Supplementary Information "Surfaces Stability and Equilibrium Crystal Morphology of Ni_2P Nanoparticle and Nanowires from *ab initio* atomistic thermodynamic approach"

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1. Vibrational contribution to the Surface free energy.

The ab initio atomistic thermodynamics provide effective approach to evaluate upper limit of the vibrational contribution ($\Delta\gamma^{vib}$) to surface free energies. The $\Delta\gamma^{vib}$ term can be obtained from the difference between the surface and bulk vibrational mode plus contributions due to the excess or deficient atoms.

$$\Delta\gamma^{vib} \approx \frac{1}{2A}\{\sum_{j=1}^{N_P^{surf}}\left[F^{vib}(T,\omega_{i,j}^{surf}) - F^{vib}(T,\omega_{i,P}^{bulkNi_2P})\right] + \sum_{j=1}^{N_{Ni}^{surf}}\left[F^{vib}(T,\omega_{i,j}^{surf}) - F^{vib}(T,\omega_{i,Ni}^{bulkNi_2P})\right] + (\frac{1}{2}N_{Ni} - N_P)\left[F^{vib}(T,\omega_{i,Ni}^{bulkNi_2P}) - F^{vib}(T,\omega_{i,Ni}^{bulkNi})\right] \quad (10)$$

where N_P^{surf} and N_{Ni}^{surf} are the number of P and Ni, respectively, at the surface. An atom whose nearest neighbour coordination is changed with respect to the bulk structure are defined as the surface atoms. The $F^{vib}(T,\omega_{i,j}^{term})$ is defined as:

$$F^{vib}(T,\omega_{i,j}^{term}) = \sum_{i}^{n} \frac{1}{2} \mathrm{h}\omega_{i,j}^{term} + k_B T \ln(1 - e^{-\beta \mathrm{h}\omega_{i,j}^{term}}) \quad (11)$$

with $\beta = 1/k_B T$. The vibrational modes $\omega_{i,j}^{surf}$, $\omega_{i,P}^{bulkNi_2P}$, $\omega_{i,Ni}^{bulkNi_2P}$ and $\omega_{i,Ni}^{bulkNi}$ represent the surface atoms, Ni in the bulk Ni_2P, P in the bulk Ni_2P, and Ni in the bulk Ni structures, respectively, and the summation includes all degrees of freedom. To estimate $\Delta\gamma^{vib}$, we first calculate the bulk vibrational modes ($\omega_{i,P}^{bulkNi_2P}$, $\omega_{i,Ni}^{bulkNi_2P}$ and $\omega_{i,Ni}^{bulkNi}$) based on frozen phonon calculations. The surface atoms (N_P^{surf} and N_{Ni}^{surf}) are defined as atoms with changed nearest neighbour coordination with respect to the bulk structure. The characteristic frequencies of surface atom are calculated by considering the changing 50 % for frequency of bulk atoms ($\omega_{i,P}^{bulkNi_2P}$, $\omega_{i,Ni}^{bulkNi_2P}$ and $\omega_{i,Ni}^{bulkNi}$) as the upper limit of $\Delta\gamma^{vib}$ contribution.

2. PDOS for Surface Atoms

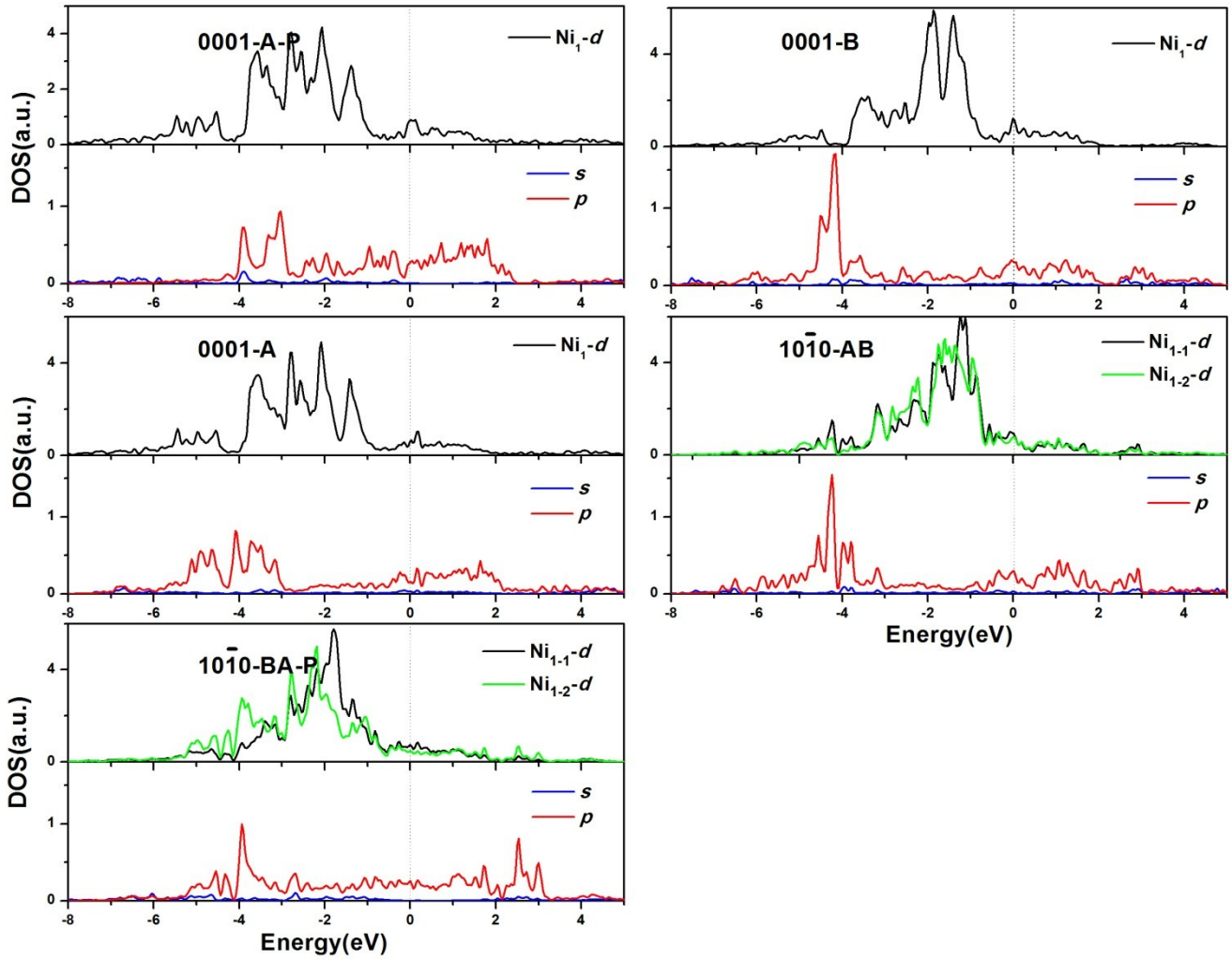

Figure S1: The partial electronic DOS (E_F=0) of Ni and P atom for (0001)-A-P, (0001)-B, (0001)-A, (10$\bar{1}$0)-AB and (10$\bar{1}$0)-BA-P structures compared with bulk PDOS.

