

## Supplementary information

### Ni spin coupling and Ni<sub>x</sub>N (x=1,4) (111) growth at low and room temperatures and different strains, using CrN (111) surface as initial substrate.

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CrN bulk was studied by local density approximation (LDA)<sup>1</sup> and general gradient approximation (GGA)<sup>2</sup>, including different Hubbard parameters ( $U_{\text{eff}}=U-J$ ), such as introduced by Cococcioni<sup>3</sup>. This test is performed with the main aim to determine which approximation provide results closer to experimental data, specifically, lattice constant and Cr magnetic moment. In fact, this way of determining the Hubbard parameter has been used in different works<sup>4-6</sup>. Note CrN bulk was modeled with an antiferromagnetic arrangement, forming by alternating single ferromagnetic layers along [100] direction with a rock-salt crystal structure, as reported in a previous work <sup>7</sup>. Additionally, a Monkhorst-Pack <sup>8</sup> grid of 10×10×10 is employed for the whole calculations. The results are listed in the **tables S1** and **S2**. According to the results, the combination LDA+U=4 eV is a good agreement with the lattice constant and Cr magnetic moment. Indeed, this Hubbard parameter has been employed in a previous work <sup>9</sup>. Therefore, this combination is employed to development the all calculations.

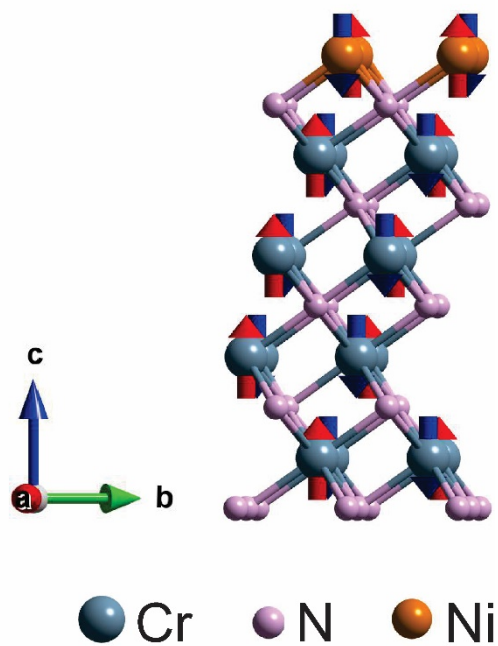
**Table S1.** Lattice constant (a) as function of the different approximations with different  $U_{\text{eff}}$  values.

	a (Å)		a (Å)	Experimental <sup>10</sup>
LDA	3.98	GGA	4.13	
LDA- $U_{\text{eff}}=1$	4.03	GGA- $U_{\text{eff}}=1$	4.18	
LDA- $U_{\text{eff}}=2$	4.10	GGA- $U_{\text{eff}}=2$	4.20	a=4.14 Å
LDA- $U_{\text{eff}}=3$	4.12	GGA- $U_{\text{eff}}=3$	4.21	
LDA- $U_{\text{eff}}=4$	<b>4.13</b>	GGA- $U_{\text{eff}}=4$	4.22	

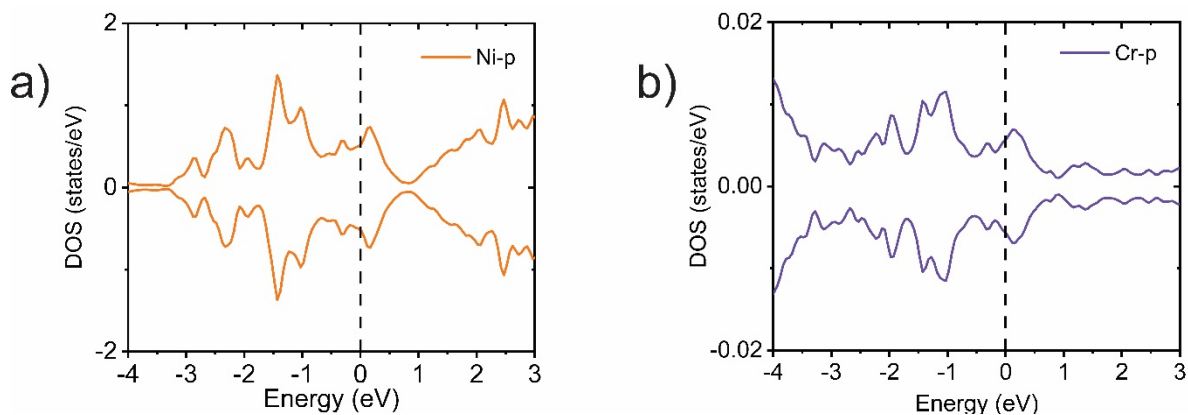
LDA- $U_{\text{eff}}=5$	4.16	GGA- $U_{\text{eff}}=5$	4.24
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**Table S2.** Cr magnetic moment ( $m_{\text{Cr}}$ ) as function of the different approximations with different  $U_{\text{eff}}$  values.

