317697	0.2302754645082814
6335	0.5000000000000000	0.7550103988112227	0.2302757940889606
6336	0.0000000000000000	0.5009881099977349	0.2702853248725603
6337	0.5000000000000000	0.5014031044564788	0.2776670678421667

6338

6339 Pure-Ni 220 Facet with Hydrogen- [Etot = -74.80999210 eV]

6340 1.01798110552312

6341	3.5450000763000000	0.0000000000000000	0.0000000000000000
6342	0.0000000000000000	5.0134000778000001	0.0000000000000000
6343	0.0000000000000000	0.0000000000000000	27.5200996398999997

6344 Ni H

6345 14 1

6346 Direct

6347	0.0000000000000000	0.5000000000000000	0.0000000000000000
6348	0.0000000000000000	0.0000000000000000	0.0910900009999978
6349	0.0000000000000000	0.5005528740471661	0.1765879707314681
6350	0.0000000000000000	0.0010249932991115	0.2613633713841779
6351	0.0000000000000000	0.0000000000000000	0.0000000000000000
6352	0.5000000000000000	0.2500000000000000	0.0455400009999991
6353	0.5000000000000000	0.7500000000000000	0.0455400009999991
6354	0.0000000000000000	0.5000000000000000	0.0910900009999978
6355	0.5000000000000000	0.7503478228563694	0.1340716236893016
6356	0.5000000000000000	0.2502320783952854	0.1340781500641768
6357	0.0000000000000000	0.0005610433605483	0.1773058967092851
6358	0.5000000000000000	0.2477519478970081	0.2235940306424027
6359	0.5000000000000000	0.7540811635547158	0.2235751529770909
6360	0.0000000000000000	0.5010386575672570	0.2614494377713896
6361	0.5000000000000000	0.5010357849091207	0.2672000694472558

6362

6363 NiCu (28.57% Cu) 220 Facet with Hydrogen- [Etot = -68.59221313 eV]

6364 0.998485100048875

6365	3.5450000763000000	0.0000000000000000	0.0000000000000000
6366	0.0000000000000000	5.0134000778000001	0.0000000000000000
6367	0.0000000000000000	0.0000000000000000	27.5200996398999997

6368 Cu Ni H

6369 4 10 1

6370 Direct

6371	0.0000000000000000	0.5000000000000000	0.0000000000000000
6372	0.0000000000000000	0.0000000000000000	0.0910900009999978
6373	0.0000000000000000	0.5005952249441492	0.1814391025104172
6374	0.0000000000000000	0.0009420864809329	0.2733180413450214
6375	0.0000000000000000	0.0000000000000000	0.0000000000000000
6376	0.5000000000000000	0.2500000000000000	0.0455400009999991
6377	0.5000000000000000	0.7500000000000000	0.0455400009999991
6378	0.0000000000000000	0.5000000000000000	0.0910900009999978
6379	0.5000000000000000	0.7510627687985263	0.1370116293832382

6380	0.5000000000000000	0.2495018696824189	0.1370111217303034
6381	0.0000000000000000	0.0005481720202027	0.1824709950709291
6382	0.5000000000000000	0.2486801224617352	0.2291948314310375
6383	0.5000000000000000	0.7529847458723182	0.2291889466524424
6384	0.0000000000000000	0.5008973721816758	0.2706697324607603
6385	0.5000000000000000	0.5009225677613642	0.2752888216974085

6386

6387 NiZn (28.57% Zn) 220 Facet with Hydrogen- [Etot = -61.77210979 eV]

6388 1.01038006037737

6389 3.5450000763000000 0.0000000000000000 0.0000000000000000

6390 0.0000000000000000 5.0134000778000001 0.0000000000000000

6391 0.0000000000000000 0.0000000000000000 27.5200996398999997

6392 Zn Ni H

6393 4 10 1

6394 Direct

6395 0.0000000000000000 0.5000000000000000 0.0000000000000000

6396 0.0000000000000000 0.0000000000000000 0.09109000099999978

6397 0.0000000000000000 0.5005942121141658 0.1811787728503376

6398 0.0000000000000000 0.0010278485597297 0.2731298547248286

6399 0.0000000000000000 0.0000000000000000 0.0000000000000000

6400 0.5000000000000000 0.2500000000000000 0.04554000099999991

6401 0.5000000000000000 0.7500000000000000 0.04554000099999991

6402 0.0000000000000000 0.5000000000000000 0.09109000099999978

6403 0.5000000000000000 0.7509025681759525 0.1366843666784519

6404 0.5000000000000000 0.2497757469533468 0.1366803870621922

6405 0.0000000000000000 0.0006162028286738 0.1820940390095771

6406 0.5000000000000000 0.2470386689075426 0.2289708177712555

6407 0.5000000000000000 0.7546793530245139 0.2289680871672530

6408 0.0000000000000000 0.5010034424687220 0.2694342630780824

6409 0.5000000000000000 0.5009137777060246 0.2727681571483842

6410

6411

6412 Sample VASP INCAR file -

6413

6414 SYSTEM = Ni Alloy (111)

6415

6416 LAECHG = .TRUE. ##### for bader charge analysis

6417 LCHARG = .TRUE. ##### to write charge densities

6418 NSIM=3 ##### NSIM>1, performance enhancement.

6419 ISYM = 2 ##### switches on the use of symmetry, memory conserving symmetrisation

6420 #NPAR=16 ##### vasp band parallelization

6421 #KPAR=16 ##### vasp k points parallelization

6422

6423 ALGO = Fast ##### Damped or default for hybrid functionals, Fast otherwise

6424 PREC = Accurate

6425 EDIFF = 1e-5 ##### electronic convergence criteria

6426 EDIFFG = -0.01 ##### ionic convergence criteria

6427 NELM=40 ##### maximum number of electronic SC (selfconsistency) steps

6428 #ISMear = -5 ##### 0: Gaussian smearing, -5 : tetrahedron method with Blöchl corrections

6429 #SIGMA = 0.05 ##### width of the smearing in eV

6430

6431 GGA = PE ##### optional for HSE if the POTCAR are PBE


```
6432 ENCUT = 400      ##### energy cut off
6433 LREAL = Auto    ##### start Auto-REAL and finish FALSE
6434 ISPIN=2         ##### 2: spin polarized 1: non-spin polarized
6435
6436 #Ionic relaxation
6437 NSW = 50         ##### number of ionic steps
6438 IBRION=2         ##### 2: conjug
```