3. The structure parameters for the most stable termination.

Table S1: Calculated Structure of 10$\bar{1}$0-AB model optimized PBE level.

Unit cell a=5.90239, b=3.41236, c=28.44182 Å, $\alpha=\beta=\gamma=90^{o}$.

	Atom name		**x**	**y**	**z**
1	P	P1	0.50932	0.39396	0.48325
2	P	P2	0.02643	0.39394	0.66228
3	P	P3	0.52069	0.39395	0.84119

4	P	P4	0.02072	0.39395	0.54327
5	P	P5	0.52643	0.39394	0.72219
6	P	P6	0.00925	0.39396	0.90121
7	P	P7	0.00745	0.89395	0.42321
8	P	P8	0.52336	0.89395	0.60300
9	P	P9	0.02336	0.89395	0.78146
10	P	P10	0.50742	0.89396	0.96126
11	Ni	Ni1	0.88229	0.39396	0.47094
12	Ni	Ni2	0.39677	0.39394	0.64898
13	Ni	Ni3	0.89216	0.39395	0.82777
14	Ni	Ni4	0.25231	0.39395	0.42850
15	Ni	Ni5	0.78383	0.39394	0.60336
16	Ni	Ni6	0.28384	0.39394	0.78111
17	Ni	Ni7	0.75223	0.39395	0.95597
18	Ni	Ni8	0.39216	0.39394	0.55670
19	Ni	Ni9	0.89677	0.39394	0.73549
20	Ni	Ni10	0.38227	0.39396	0.91352
21	Ni	Ni11	0.72850	0.89395	0.53460
22	Ni	Ni12	0.22554	0.89394	0.71053
23	Ni	Ni13	0.69629	0.89396	0.88535
24	Ni	Ni14	0.60927	0.89396	0.43988
25	Ni	Ni15	0.12753	0.89394	0.60354
26	Ni	Ni16	0.62755	0.89394	0.78092
27	Ni	Ni17	0.10922	0.89396	0.94459
28	Ni	Ni18	0.19631	0.89395	0.49912
29	Ni	Ni19	0.72554	0.89394	0.67394
30	Ni	Ni20	0.22850	0.89395	0.84986

Table S2: The surface structure of $10\bar{1}0$-BA-P optimized in PBE level.

Unit cell a=5.90239, b=3.41236, c=8.44182 Å, $\alpha=\beta=\gamma=90^{o}$.

	Atom name		**x**	**y**	**z**
1	P	P1	0.16938	0.00000	0.16356
2	P	P2	0.50733	0.00000	0.29614
3	P	P3	0.00000	0.00000	0.43648
4	P	P4	0.50112	0.00000	0.57757
5	P	P5	0.01170	-0.00000	0.71982
6	P	P6	0.51169	0.00000	0.20046
7	P	P7	0.00116	-0.00000	0.34271
8	P	P8	0.50000	0.00000	0.48381

9	P	P9	0.00734	-0.00000	0.62414
10	P	P10	0.66938	-0.00000	0.75674
11	P	P11	-0.00316	0.50000	0.24851
12	P	P12	0.50000	0.50000	0.38915
13	P	P13	0.00000	0.50000	0.53114
14	P	P14	0.49683	0.50000	0.67178
15	Ni	Ni1	0.87262	0.00000	0.28512
16	Ni	Ni2	0.37034	0.00000	0.42597
17	Ni	Ni3	0.87097	0.00000	0.56732
18	Ni	Ni4	0.39498	-0.00000	0.71021
19	Ni	Ni5	0.26243	0.00000	0.25173
20	Ni	Ni6	0.75932	0.00000	0.38915
21	Ni	Ni7	0.25932	0.00000	0.53114
22	Ni	Ni8	0.76238	-0.00000	0.66857
23	Ni	Ni9	0.89499	0.00000	0.21008
24	Ni	Ni10	0.37100	-0.00000	0.35296
25	Ni	Ni11	0.87034	0.00000	0.49432
26	Ni	Ni12	0.37259	-0.00000	0.63516
27	Ni	Ni13	0.25197	0.50000	0.20094
28	Ni	Ni14	0.69394	0.50000	0.33275
29	Ni	Ni15	0.19911	0.50000	0.47459
30	Ni	Ni16	0.68851	0.50000	0.61388
31	Ni	Ni17	0.60793	0.50000	0.25031
32	Ni	Ni18	0.10179	0.50000	0.38915
33	Ni	Ni19	0.60179	0.50000	0.53114
34	Ni	Ni20	0.10791	0.50000	0.66997
35	Ni	Ni21	0.18852	0.50000	0.30640
36	Ni	Ni22	0.69911	0.50000	0.44569
37	Ni	Ni23	0.19395	0.50000	0.58753
38	Ni	Ni24	0.75191	0.50000	0.71934

Table S3: The surface structure of 0001-A optimized in PBE level.

Unit cell a=5.90239, b=5.90239, c=30.47416 Å, $\alpha=\beta=90^{o}$, $\gamma=120^{o}$.

	Atom name		**x**	**y**	**z**
1	P	P1	0.33333	0.66667	0.00319
2	P	P2	0.66667	0.33333	0.00319
3	P	P3	0.00000	0.00000	0.05790
4	P	P4	0.33333	0.66667	0.11287
5	P	P5	0.66667	0.33333	0.11287
6	P	P6	-0.00000	1.00000	0.16911
7	P	P7	0.33333	0.66667	0.22395