	$m_{\text{Cr}}(\mu_{\text{B}})$		$m_{\text{Cr}}(\mu_{\text{B}})$	Experimental <sup>11</sup>
LDA	1.48	GGA	2.05	
LDA- $U_{\text{eff}}=1$	1.95	GGA- $U_{\text{eff}}=1$	2.32	
LDA- $U_{\text{eff}}=2$	2.28	GGA- $U_{\text{eff}}=2$	2.41	$m_{\text{Cr}}=2.36 \mu_{\text{B}}$
LDA- $U_{\text{eff}}=3$	2.38	GGA- $U_{\text{eff}}=3$	2.47	
LDA- $U_{\text{eff}}=4$	<b>2.47</b>	GGA- $U_{\text{eff}}=4$	2.55	
LDA- $U_{\text{eff}}=5$	2.55	GGA- $U_{\text{eff}}=5$	2.63	



**Figure S1.** Spin configuration of NiN model. The red and blues arrows represent the spins up and down, respectively.



**Figure S2.** Projected density of states for first two layer: a) Ni-p and b) Cr-p of NiN model.

In addition, the atomic positions, in xyz format, the different structures are presented, with the aim of the reader can reproduce our data. Figure S1 is helpfully to build the spin arrangement for each structure.

Model: A full Ni adsorption at H3 site

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Ni	1.324877	0.924132	5.615734
Ni	-0.145121	3.461629	5.616427
Ni	4.242715	0.928313	5.616391
Ni	2.787416	3.457323	5.615734
Cr	5.668386	0.105201	7.419344
Cr	4.206172	2.638326	7.420658
Cr	2.743522	0.104953	7.420658
Cr	1.280453	2.638574	7.419380
N	-0.090395	1.741108	8.612111
N	-1.552494	4.274177	8.612622
N	2.835446	1.740799	8.612622
N	1.372258	4.274496	8.612111
Cr	1.385881	0.888777	9.820870

Cr	-0.076616	3.422078	9.821162
Cr	4.311334	0.888695	9.821162
Cr	2.848537	3.422169	9.820870
N	5.778224	0.041786	11.014259
N	4.315467	2.575234	11.014295
N	2.852814	0.041846	11.014295
N	1.390284	2.575163	11.014295
Cr	-0.096506	1.744640	12.222580
Cr	-1.559164	4.278028	12.222617
Cr	2.828794	1.744640	12.222617
Cr	1.366144	4.278022	12.222580
N	1.411343	0.874083	13.423270
N	-0.051298	3.407461	13.423234
N	4.336652	0.874078	13.423270
N	2.873993	3.407466	13.423270
Cr	5.813899	0.021189	14.635645
Cr	4.351257	2.554567	14.635645
Cr	2.888608	0.021184	14.635645
Cr	1.425949	2.554572	14.635645
N	-0.013696	1.696829	15.842615
N	-1.476337	4.230207	15.842580
N	2.911613	1.696824	15.842580
N	1.448954	4.230212	15.842615
Cr	1.480646	0.834071	17.051886
Cr	0.017997	3.367454	17.051886
Cr	4.405946	0.834071	17.051886
Cr	2.943296	3.367454	17.051886
N	0.000000	0.000000	18.255899
N	-2.925300	5.066766	18.255899

N	5.850600	0.000000	18.255899
N	2.925300	5.066766	18.255899
N	-1.462650	2.533383	18.255899
N	4.387950	2.533383	18.255899
N	2.925300	0.000000	18.255899
N	0.000000	5.066766	18.255899
N	1.462650	2.533383	18.255899
Cr	-0.014986	1.697574	19.456919
Cr	-1.477636	4.230957	19.456919
Cr	2.910314	1.697574	19.456919
Cr	1.447664	4.230957	19.456919
N	1.478251	0.835454	20.666372
N	0.015592	3.368842	20.666372
N	4.403542	0.835459	20.666372
N	2.940901	3.368837	20.666372
Cr	-2.884536	5.043231	21.871664
Cr	-1.421895	2.509853	21.871664
Cr	0.040755	5.043236	21.871664
Cr	1.503414	2.509848	21.871664
N	0.054984	1.657177	23.084877
N	-1.407674	4.190565	23.084877
N	2.980275	1.657182	23.084877
N	1.517634	4.190560	23.084877
Cr	1.564527	0.785643	24.286152
Cr	0.101877	3.319026	24.286114
Cr	4.489835	0.785637	24.286114
Cr	3.027182	3.319026	24.286152
N	-2.847800	5.022021	25.497429
N	-1.385085	2.488608	25.497429