8	P	P8	0.66667	0.33333	0.22395
9	P	P9	0.00000	0.00000	0.27994
10	P	P10	0.33333	0.66667	0.33593
11	P	P11	0.66667	0.33333	0.33593
12	P	P12	0.00000	1.00000	0.39077
13	P	P13	0.33333	0.66667	0.44702
14	P	P14	0.66667	0.33334	0.44702
15	P	P15	0.00000	0.00000	0.50198
16	P	P16	0.33333	0.66667	0.55670
17	P	P17	0.66667	0.33333	0.55670
18	Ni	Ni1	0.26633	-0.00000	0.00828
19	Ni	Ni2	-0.00000	0.26633	0.00828
20	Ni	Ni3	0.73367	0.73367	0.00828
21	Ni	Ni4	0.60227	0.00000	0.06049
22	Ni	Ni5	0.00000	0.60227	0.06049
23	Ni	Ni6	0.39773	0.39773	0.06049
24	Ni	Ni7	0.25977	0.00000	0.11476
25	Ni	Ni8	0.00000	0.25977	0.11476
26	Ni	Ni9	0.74023	0.74023	0.11476
27	Ni	Ni10	0.60250	0.00000	0.16926
28	Ni	Ni11	0.00000	0.60250	0.16926
29	Ni	Ni12	0.39750	0.39750	0.16926
30	Ni	Ni13	0.25932	0.00000	0.22395
31	Ni	Ni14	0.00000	0.25932	0.22395
32	Ni	Ni15	0.74068	0.74068	0.22395
33	Ni	Ni16	0.60179	0.00000	0.27994
34	Ni	Ni17	0.00000	0.60179	0.27994
35	Ni	Ni18	0.39821	0.39821	0.27994
36	Ni	Ni19	0.25932	0.00000	0.33593
37	Ni	Ni20	0.00000	0.25932	0.33593
38	Ni	Ni21	0.74068	0.74068	0.33593
39	Ni	Ni22	0.60249	-0.00000	0.39062
40	Ni	Ni23	0.00000	0.60249	0.39062
41	Ni	Ni24	0.39751	0.39751	0.39062
42	Ni	Ni25	0.25977	0.00000	0.44512
43	Ni	Ni26	1.00000	0.25976	0.44512
44	Ni	Ni27	0.74023	0.74023	0.44512
45	Ni	Ni28	0.60226	-0.00000	0.49940
46	Ni	Ni29	1.00000	0.60226	0.49940
47	Ni	Ni30	0.39774	0.39774	0.49940
48	Ni	Ni31	0.26633	0.00000	0.55161
49	Ni	Ni32	-0.00000	0.26633	0.55161
50	Ni	Ni33	0.73367	0.73367	0.55161

Table S4: The surface structure of 0001-A-P optimized in PBE level.

Unit cell a=5.90239, b=5.90239, c=33.60000 Å, $\alpha=\beta=90^{o}$, $\gamma=120^{o}$.

	Atom	name	x	y	z
1	P	P1	1.00000	0.00000	0.05959
2	P	P2	0.33333	0.66667	0.10390
3	P	P3	0.66667	0.33333	0.10390
4	P	P4	1.00000	0.00000	0.15488
5	P	P5	0.33333	0.66667	0.20425
6	P	P6	0.66667	0.33333	0.20425
7	P	P7	1.00000	0.00000	0.25496
8	P	P8	0.33333	0.66667	0.30467
9	P	P9	0.66667	0.33333	0.30467
10	P	P10	0.00000	0.00000	0.35545
11	P	P11	0.33333	0.66667	0.40623
12	P	P12	0.66667	0.33333	0.40623
13	P	P13	-0.00000	-0.00000	0.45595
14	P	P14	0.33333	0.66667	0.50666
15	P	P15	0.66667	0.33333	0.50666
16	P	P16	1.00000	0.00000	0.55603
17	P	P17	0.33333	0.66667	0.60701
18	P	P18	0.66667	0.33333	0.60701
19	P	P19	1.00000	0.00000	0.65132
20	Ni	Ni1	0.26161	0.00000	0.10646
21	Ni	Ni2	1.00000	0.26161	0.10646
22	Ni	Ni3	0.73839	0.73839	0.10646
23	Ni	Ni4	0.60239	0.00000	0.15578
24	Ni	Ni5	1.00000	0.60239	0.15578
25	Ni	Ni6	0.39761	0.39761	0.15578
26	Ni	Ni7	0.26084	0.00000	0.20527
27	Ni	Ni8	1.00000	0.26084	0.20527
28	Ni	Ni9	0.73916	0.73916	0.20527
29	Ni	Ni10	0.60301	0.00000	0.25472
30	Ni	Ni11	1.00000	0.60301	0.25472
31	Ni	Ni12	0.39699	0.39699	0.25472
32	Ni	Ni13	0.25932	0.00000	0.30467
33	Ni	Ni14	0.00000	0.25932	0.30467
34	Ni	Ni15	0.74068	0.74068	0.30467
35	Ni	Ni16	0.60179	0.00000	0.35545
36	Ni	Ni17	0.00000	0.60179	0.35545
37	Ni	Ni18	0.39821	0.39821	0.35545
38	Ni	Ni19	0.25932	0.00000	0.40623
39	Ni	Ni20	0.00000	0.25932	0.40623

40	Ni	Ni21	0.74068	0.74068	0.40623
41	Ni	Ni22	0.60301	0.00000	0.45619
42	Ni	Ni23	1.00000	0.60302	0.45619
43	Ni	Ni24	0.39698	0.39699	0.45619
44	Ni	Ni25	0.26084	0.00000	0.50564
45	Ni	Ni26	1.00000	0.26085	0.50564
46	Ni	Ni27	0.73915	0.73915	0.50564
47	Ni	Ni28	0.60240	0.00000	0.55513
48	Ni	Ni29	1.00000	0.60240	0.55513
49	Ni	Ni30	0.39760	0.39760	0.55513
50	Ni	Ni31	0.26161	0.00000	0.60445
51	Ni	Ni32	1.00000	0.26161	0.60445
52	Ni	Ni33	0.73839	0.73839	0.60445

Table S5: The surface structure of 0001-B optimized in PBE level.

Unit cell a=5.90239, b=5.90239, c=30.71124 Å, $\alpha=\beta=90^{o}$, $\gamma=120^{o}$.

Atom		**name**	**x**	**y**	**z**
1	P	P1	1.00000	1.00000	0.05591
2	P	P2	0.33333	0.66667	0.11023
3	P	P3	0.66666	0.33333	0.11023
4	P	P4	1.00000	-0.00000	0.16913
5	P	P5	0.33333	0.66667	0.22266
6	P	P6	0.66667	0.33333	0.22266
7	P	P7	0.00000	0.00000	0.27778
8	P	P8	0.33333	0.66667	0.33333
9	P	P9	0.66667	0.33333	0.33333
10	P	P10	0.00000	0.00000	0.38889
11	P	P11	0.33333	0.66667	0.44402
12	P	P12	0.66667	0.33333	0.44402
13	P	P13	1.00000	1.00000	0.49756
14	P	P14	0.33333	0.66667	0.55646
15	P	P15	0.66667	0.33333	0.55646
16	P	P16	1.00000	1.00000	0.61078
17	Ni	Ni1	0.61850	-0.00000	0.06798
18	Ni	Ni2	-0.00000	0.61850	0.06798
19	Ni	Ni3	0.38150	0.38150	0.06798
20	Ni	Ni4	0.25987	-0.00000	0.11641
21	Ni	Ni5	-0.00000	0.25987	0.11641
22	Ni	Ni6	0.74013	0.74013	0.11641
23	Ni	Ni7	0.60159	1.00000	0.16944
24	Ni	Ni8	1.00000	0.60159	0.16944
25	Ni	Ni9	0.39841	0.39841	0.16944