N	0.077559	5.021981	25.497429
N	1.540141	2.488643	25.497429
Cr	0.081461	1.641901	26.690525
Cr	-1.381277	4.175324	26.690346
Cr	3.006653	1.641956	26.690308
Cr	1.544102	4.175268	26.690525
N	1.555716	0.790740	27.901150
N	0.092776	3.324280	27.900856
N	4.480717	0.790902	27.900747
N	3.018357	3.324107	27.901150
Cr	-2.744920	4.962624	29.092274
Cr	-1.282524	2.429377	29.091505
Cr	0.180134	4.962775	29.091505
Cr	1.643074	2.429215	29.092344
Ni	0.127953	1.614981	30.896612
Ni	-1.330069	4.145760	30.896101
Ni	3.057933	1.612346	30.896246
Ni	1.590661	4.148465	30.896612

Model: A full Ni adsorption at T4 site

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Ni	-0.217394	1.814171	5.613105
Ni	-1.681483	4.348648	5.612849
Ni	2.706625	1.815174	5.612849
Ni	1.245490	4.347949	5.613105
Cr	5.710089	0.081124	7.427742
Cr	4.247331	2.614583	7.427486
Cr	2.784669	0.081180	7.427486

Cr	1.322104	2.614527	7.427705
N	-0.057304	1.722006	8.620472
N	-1.520076	4.255460	8.620436
N	2.867899	1.722062	8.620436
N	1.405346	4.255389	8.620472
Cr	1.412224	0.873581	9.831861
Cr	-0.050447	3.406969	9.831823
Cr	4.337503	0.873586	9.831823
Cr	2.874868	3.406954	9.831861
N	5.800639	0.028845	11.021708
N	4.338006	2.562218	11.021708
N	2.875356	0.028835	11.021708
N	1.412680	2.562233	11.021708
Cr	-0.077585	1.733716	12.230139
Cr	-1.540235	4.267098	12.230139
Cr	2.847715	1.733716	12.230139
Cr	1.385065	4.267098	12.230139
N	1.424320	0.866594	13.429150
N	-0.038336	3.399977	13.429150
N	4.349614	0.866594	13.429150
N	2.886967	3.399972	13.429150
Cr	5.821060	0.017055	14.641560
Cr	4.358410	2.550438	14.641560
Cr	2.895760	0.017055	14.641560
Cr	1.433110	2.550438	14.641560
N	-0.009923	1.694651	15.846486
N	-1.472581	4.228039	15.846522
N	2.915377	1.694651	15.846522
N	1.452728	4.228034	15.846486

Cr	1.480919	0.833914	17.055063
Cr	0.018269	3.367296	17.055027
Cr	4.406218	0.833914	17.055027
Cr	2.943568	3.367296	17.055063
N	0.000000	0.000000	18.255899
N	-2.925300	5.066766	18.255899
N	5.850600	0.000000	18.255899
N	2.925300	5.066766	18.255899
N	-1.462650	2.533383	18.255899
N	4.387950	2.533383	18.255899
N	2.925300	0.000000	18.255899
N	0.000000	5.066766	18.255899
N	1.462650	2.533383	18.255899
Cr	-0.018268	1.699469	19.456774
Cr	-1.480918	4.232852	19.456774
Cr	2.907032	1.699469	19.456774
Cr	1.444381	4.232852	19.456774
N	1.472573	0.838732	20.665167
N	0.009923	3.372115	20.665167
N	4.397882	0.838727	20.665167
N	2.935223	3.372115	20.665167
Cr	-2.895760	5.049711	21.870058
Cr	-1.433110	2.516328	21.870058
Cr	0.029540	5.049711	21.870058
Cr	1.492190	2.516328	21.870058
N	0.038333	1.666794	23.082468
N	-1.424314	4.200171	23.082468
N	2.963636	1.666789	23.082468
N	1.500980	4.200171	23.082468



Cr	1.540235	0.799667	24.281662
Cr	0.077585	3.333050	24.281696
Cr	4.465535	0.799667	24.281696
Cr	3.002885	3.333050	24.281662
N	-2.875338	5.037920	25.490128
N	-1.412706	2.504548	25.490166
N	0.049944	5.037931	25.490166
N	1.512620	2.504533	25.490166
Cr	0.050432	1.659812	26.680084
Cr	-1.412203	4.193179	26.680120
Cr	2.975747	1.659796	26.680120
Cr	1.513076	4.193184	26.680084
N	1.519954	0.811377	27.891399
N	0.057400	3.344704	27.891436
N	4.445376	0.811306	27.891436
N	2.982604	3.344759	27.891399
Cr	-2.784789	4.985642	29.084095
Cr	-1.322031	2.452183	29.084349
Cr	0.140631	4.985586	29.084349
Cr	1.603196	2.452239	29.084167
Ni	1.679810	0.718817	30.898767
Ni	0.218675	3.251592	30.899021
Ni	4.606782	0.718118	30.899021
Ni	3.142691	3.252600	30.898767

Model: A full Ni incorporation at H3 site.

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Cr	1.385311	0.889116	5.526243
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Cr	-0.077353	3.422504	5.526243
Cr	4.310605	0.889116	5.526280
Cr	2.847958	3.422494	5.526243
Ni	5.764464	0.049730	7.658533
Ni	4.301797	2.583133	7.658533
Ni	2.839138	0.049735	7.658533
Ni	1.376506	2.583118	7.658496
N	-0.086425	1.738823	8.598018
N	-1.549063	4.272196	8.598018
N	2.838895	1.738808	8.598018
N	1.376222	4.272201	8.598018
Cr	1.382538	0.890717	9.820104
Cr	-0.080144	3.424115	9.820104
Cr	4.307796	0.890737	9.820104
Cr	2.845185	3.424095	9.820104
N	5.764728	0.049578	11.018020
N	4.302078	2.582961	11.018020
N	2.839428	0.049578	11.018020
N	1.376778	2.582961	11.018020
Cr	-0.103070	1.748429	12.221813
Cr	-1.565720	4.281812	12.221813
Cr	2.822230	1.748429	12.221813
Cr	1.359580	4.281812	12.221813
N	1.402936	0.878937	13.426594
N	-0.059714	3.412320	13.426594
N	4.328236	0.878937	13.426594
N	2.865586	3.412320	13.426594
Cr	5.813618	0.021351	14.635135
Cr	4.350968	2.554734	14.635135

Cr	2.888318	0.021351	14.635135
Cr	1.425668	2.554734	14.635135
N	-0.015592	1.697924	15.844075
N	-1.478241	4.231307	15.844075
N	2.909708	1.697924	15.844075
N	1.447058	4.231307	15.844075
Cr	1.480243	0.834304	17.052544
Cr	0.017593	3.367687	17.052544
Cr	4.405543	0.834304	17.052544
Cr	2.942893	3.367687	17.052544
N	0.000000	0.000000	18.255899
N	-2.925300	5.066766	18.255899
N	5.850600	0.000000	18.255899
N	2.925300	5.066766	18.255899
N	-1.462650	2.533383	18.255899
N	4.387950	2.533383	18.255899
N	2.925300	0.000000	18.255899
N	0.000000	5.066766	18.255899
N	1.462650	2.533383	18.255899
Cr	-0.017593	1.699079	19.459291
Cr	-1.480242	4.232462	19.459291
Cr	2.907707	1.699079	19.459291
Cr	1.445057	4.232462	19.459291
N	1.478242	0.835459	20.667578
N	0.015592	3.368842	20.667578
N	4.403542	0.835459	20.667578
N	2.940892	3.368842	20.667578
Cr	-2.888318	5.045414	21.876518
Cr	-1.425668	2.512032	21.876518

Cr	0.036982	5.045414	21.876518
Cr	1.499632	2.512032	21.876518
N	0.059714	1.654446	23.085022
N	-1.402936	4.187829	23.085022
N	2.985014	1.654446	23.085022
N	1.522364	4.187829	23.085022
Cr	1.565720	0.784953	24.289986
Cr	0.103070	3.318336	24.289986
Cr	4.491020	0.784953	24.289986
Cr	3.028370	3.318336	24.289986
N	-2.839427	5.017188	25.493853
N	-1.376778	2.483805	25.493853
N	0.085872	5.017188	25.493853
N	1.548522	2.483805	25.493853
Cr	0.080115	1.642671	26.691839
Cr	-1.382497	4.176028	26.691839
Cr	3.005445	1.642650	26.691839
Cr	1.542763	4.176049	26.691839
N	1.549078	0.794565	27.913855
N	0.086405	3.327958	27.913855
N	4.474363	0.794570	27.913855
N	3.011725	3.327943	27.913855
Ni	-2.839164	5.017035	28.853340
Ni	-1.376497	2.483632	28.853340
Ni	0.086162	5.017030	28.853340
Ni	1.548794	2.483648	28.853340
Cr	0.077342	1.644272	30.985628
Cr	-1.385305	4.177649	30.985592
Cr	3.002654	1.644262	30.985628

Cr 1.539989 4.177649 30.985628

Model: A full Ni incorporation at T4 site.