26	Ni	Ni10	0.26072	-0.00000	0.22355
27	Ni	Ni11	-0.00000	0.26072	0.22355
28	Ni	Ni12	0.73928	0.73928	0.22355
29	Ni	Ni13	0.60179	0.00000	0.27778
30	Ni	Ni14	0.00000	0.60179	0.27778
31	Ni	Ni15	0.39821	0.39821	0.27778
32	Ni	Ni16	0.25932	0.00000	0.33333
33	Ni	Ni17	0.00000	0.25932	0.33333
34	Ni	Ni18	0.74068	0.74068	0.33333
35	Ni	Ni19	0.60179	0.00000	0.38889
36	Ni	Ni20	0.00000	0.60179	0.38889
37	Ni	Ni21	0.39821	0.39821	0.38889
38	Ni	Ni22	0.26071	-0.00000	0.44313
39	Ni	Ni23	-0.00000	0.26071	0.44313
40	Ni	Ni24	0.73929	0.73929	0.44313
41	Ni	Ni25	0.60158	1.00000	0.49726
42	Ni	Ni26	1.00000	0.60158	0.49726
43	Ni	Ni27	0.39842	0.39842	0.49726
44	Ni	Ni28	0.25986	-0.00000	0.55028
45	Ni	Ni29	1.00000	0.25986	0.55028
46	Ni	Ni30	0.74014	0.74014	0.55028
47	Ni	Ni31	0.61849	-0.00000	0.59871
48	Ni	Ni32	1.00000	0.61849	0.59871
49	Ni	Ni33	0.38151	0.38151	0.59871

Table S6: The surface structure of $10\bar{1}2$-NiP2 optimized in PBE level.

Unit cell a= 17.05350, b=5.90239, c=24.0000 Å, $\alpha=\beta=\gamma=90^{o}$.

Atom	**name**	**x**	**y**	**z**
1	P	P1	0.77995	0.94218	0.25340
2	P	P2	0.61003	0.43747	0.07863
3	P	P3	0.95967	0.41918	0.42210
4	P	P4	0.58008	0.94215	0.18238
5	P	P5	0.40001	0.44288	0.01383
6	P	P6	0.76101	0.43618	0.35526
7	P	P7	0.62414	0.94555	0.33824
8	P	P8	0.44274	0.43817	0.16887
9	P	P9	0.27995	0.44218	0.25340
10	P	P10	0.11003	0.93730	0.07854
11	P	P11	0.45956	0.91885	0.42214
12	P	P12	0.08008	0.44215	0.18238
13	P	P13	0.89996	0.94270	0.01385

14	P	P14	0.26115	0.93648	0.35547
15	P	P15	0.12477	0.44533	0.33846
16	P	P16	0.94280	0.93807	0.16890
17	P	P17	0.21934	0.93982	0.19835
18	P	P18	0.38993	0.43718	0.37229
19	P	P19	0.04073	0.41813	0.02820
20	P	P20	0.41992	0.94215	0.26762
21	P	P21	0.60007	0.44318	0.43644
22	P	P22	0.23921	0.43551	0.09529
23	P	P23	0.37541	0.94503	0.11220
24	P	P24	0.55681	0.43843	0.28148
25	P	P25	0.71934	0.43984	0.19842
26	P	P26	0.88937	0.93692	0.37240
27	P	P27	0.54076	0.91820	0.02824
28	P	P28	0.91992	0.44215	0.26762
29	P	P29	0.10008	0.94287	0.43663
30	P	P30	0.73921	0.93560	0.09536
31	P	P31	0.87543	0.44485	0.11220
32	P	P32	0.05697	0.93995	0.28167
33	Ni	Ni1	0.61391	0.07732	0.09668
34	Ni	Ni2	0.97888	0.05666	0.42743
35	Ni	Ni3	0.47094	0.20744	0.07463
36	Ni	Ni4	0.84135	0.24762	0.41155
37	Ni	Ni5	0.58008	0.34039	0.18238
38	Ni	Ni6	0.69062	0.24201	0.28450
39	Ni	Ni7	0.50984	0.74444	0.11915
40	Ni	Ni8	0.65259	0.75283	0.25056
41	Ni	Ni9	0.41249	0.83042	0.02938
42	Ni	Ni10	0.75840	0.84119	0.34792
43	Ni	Ni11	0.32028	0.18208	0.05459
44	Ni	Ni12	0.45341	0.07183	0.18081
45	Ni	Ni13	0.84187	0.17954	0.30732
46	Ni	Ni14	0.70675	0.07183	0.18396
47	Ni	Ni15	0.21818	0.08320	0.43164
48	Ni	Ni16	0.86752	0.06410	0.10421
49	Ni	Ni17	0.11396	0.57723	0.09665
50	Ni	Ni18	0.47884	0.55645	0.42790
51	Ni	Ni19	0.97094	0.70723	0.07460
52	Ni	Ni20	0.34134	0.74698	0.41161
53	Ni	Ni21	0.08008	0.84039	0.18238
54	Ni	Ni22	0.19151	0.74212	0.28478
55	Ni	Ni23	0.00967	0.24502	0.11911
56	Ni	Ni24	0.15163	0.24308	0.25027
57	Ni	Ni25	0.91241	0.33031	0.02934
58	Ni	Ni26	0.25860	0.34120	0.34802

59	Ni	Ni27	0.82026	0.68197	0.05464
60	Ni	Ni28	0.95341	0.57183	0.18081
61	Ni	Ni29	0.34191	0.67964	0.30729
62	Ni	Ni30	0.20675	0.57183	0.18396
63	Ni	Ni31	0.71810	0.58323	0.43138
64	Ni	Ni32	0.36749	0.56428	0.10419
65	Ni	Ni33	0.38628	0.07747	0.35350
66	Ni	Ni34	0.02142	0.05554	0.02240
67	Ni	Ni35	0.52910	0.20800	0.37561
68	Ni	Ni36	0.15902	0.24598	0.03911
69	Ni	Ni37	0.41992	0.34039	0.26762
70	Ni	Ni38	0.30955	0.24289	0.16615
71	Ni	Ni39	0.49087	0.74642	0.33106
72	Ni	Ni40	0.34837	0.74308	0.19973
73	Ni	Ni41	0.58787	0.83067	0.42111
74	Ni	Ni42	0.24179	0.84121	0.10296
75	Ni	Ni43	0.67967	0.18268	0.39568
76	Ni	Ni44	0.54659	0.07183	0.26919
77	Ni	Ni45	0.15882	0.17878	0.14342
78	Ni	Ni46	0.29325	0.07183	0.26604
79	Ni	Ni47	0.78183	0.08306	0.01921
80	Ni	Ni48	0.13288	0.06489	0.34616
81	Ni	Ni49	0.88626	0.57765	0.35344
82	Ni	Ni50	0.52148	0.55560	0.02239
83	Ni	Ni51	0.02937	0.70702	0.37580
84	Ni	Ni52	0.65906	0.74607	0.03921
85	Ni	Ni53	0.91992	0.84039	0.26762
86	Ni	Ni54	0.80962	0.74279	0.16618
87	Ni	Ni55	0.99166	0.25032	0.33096
88	Ni	Ni56	0.84837	0.24308	0.19973
89	Ni	Ni57	0.08802	0.33077	0.42139
90	Ni	Ni58	0.74182	0.34113	0.10302
91	Ni	Ni59	0.17995	0.68259	0.39605
92	Ni	Ni60	0.04892	0.57420	0.26911
93	Ni	Ni61	0.65888	0.67865	0.14362
94	Ni	Ni62	0.79325	0.57183	0.26604
95	Ni	Ni63	0.28185	0.58319	0.01916
96	Ni	Ni64	0.63275	0.56503	0.34575
97	Ni	Ni65	0.00000	0.18285	0.22500
98	Ni	Ni66	0.50000	0.68285	0.22500

Table S7: The surface structure of $10\bar{1}3$-NiP2 optimized in PBE level.