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Cr -0.080571 1.735453 5.538329

Cr -1.543236 4.268831 5.538292

Cr 2.844731 1.735438 5.538329

Cr 1.382067 4.268816 5.538329

Ni 5.758611 0.053110 7.655137

Ni 4.295949 2.586513 7.655100

Ni 2.833287 0.053110 7.655100

Ni 1.370635 2.586508 7.655100

N -0.077573 1.733705 8.596630

N -1.540217 4.267088 8.596630

N 2.847724 1.733711 8.596594

N 1.385086 4.267093 8.596630

Cr 1.384465 0.889597 9.819227

Cr -0.078170 3.422975 9.819227

Cr 4.309771 0.889597 9.819227

Cr 2.847118 3.422985 9.819227

N 5.770406 0.046300 11.017179

N 4.307756 2.579683 11.017179

N 2.845106 0.046300 11.017179

N 1.382456 2.579683 11.017179

Cr -0.098989 1.746073 12.219878

Cr -1.561639 4.279456 12.219878

Cr 2.826311 1.746073 12.219878

Cr 1.363661 4.279456 12.219878

N	1.407350	0.876388	13.424220
N	-0.055300	3.409771	13.424220
N	4.332650	0.876388	13.424220
N	2.870001	3.409771	13.424220
Cr	5.815874	0.020049	14.632870
Cr	4.353230	2.553432	14.632870
Cr	2.890576	0.020044	14.632870
Cr	1.427924	2.553432	14.632870
N	-0.013968	1.696987	15.842360
N	-1.476618	4.230370	15.842360
N	2.911332	1.696987	15.842360
N	1.448682	4.230370	15.842360
Cr	1.480567	0.834116	17.051668
Cr	0.017918	3.367499	17.051668
Cr	4.405868	0.834116	17.051668
Cr	2.943218	3.367499	17.051668
N	0.000000	0.000000	18.255899
N	-2.925300	5.066766	18.255899
N	5.850600	0.000000	18.255899
N	2.925300	5.066766	18.255899
N	-1.462650	2.533383	18.255899
N	4.387950	2.533383	18.255899
N	2.925300	0.000000	18.255899
N	0.000000	5.066766	18.255899
N	1.462650	2.533383	18.255899
Cr	-0.017917	1.699267	19.460169
Cr	-1.480567	4.232649	19.460169
Cr	2.907382	1.699267	19.460169
Cr	1.444733	4.232649	19.460169

N	1.476618	0.836396	20.669292
N	0.013968	3.369779	20.669292
N	4.401918	0.836396	20.669292
N	2.939268	3.369779	20.669292
Cr	-2.890574	5.046717	21.878746
Cr	-1.427929	2.513334	21.878746
Cr	0.034724	5.046721	21.878746
Cr	1.497376	2.513334	21.878746
N	0.055300	1.656995	23.087360
N	-1.407350	4.190378	23.087360
N	2.980600	1.656995	23.087360
N	1.517950	4.190378	23.087360
Cr	1.561639	0.787310	24.291958
Cr	0.098989	3.320692	24.291958
Cr	4.486939	0.787310	24.291958
Cr	3.024289	3.320692	24.291958
N	-2.845106	5.020466	25.494692
N	-1.382456	2.487083	25.494692
N	0.080194	5.020466	25.494692
N	1.542844	2.487083	25.494692
Cr	0.078182	1.643780	26.692717
Cr	-1.384471	4.177168	26.692717
Cr	3.003470	1.643790	26.692717
Cr	1.540835	4.177168	26.692717
N	1.540214	0.799672	27.915243
N	0.077576	3.333055	27.915277
N	4.465517	0.799678	27.915243
N	3.002870	3.333066	27.915243
Ni	-2.833311	5.013656	28.856735

Ni	-1.370649	2.480253	28.856735
Ni	0.092013	5.013656	28.856735
Ni	1.554665	2.480258	28.856735
Cr	1.543233	0.797950	30.973543
Cr	0.080569	3.331328	30.973543
Cr	4.468536	0.797935	30.973581
Cr	3.005872	3.331312	30.973543

Model: 3NiN-N

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N	1.320021	0.926828	6.451141
N	-0.143612	3.460758	6.457665
N	4.244338	0.927375	6.457459
N	2.782653	3.460181	6.451141
Ni	2.781486	0.083065	6.957503
Ni	1.320656	2.615363	6.950276
Ni	5.708588	0.081990	6.950070
Ni	4.244107	2.616397	6.957503
N	2.788042	0.079199	8.825089
N	1.322631	2.614223	8.815386
N	5.710624	0.080815	8.815097
N	4.250736	2.612648	8.825089
Ni	-0.135076	1.766796	9.544021
Ni	-1.604562	4.304238	9.543443
Ni	2.783484	1.770799	9.543443
Ni	1.327671	4.300346	9.544021
N	-0.117603	1.756840	11.401739
N	-1.578901	4.289423	11.401698



N	2.809022	1.756055	11.401698
N	1.345030	4.290193	11.401739
Ni	1.347449	0.910969	12.301818
Ni	-0.115125	3.444311	12.302726
Ni	4.272824	0.910928	12.302726
Ni	2.810104	3.444352	12.301818
N	5.737189	0.065478	13.426523
N	4.273776	2.599291	13.426316
N	2.811134	0.065924	13.426316
N	1.349257	2.598850	13.426523
Cr	-0.104184	1.749073	14.620682
Cr	-1.566843	4.282461	14.620641
Cr	2.821106	1.749078	14.620641
Cr	1.358465	4.282456	14.620682
N	1.387089	0.888082	15.831110
N	-0.075370	3.421359	15.831152
N	4.312580	0.887976	15.831152
N	2.849742	3.421470	15.831110
Cr	5.801130	0.028561	17.035963
Cr	4.338498	2.561934	17.036005
Cr	2.875848	0.028551	17.036005
Cr	1.413180	2.561944	17.035963
N	-0.027703	1.704916	18.244328
N	-1.490317	4.238278	18.244328
N	2.897633	1.704896	18.244328
N	1.434948	4.238299	18.244328
Cr	1.476057	0.836721	19.447323
Cr	0.013398	3.370108	19.447323
Cr	4.401348	0.836726	19.447323

Cr	2.938707	3.370104	19.447323
N	0.000000	0.000000	20.645899
N	-2.925300	5.066766	20.645899
N	5.850600	0.000000	20.645899
N	2.925300	5.066766	20.645899
N	-1.462650	2.533383	20.645899
N	4.387950	2.533383	20.645899
N	2.925300	0.000000	20.645899
N	0.000000	5.066766	20.645899
N	1.462650	2.533383	20.645899
Cr	-0.013442	1.696683	21.845549
Cr	-1.476091	4.230065	21.845549
Cr	2.911858	1.696683	21.845549
Cr	1.449208	4.230065	21.845549
N	1.489984	0.828680	23.049246
N	0.027282	3.362093	23.049246
N	4.415231	0.828710	23.049246
N	2.952634	3.362062	23.049246
Cr	-2.876198	5.038417	24.258394
Cr	-1.413566	2.505044	24.258354
Cr	0.049084	5.038427	24.258354
Cr	1.511751	2.505034	24.258394
N	0.075016	1.645615	25.464403
N	-1.387850	4.179119	25.464363
N	3.000100	1.645736	25.464363
N	1.537663	4.178992	25.464403
Cr	1.566238	0.784655	26.675657
Cr	0.103597	3.318032	26.675657
Cr	4.491547	0.784649	26.675657

Cr	3.028888	3.318038	26.675657
N	-2.812600	5.001698	27.870850
N	-1.349096	2.467819	27.871096
N	0.113563	5.001207	27.871096
N	1.575350	2.468316	27.870850
Ni	0.114529	1.622799	28.996050
Ni	-1.348209	4.156232	28.995018
Ni	3.039741	1.622850	28.995018
Ni	1.577178	4.156182	28.996050
N	1.579644	0.776908	29.895798
N	0.115482	3.311167	29.895882
N	4.503438	0.777784	29.895882
N	3.042300	3.310300	29.895798
Ni	1.597319	0.766744	31.754219
Ni	0.142333	3.295668	31.754837
Ni	4.530257	0.762300	31.754837
Ni	3.059940	3.300076	31.754219
N	-1.325518	2.454220	32.473190
N	-2.785069	4.985804	32.484215
N	1.602863	2.452431	32.484341
N	0.137124	4.987587	32.473190
Ni	-1.318494	2.450141	34.340488
Ni	-2.783130	4.984684	34.348705
Ni	1.604811	2.451306	34.348747
Ni	0.144168	4.983544	34.340488
N	0.142807	1.606459	34.846725
N	-1.318731	4.139213	34.839584
N	3.069207	1.605840	34.839626
N	1.605463	4.139862	34.846725