Unit cell a=22.88473, b=5.90239, c=20.8000 Å, $\alpha=\beta=\gamma=90^{o}$.

	Atom	name	x	y	z
1	P	P1	0.16779	0.97711	0.06395
2	P	P2	0.03519	0.97546	0.13521
3	P	P3	0.90004	0.97950	0.20716
4	P	P4	0.76663	0.97950	0.28045
5	P	P5	0.63479	0.00639	0.35708
6	P	P6	0.47434	0.98617	0.44335
7	P	P7	0.08915	0.03578	0.45591
8	P	P8	0.23030	0.99473	0.39456
9	P	P9	0.36558	0.98017	0.31873
10	P	P10	0.66781	0.47698	0.06408
11	P	P11	0.53521	0.47562	0.13515
12	P	P12	0.40004	0.47950	0.20716
13	P	P13	0.26663	0.47950	0.28045
14	P	P14	0.13487	0.50748	0.35721
15	P	P15	0.97383	0.48535	0.44358
16	P	P16	0.58912	0.53492	0.45602
17	P	P17	0.73003	0.49427	0.39423
18	P	P18	0.86563	0.48014	0.31882
19	P	P19	0.83221	0.97681	0.42346
20	P	P20	0.96509	0.97516	0.35225
21	P	P21	0.10151	0.98158	0.28017
22	P	P22	0.23337	0.97950	0.20716
23	P	P23	0.36526	0.00642	0.13049
24	P	P24	0.52582	0.98598	0.04424
25	P	P25	0.91094	0.03492	0.03160
26	P	P26	0.77000	0.99438	0.09333
27	P	P27	0.63449	0.98009	0.16882
28	P	P28	0.33236	0.47722	0.42356
29	P	P29	0.46486	0.47576	0.35245
30	P	P30	0.59996	0.47950	0.28045
31	P	P31	0.73337	0.47950	0.20716
32	P	P32	0.86524	0.50639	0.13049
33	P	P33	0.02579	0.48583	0.04422
34	P	P34	0.41098	0.53496	0.03160
35	P	P35	0.27003	0.49437	0.09333
36	P	P36	0.13445	0.48029	0.16870
37	P	P37	0.50000	0.97947	0.24380
38	P	P38	0.00000	0.47947	0.24380
39	Ni	Ni1	0.67955	0.11752	0.08217
40	Ni	Ni2	0.53934	0.09349	0.14980
41	Ni	Ni3	0.40742	0.10915	0.22343

42	Ni	Ni4	0.27339	0.10628	0.29408
43	Ni	Ni5	0.14093	0.13830	0.36872
44	Ni	Ni6	-0.00200	0.12029	0.44077
45	Ni	Ni7	0.58053	0.30734	0.05556
46	Ni	Ni8	0.44496	0.31607	0.11536
47	Ni	Ni9	0.30781	0.29747	0.18435
48	Ni	Ni10	0.17314	0.28040	0.25807
49	Ni	Ni11	0.03784	0.24604	0.32276
50	Ni	Ni12	0.90084	0.25522	0.39881
51	Ni	Ni13	0.65633	0.27204	0.42494
52	Ni	Ni14	0.79655	0.22906	0.35490
53	Ni	Ni15	0.93330	0.22016	0.28045
54	Ni	Ni16	0.07096	0.41618	0.43073
55	Ni	Ni17	0.23129	0.38780	0.37894
56	Ni	Ni18	0.36471	0.37932	0.31255
57	Ni	Ni19	0.17960	0.61764	0.08208
58	Ni	Ni20	0.03930	0.59342	0.14978
59	Ni	Ni21	0.90742	0.60915	0.22343
60	Ni	Ni22	0.77348	0.60627	0.29401
61	Ni	Ni23	0.64052	0.63686	0.36842
62	Ni	Ni24	0.49803	0.62070	0.44093
63	Ni	Ni25	0.08051	0.80728	0.05557
64	Ni	Ni26	0.94492	0.81599	0.11533
65	Ni	Ni27	0.80782	0.79744	0.18432
66	Ni	Ni28	0.67314	0.78040	0.25807
67	Ni	Ni29	0.53762	0.74773	0.32300
68	Ni	Ni30	0.40094	0.75604	0.39891
69	Ni	Ni31	0.15652	0.77296	0.42508
70	Ni	Ni32	0.29671	0.72929	0.35495
71	Ni	Ni33	0.43330	0.72016	0.28045
72	Ni	Ni34	0.57144	0.91521	0.43116
73	Ni	Ni35	0.73098	0.88715	0.37874
74	Ni	Ni36	0.86473	0.87914	0.31256
75	Ni	Ni37	0.32072	0.11768	0.40544
76	Ni	Ni38	0.46069	0.09363	0.33780
77	Ni	Ni39	0.59258	0.10915	0.26417
78	Ni	Ni40	0.72659	0.10623	0.19357
79	Ni	Ni41	0.85952	0.13686	0.11919
80	Ni	Ni42	0.00207	0.12030	0.04670
81	Ni	Ni43	0.41965	0.30757	0.43213
82	Ni	Ni44	0.55508	0.31604	0.37229
83	Ni	Ni45	0.69221	0.29754	0.30322
84	Ni	Ni46	0.82686	0.28040	0.22954
85	Ni	Ni47	0.96245	0.24734	0.16465
86	Ni	Ni48	0.09918	0.25580	0.08867

87	Ni	Ni49	0.34374	0.27211	0.06263
88	Ni	Ni50	0.20348	0.22910	0.13262
89	Ni	Ni51	0.06670	0.22016	0.20716
90	Ni	Ni52	0.92871	0.41497	0.05653
91	Ni	Ni53	0.76907	0.38725	0.10888
92	Ni	Ni54	0.63534	0.37928	0.17506
93	Ni	Ni55	0.82048	0.61733	0.40544
94	Ni	Ni56	0.96104	0.59301	0.33792
95	Ni	Ni57	0.09258	0.60915	0.26417
96	Ni	Ni58	0.22654	0.60628	0.19356
97	Ni	Ni59	0.35954	0.63691	0.11919
98	Ni	Ni60	0.50209	0.62052	0.04667
99	Ni	Ni61	0.91952	0.80737	0.43183
100	Ni	Ni62	0.05566	0.81793	0.37172
101	Ni	Ni63	0.19253	0.79621	0.30358
102	Ni	Ni64	0.32686	0.78040	0.22954
103	Ni	Ni65	0.46243	0.74755	0.16463
104	Ni	Ni66	0.59920	0.75579	0.08872
105	Ni	Ni67	0.84370	0.77205	0.06264
106	Ni	Ni68	0.70349	0.72908	0.13265
107	Ni	Ni69	0.56670	0.72016	0.20716
108	Ni	Ni70	0.42872	0.91517	0.05650
109	Ni	Ni71	0.26911	0.88728	0.10891
110	Ni	Ni72	0.13528	0.87920	0.17480
111	Ni	Ni73	0.50000	0.37771	0.24380
112	Ni	Ni74	0.00000	0.87771	0.24380

Table S8: The surface structure of $10\bar{1}1$-NiP1 optimized in PBE level.