Model: 3Ni<sub>4</sub>N-N

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N	2.871814	1.719802	7.119201
Ni	1.229047	1.196446	7.220696
Ni	0.077058	3.333354	7.502678
Ni	4.351070	0.865753	7.176019
Ni	2.503671	3.404157	7.220696
N	5.794917	0.032149	8.182672
Ni	-0.147997	1.492325	9.135687
Ni	-1.701211	4.360038	8.906848
Ni	2.895772	1.705970	8.992363
Ni	1.558910	4.448772	9.135687
N	-0.089210	3.429349	9.456565
Ni	5.810450	0.023180	10.880182
Ni	-1.468231	2.734817	10.643457
Ni	-0.177238	4.970882	10.643457
Ni	1.264464	2.647806	10.616162
N	2.845082	1.735236	10.978374
Ni	1.531298	1.008352	12.410705
Ni	-0.085831	3.427398	12.495806
Ni	4.146381	0.983930	12.414875
Ni	2.817690	3.236447	12.410705
N	5.774364	0.044015	13.487966
N	4.327142	2.590075	13.474339
N	2.845799	0.024315	13.474339
N	1.338778	2.604900	13.486025
Cr	-0.098919	1.739821	14.620766

Cr	-1.589774	4.295700	14.588887
Cr	2.838272	1.739167	14.662264
Cr	1.369111	4.282522	14.620766
N	1.389172	0.878354	15.838378
N	-0.053553	3.408763	15.801710
N	4.332475	0.876490	15.836684
N	2.859209	3.424531	15.838378
Cr	5.807537	0.024863	17.037161
Cr	4.344790	2.561889	17.035303
Cr	2.879034	0.023125	17.035303
Cr	1.416585	2.559978	17.033197
N	-0.019398	1.702337	18.243914
N	-1.479532	4.232051	18.240196
N	2.908418	1.698669	18.233095
N	1.441334	4.232396	18.243914
Cr	1.477320	0.836001	19.446785
Cr	0.014837	3.369278	19.447073
Cr	4.402708	0.835940	19.446289
Cr	2.939962	3.369369	19.446785
N	0.000000	0.000000	20.645899
N	-2.925300	5.066766	20.645899
N	5.850600	0.000000	20.645899
N	2.925300	5.066766	20.645899
N	-1.462650	2.533383	20.645899
N	4.387950	2.533383	20.645899
N	2.925300	0.000000	20.645899
N	0.000000	5.066766	20.645899
N	1.462650	2.533383	20.645899
Cr	-0.014863	1.697513	21.847738

Cr	-1.477610	4.230942	21.848234
Cr	2.910270	1.697600	21.847406
Cr	1.447778	4.230881	21.847738
N	1.483698	0.834542	23.051476
N	0.016566	3.368279	23.062376
N	4.404551	0.834876	23.055235
N	2.944414	3.364576	23.051476
Cr	-2.882736	5.042192	24.259634
Cr	-1.420019	2.505176	24.261532
Cr	0.045743	5.043950	24.261532
Cr	1.508232	2.507066	24.263638
N	0.065623	1.642519	25.459202
N	-1.407639	4.190545	25.460854
N	2.978379	1.658276	25.495993
N	1.535648	4.188675	25.459202
Cr	1.555452	0.784741	26.677721
Cr	0.086221	3.328064	26.636181
Cr	4.514390	0.771461	26.709682
Cr	3.023421	3.327335	26.677721
N	-2.850204	5.023409	27.810232
N	-1.402547	2.477081	27.824520
N	0.078811	5.042866	27.824520
N	1.585776	2.462296	27.812916
Ni	0.106586	1.831443	28.801029
Ni	-1.221880	4.083296	28.924904
Ni	3.010482	1.639742	28.802391
Ni	1.392516	4.058738	28.888567
N	0.079296	3.332062	30.320070
Ni	-2.886853	5.044568	30.415951

Ni	4.392391	2.333124	30.655071
Ni	3.100950	0.096284	30.655071
Ni	1.659608	2.419669	30.682945
N	3.013386	1.638065	31.833540
Ni	1.364076	0.619610	32.166309
Ni	0.029449	3.360842	32.305794
Ni	4.624905	0.707655	32.391102
Ni	3.070740	3.575637	32.410591
N	-2.871775	5.035864	33.035503
Ni	0.419781	1.663824	34.077911
Ni	-1.428078	4.202345	34.122799
Ni	2.845802	1.734820	33.835037
Ni	1.694275	3.871313	34.077911
N	0.051249	3.348256	34.178955

Model: Ni<sub>4</sub>N (111) Surface

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Ni<sub>4</sub>N\ (1\1\1)

Ni	-0.000026	2.998195	8.560019
Ni	0.000000	0.000000	10.679905
Ni	-2.596500	4.497270	10.679905
Ni	5.193000	0.000000	10.679905
Ni	2.596500	4.497270	10.679905
Ni	2.596526	1.499075	12.800196
Ni	-0.000026	2.998195	14.920081
Ni	0.000000	0.000000	17.039967
Ni	-2.596500	4.497270	17.039967
Ni	5.193000	0.000000	17.039967
Ni	2.596500	4.497270	17.039967

Ni	2.596526	1.499075	19.160255
Ni	-0.000026	2.998195	21.280144
Ni	0.000000	0.000000	23.400433
Ni	-2.596500	4.497270	23.400433
Ni	5.193000	0.000000	23.400433
Ni	2.596500	4.497270	23.400433
Ni	2.596526	1.499075	25.520319
Ni	-0.000026	2.998195	27.640205
Ni	0.000000	0.000000	29.760494
Ni	-2.596500	4.497270	29.760494
Ni	5.193000	0.000000	29.760494
Ni	2.596500	4.497270	29.760494
Ni	2.596526	1.499075	31.880381
Ni	2.596474	2.998195	8.560019
Ni	2.596500	0.000000	10.679905
Ni	0.000000	4.497270	10.679905
Ni	0.000026	1.499075	12.800196
Ni	2.596474	2.998195	14.920081
Ni	2.596500	0.000000	17.039967
Ni	0.000000	4.497270	17.039967
Ni	0.000026	1.499075	19.160255
Ni	2.596474	2.998195	21.280144
Ni	2.596500	0.000000	23.400433
Ni	0.000000	4.497270	23.400433
Ni	0.000026	1.499075	25.520319
Ni	2.596474	2.998195	27.640205
Ni	2.596500	0.000000	29.760494
Ni	0.000000	4.497270	29.760494
Ni	0.000026	1.499075	31.880381



Ni	3.894724	0.749560	8.560019
Ni	1.298250	2.248635	10.679905
Ni	-1.298224	3.747710	12.800196
Ni	3.894724	0.749560	14.920081
Ni	1.298250	2.248635	17.039967
Ni	-1.298224	3.747710	19.160255
Ni	3.894724	0.749560	21.280144
Ni	1.298250	2.248635	23.400433
Ni	-1.298224	3.747710	25.520319
Ni	3.894724	0.749560	27.640205
Ni	1.298250	2.248635	29.760494
Ni	-1.298224	3.747710	31.880381
Ni	1.298224	0.749560	8.560019
Ni	-1.298250	2.248635	10.679905
Ni	3.894750	2.248635	10.679905
Ni	1.298276	3.747710	12.800196
Ni	1.298224	0.749560	14.920081
Ni	-1.298250	2.248635	17.039967
Ni	3.894750	2.248635	17.039967
Ni	1.298276	3.747710	19.160255
Ni	1.298224	0.749560	21.280144
Ni	-1.298250	2.248635	23.400433
Ni	3.894750	2.248635	23.400433
Ni	1.298276	3.747710	25.520319
Ni	1.298224	0.749560	27.640205
Ni	-1.298250	2.248635	29.760494
Ni	3.894750	2.248635	29.760494
Ni	1.298276	3.747710	31.880381
N	0.000000	0.000000	7.500076

N	-2.596500	4.497270	7.500076
N	5.193000	0.000000	7.500076
N	2.596500	4.497270	7.500076
N	2.596526	1.499075	9.619963
N	-0.000026	2.998195	11.740252
N	0.000000	0.000000	13.860137
N	-2.596500	4.497270	13.860137
N	5.193000	0.000000	13.860137
N	2.596500	4.497270	13.860137
N	2.596526	1.499075	15.980024
N	-0.000026	2.998195	18.100315
N	0.000000	0.000000	20.220200
N	-2.596500	4.497270	20.220200
N	5.193000	0.000000	20.220200
N	2.596500	4.497270	20.220200
N	2.596526	1.499075	22.340086
N	-0.000026	2.998195	24.460375
N	0.000000	0.000000	26.580261
N	-2.596500	4.497270	26.580261
N	5.193000	0.000000	26.580261
N	2.596500	4.497270	26.580261
N	2.596526	1.499075	28.700146
N	-0.000026	2.998195	30.820436
N	0.000000	0.000000	32.940323
N	-2.596500	4.497270	32.940323
N	5.193000	0.000000	32.940323
N	2.596500	4.497270	32.940323

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