Unit cell a=12.29177, b=5.90239, c=29.4000 Å, $\alpha=\beta=\gamma=90^{o}$.

Atom		**name**	**x**	**y**	**z**
1	P	P1	0.14524	0.00865	0.15094
2	P	P2	0.83996	0.00910	0.34144
3	P	P3	0.55397	0.99177	0.52659
4	P	P4	0.79482	0.50534	0.05138
5	P	P5	0.49332	0.51007	0.24587
6	P	P6	0.19447	0.50887	0.43670
7	P	P7	0.83458	0.01050	0.13410
8	P	P8	0.53154	0.01003	0.32631
9	P	P9	0.23882	0.00994	0.51901
10	P	P10	0.02271	0.50886	0.11939
11	P	P11	0.72389	0.51009	0.31022

12	P	P12	0.42236	0.50536	0.50470
13	P	P13	0.66320	0.99176	0.02950
14	P	P14	0.37724	0.00909	0.21464
15	P	P15	0.07195	0.00865	0.40514
16	P	P16	0.47835	0.50990	0.03707
17	P	P17	0.18568	0.51008	0.22978
18	P	P18	0.88261	0.51051	0.42198
19	P	P19	0.29482	0.00535	0.05139
20	P	P20	0.99331	0.01005	0.24586
21	P	P21	0.69447	0.00887	0.43670
22	P	P22	0.64524	0.50862	0.15094
23	P	P23	0.33997	0.50908	0.34144
24	P	P24	0.05397	0.49178	0.52659
25	P	P25	0.97835	0.00991	0.03707
26	P	P26	0.68568	0.01003	0.22978
27	P	P27	0.38261	0.01049	0.42198
28	P	P28	0.16320	0.49177	0.02950
29	P	P29	0.87724	0.50908	0.21464
30	P	P30	0.57195	0.50863	0.40515
31	P	P31	0.52271	0.00886	0.11939
32	P	P32	0.22390	0.01011	0.31022
33	P	P33	0.92235	0.00537	0.50470
34	P	P34	0.33458	0.51051	0.13410
35	P	P35	0.03153	0.51008	0.32631
36	P	P36	0.73882	0.50994	0.51901
37	Ni	Ni1	0.26184	0.24928	0.18365
38	Ni	Ni2	0.95535	0.24928	0.37244
39	Ni	Ni3	0.81358	0.13619	0.06121
40	Ni	Ni4	0.51892	0.13970	0.25301
41	Ni	Ni5	0.21511	0.13320	0.44210
42	Ni	Ni6	0.90667	0.75344	0.08586
43	Ni	Ni7	0.60862	0.75075	0.27805
44	Ni	Ni8	0.31051	0.75344	0.47022
45	Ni	Ni9	0.61412	0.28052	0.07543
46	Ni	Ni10	0.32340	0.31095	0.26822
47	Ni	Ni11	0.01770	0.30748	0.45480
48	Ni	Ni12	0.83016	0.40778	0.13272
49	Ni	Ni13	0.53154	0.40827	0.32631
50	Ni	Ni14	0.23295	0.40151	0.51017
51	Ni	Ni15	0.00209	0.13318	0.11398
52	Ni	Ni16	0.69828	0.13973	0.30307
53	Ni	Ni17	0.40361	0.13621	0.49488
54	Ni	Ni18	0.04886	0.30437	0.19309
55	Ni	Ni19	0.74354	0.30796	0.38309
56	Ni	Ni20	0.64026	0.63539	0.02712

57	Ni	Ni21	0.35213	0.64124	0.20682
58	Ni	Ni22	0.05050	0.64003	0.39793
59	Ni	Ni23	0.16668	0.64003	0.15816
60	Ni	Ni24	0.86509	0.64124	0.34926
61	Ni	Ni25	0.57691	0.63540	0.52898
62	Ni	Ni26	0.69949	0.80747	0.10129
63	Ni	Ni27	0.39382	0.81098	0.28787
64	Ni	Ni28	0.10308	0.78054	0.48067
65	Ni	Ni29	0.97364	0.80794	0.17299
66	Ni	Ni30	0.66833	0.80436	0.36300
67	Ni	Ni31	0.48420	0.90150	0.04592
68	Ni	Ni32	0.18568	0.90832	0.22978
69	Ni	Ni33	0.88703	0.90779	0.42335
70	Ni	Ni34	0.40667	0.25344	0.08586
71	Ni	Ni35	0.10860	0.25074	0.27804
72	Ni	Ni36	0.81051	0.25345	0.47022
73	Ni	Ni37	0.66667	0.14000	0.15816
74	Ni	Ni38	0.36509	0.14123	0.34927
75	Ni	Ni39	0.07690	0.13540	0.52898
76	Ni	Ni40	0.76184	0.74925	0.18364
77	Ni	Ni41	0.45536	0.74925	0.37244
78	Ni	Ni42	0.47364	0.30795	0.17300
79	Ni	Ni43	0.16833	0.30437	0.36300
80	Ni	Ni44	0.98421	0.40150	0.04592
81	Ni	Ni45	0.68568	0.40827	0.22978
82	Ni	Ni46	0.38703	0.40778	0.42336
83	Ni	Ni47	0.14026	0.13540	0.02712
84	Ni	Ni48	0.85213	0.14123	0.20681
85	Ni	Ni49	0.55051	0.14001	0.39793
86	Ni	Ni50	0.19949	0.30748	0.10129
87	Ni	Ni51	0.89381	0.31097	0.28787
88	Ni	Ni52	0.60308	0.28053	0.48067
89	Ni	Ni53	0.50209	0.63317	0.11398
90	Ni	Ni54	0.19830	0.63975	0.30308
91	Ni	Ni55	0.90361	0.63622	0.49488
92	Ni	Ni56	0.31358	0.63619	0.06121
93	Ni	Ni57	0.01891	0.63976	0.25301
94	Ni	Ni58	0.71511	0.63320	0.44210
95	Ni	Ni59	0.54887	0.80432	0.19309
96	Ni	Ni60	0.24355	0.80796	0.38309
97	Ni	Ni61	0.11412	0.78052	0.07543
98	Ni	Ni62	0.82340	0.81101	0.26822
99	Ni	Ni63	0.51769	0.80746	0.45480
100	Ni	Ni64	0.33017	0.90779	0.13273
101	Ni	Ni65	0.03154	0.90832	0.32631

102	Ni	Ni66	0.73295	0.90151	0.51017

Table S9: The surface structure of $20\bar{2}1$-NiP1 optimized in PBE level.

Unit cell a=10.77749, b=5.90239, c= 28.66737 Å, $\alpha=\beta=\gamma=90^{o}$.

	Atom name		**x**	**y**	**z**
1	P	P1	0.79917	0.00754	0.05505
2	P	P2	0.71257	0.00816	0.17049
3	P	P3	0.61826	0.00768	0.28122
4	P	P4	0.52009	0.00580	0.39298
5	P	P5	0.43326	0.01317	0.50270
6	P	P6	0.26301	0.51513	0.11495
7	P	P7	0.16775	0.50794	0.22486
8	P	P8	0.06849	0.50687	0.33733
9	P	P9	0.97303	0.50704	0.44991
10	P	P10	0.90139	0.51031	0.55264
11	P	P11	0.38639	0.08922	0.04405
12	P	P12	0.36951	0.00839	0.18713
13	P	P13	0.26823	0.00765	0.30004
14	P	P14	0.16697	0.00692	0.41264
15	P	P15	0.15003	0.08789	0.55562
16	P	P16	0.63505	0.51132	0.04713
17	P	P17	0.56337	0.50734	0.14990
18	P	P18	0.46830	0.50772	0.26240
19	P	P19	0.36844	0.50737	0.37477
20	P	P20	0.27334	0.51436	0.48489
21	P	P21	0.10343	0.01384	0.09715
22	P	P22	0.01641	0.00700	0.20705
23	P	P23	0.91819	0.00773	0.31886
24	P	P24	0.82434	0.00779	0.42925
25	P	P25	0.73740	0.00666	0.54482
26	P	P26	0.02799	0.52393	0.02483
27	P	P27	0.90230	0.50623	0.13186
28	P	P28	0.81835	0.50771	0.24358
29	P	P29	0.71810	0.50771	0.35649
30	P	P30	0.63430	0.50516	0.46795
31	P	P31	0.50832	0.52331	0.57496
32	Ni	Ni1	0.95363	0.25664	0.07615
33	Ni	Ni2	0.86360	0.24533	0.18952
34	Ni	Ni3	0.76822	0.24837	0.30004
35	Ni	Ni4	0.67346	0.24347	0.41010

36	Ni	Ni5	0.58303	0.25600	0.52380
37	Ni	Ni6	0.29342	0.13638	0.12063
38	Ni	Ni7	0.20155	0.13820	0.22995
39	Ni	Ni8	0.10144	0.13733	0.34185
40	Ni	Ni9	0.00463	0.13929	0.45336
41	Ni	Ni10	0.93441	0.14114	0.54912
42	Ni	Ni11	0.48695	0.76912	0.04663
43	Ni	Ni12	0.41768	0.75234	0.13169
44	Ni	Ni13	0.31836	0.74838	0.24359
45	Ni	Ni14	0.21753	0.74783	0.35507
46	Ni	Ni15	0.11852	0.75192	0.46834
47	Ni	Ni16	0.04945	0.76791	0.55334
48	Ni	Ni17	0.19014	0.30819	0.05228
49	Ni	Ni18	0.08744	0.29063	0.15659
50	Ni	Ni19	0.99750	0.30858	0.26606
51	Ni	Ni20	0.89882	0.30754	0.37678
52	Ni	Ni21	0.80461	0.31172	0.48692
53	Ni	Ni22	0.44184	0.40224	0.08072
54	Ni	Ni23	0.36899	0.40640	0.18840
55	Ni	Ni24	0.26823	0.40589	0.30004
56	Ni	Ni25	0.16822	0.40680	0.41144
57	Ni	Ni26	0.09488	0.40125	0.51917
58	Ni	Ni27	0.60211	0.14204	0.05077
59	Ni	Ni28	0.53225	0.13955	0.14646
60	Ni	Ni29	0.43500	0.13736	0.25822
61	Ni	Ni30	0.33498	0.13727	0.37017
62	Ni	Ni31	0.24352	0.13535	0.47904
63	Ni	Ni32	0.73201	0.31256	0.11284
64	Ni	Ni33	0.63812	0.30695	0.22331
65	Ni	Ni34	0.53895	0.30859	0.33401
66	Ni	Ni35	0.44988	0.28902	0.44334
67	Ni	Ni36	0.34644	0.30737	0.54745
68	Ni	Ni37	0.07290	0.63152	0.10073
69	Ni	Ni38	0.98423	0.63775	0.20123
70	Ni	Ni39	0.88489	0.63737	0.31468
71	Ni	Ni40	0.79166	0.63654	0.42301
72	Ni	Ni41	0.70480	0.62129	0.53942
73	Ni	Ni42	0.83175	0.62191	0.06032
74	Ni	Ni43	0.74457	0.63573	0.17678
75	Ni	Ni44	0.65156	0.63738	0.28540
76	Ni	Ni45	0.55194	0.63668	0.39879
77	Ni	Ni46	0.46356	0.63107	0.49894
78	Ni	Ni47	0.25260	0.81237	0.06173
79	Ni	Ni48	0.19061	0.80688	0.16838
80	Ni	Ni49	0.08909	0.80861	0.27756

81	Ni	Ni50	0.99152	0.81028	0.38948
82	Ni	Ni51	0.88211	0.81112	0.49568
83	Ni	Ni52	0.65442	0.81155	0.10415
84	Ni	Ni53	0.54530	0.81132	0.21044
85	Ni	Ni54	0.44737	0.80863	0.32252
86	Ni	Ni55	0.34430	0.80262	0.43103
87	Ni	Ni56	0.28405	0.81158	0.53810
88	Ni	Ni57	-0.00503	0.88745	0.03723
89	Ni	Ni58	0.89858	0.90815	0.13138
90	Ni	Ni59	0.81835	0.90594	0.24358
91	Ni	Ni60	0.71601	0.90322	0.35457
92	Ni	Ni61	0.63774	0.90783	0.46841
93	Ni	Ni62	0.54155	0.88657	0.56261

Table S10: The surface structure of $20\bar{2}3$-NiP1 optimized in PBE level.

Unit cell a= 14.46755, b=5.90239, c=24.15687 Å, $\alpha=\beta=\gamma=90^{o}$.

Atom		**name**	**x**	**y**	**z**
1	P	P1	0.24511	0.30150	0.04701
2	P	P2	0.08622	0.31050	0.14463
3	P	P3	0.92690	0.30768	0.24215
4	P	P4	0.76000	0.30768	0.34197
5	P	P5	0.59930	0.30874	0.44025
6	P	P6	0.43221	0.29132	0.53788
7	P	P7	0.68727	0.81018	0.08863
8	P	P8	0.51237	0.80671	0.19204
9	P	P9	0.34346	0.80769	0.29207
10	P	P10	0.17416	0.80809	0.39189
11	P	P11	-0.00142	0.80709	0.50421
12	P	P12	0.83969	0.32926	0.08710
13	P	P13	0.67636	0.31144	0.19313
14	P	P14	0.51013	0.30765	0.29207
15	P	P15	0.34387	0.31143	0.39100
16	P	P16	0.18052	0.32928	0.49702
17	P	P17	0.02160	0.80712	0.07992
18	P	P18	0.84607	0.80812	0.19224
19	P	P19	0.67679	0.80772	0.29206
20	P	P20	0.50784	0.80669	0.39210
21	P	P21	0.33290	0.81017	0.49551
22	P	P22	0.58801	0.29130	0.04624
23	P	P23	0.42092	0.30877	0.14388
24	P	P24	0.26024	0.30773	0.24216

25	P	P25	0.09335	0.30773	0.34198
26	P	P26	0.93399	0.31051	0.43952
27	P	P27	0.77507	0.30145	0.53712
28	P	P28	0.42474	0.81225	0.04344
29	P	P29	0.25534	0.80283	0.14142
30	P	P30	0.09357	0.80771	0.24216
31	P	P31	0.92668	0.80771	0.34197
32	P	P32	0.76487	0.80281	0.44272
33	P	P33	0.59546	0.81221	0.54069
34	Ni	Ni1	0.33624	0.54705	0.08989
35	Ni	Ni2	0.17334	0.54562	0.19504
36	Ni	Ni3	0.01012	0.54837	0.29206
37	Ni	Ni4	0.84689	0.54561	0.38910
38	Ni	Ni5	0.68396	0.54701	0.49424
39	Ni	Ni6	0.69055	0.45138	0.10581
40	Ni	Ni7	0.52520	0.44052	0.20424
41	Ni	Ni8	0.36194	0.43733	0.30315
42	Ni	Ni9	0.19758	0.43833	0.40181
43	Ni	Ni10	0.03434	0.44818	0.50024
44	Ni	Ni11	0.92178	0.05438	0.05533
45	Ni	Ni12	0.76272	0.05293	0.14600
46	Ni	Ni13	0.59358	0.04838	0.24216
47	Ni	Ni14	0.42668	0.04838	0.34198
48	Ni	Ni15	0.25748	0.05291	0.43813
49	Ni	Ni16	0.09844	0.05435	0.52877
50	Ni	Ni17	0.51562	0.57464	0.09874
51	Ni	Ni18	0.35430	0.60006	0.20163
52	Ni	Ni19	0.19299	0.60858	0.30178
53	Ni	Ni20	0.02808	0.60620	0.39807
54	Ni	Ni21	0.86240	0.58600	0.49557
55	Ni	Ni22	0.84576	0.70863	0.09989
56	Ni	Ni23	0.67599	0.70967	0.19318
57	Ni	Ni24	0.51013	0.70589	0.29207
58	Ni	Ni25	0.34421	0.70966	0.39092
59	Ni	Ni26	0.17442	0.70860	0.48423
60	Ni	Ni27	0.98587	0.44821	0.08392
61	Ni	Ni28	0.82265	0.43833	0.18231
62	Ni	Ni29	0.65831	0.43736	0.28098
63	Ni	Ni30	0.49503	0.44053	0.37987
64	Ni	Ni31	0.32969	0.45141	0.47832
65	Ni	Ni32	0.15780	0.58605	0.08856
66	Ni	Ni33	0.99214	0.60617	0.18608
67	Ni	Ni34	0.82726	0.60859	0.28235
68	Ni	Ni35	0.66592	0.60007	0.38250
69	Ni	Ni36	0.50460	0.57468	0.48536

70	Ni	Ni37	0.56681	0.92777	0.04399
71	Ni	Ni38	0.40598	0.92741	0.13611
72	Ni	Ni39	0.24176	0.93737	0.23108
73	Ni	Ni40	0.07487	0.93737	0.33089
74	Ni	Ni41	0.91444	0.92740	0.42996
75	Ni	Ni42	0.73846	0.94893	0.52540
76	Ni	Ni43	0.28174	0.94899	0.05873
77	Ni	Ni44	0.10576	0.92740	0.15417
78	Ni	Ni45	0.94538	0.93738	0.25324
79	Ni	Ni46	0.77848	0.93738	0.35305
80	Ni	Ni47	0.61421	0.92739	0.44803
81	Ni	Ni48	0.45340	0.92777	0.54013
82	Ni	Ni49	0.72799	0.12096	0.04701
83	Ni	Ni50	0.57808	0.11562	0.13808
84	Ni	Ni51	0.41071	0.10861	0.23245
85	Ni	Ni52	0.24382	0.10861	0.33226
86	Ni	Ni53	0.07567	0.13094	0.42611
87	Ni	Ni54	0.91196	0.13957	0.52000
88	Ni	Ni55	0.10824	0.13960	0.06415
89	Ni	Ni56	0.94453	0.13081	0.15800
90	Ni	Ni57	0.77644	0.10863	0.25187
91	Ni	Ni58	0.60954	0.10863	0.35169
92	Ni	Ni59	0.44215	0.11570	0.44604
93	Ni	Ni60	0.29224	0.12103	0.53711
94	Ni	Ni61	0.43448	0.19896	0.05601
95	Ni	Ni62	0.25599	0.20465	0.14576
96	Ni	Ni63	0.09358	0.20594	0.24216
97	Ni	Ni64	0.92668	0.20594	0.34197
98	Ni	Ni65	0.76422	0.20459	0.43837
99	Ni	Ni66	0.58572	0.19895	0.52813

Table S11: Atomic displacements along the surface normal upon the surface relaxation; relative shifts of atoms are reported (in Å) for the (0001)-A, (0001)-B, (0001)-A-P, $(10\bar{1}0)$-AB, and $(10\bar{1}0)$-BA-P surfaces with respect to Ni_2P bulk interlayer distances.

	d_{P1-P2}	d_{P1-Ni1}	d_{P2-Ni2}	d_{P3-Ni3}	d_{P4-Ni4}
(0001)-A		0.155	0.079	0.002	0.005
(0001)-B		0.371	0.190	0.009	0.027
(0001)-A-P	-0.217		0.210	0.030	0.034
	d_{P1-P2}	$d_{P1-Ni1-1/Ni1-2}$	$d_{P2-Ni2-1/Ni2-2}$	$d_{P3-Ni3-1/Ni3-2}$	$d_{P4-Ni4-1/Ni4-2}$
$(10\bar{1}0)$-AB		0.150/0.474	0.120/-0.029	0.004/-0.084	0.015/0.010
$(10\bar{1}0)$-BA-P	-0.399		-0.014/-0.343	0.065/0.116	0.045/0.037