Supporting information

Phase relations, mechanical and electronic properties of nickel borides, carbides, and nitrides from ab initio calculations

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Table S1: Energies above hull of the considered iron borides.

Compound	Energy above hull (eV/atom)					
	0 GPa	50 GPa	100 GPa	200 GPa	300 GPa	400 GPa
$Ni_{23}B_6$	0.0157	0.0473	0.0525	0.0657	0.0668	0.0679
Ni_3B	0	0	0.0066	0.0526	0.0578	0.0631
Ni_7B_3	0.0197	0.0736	0.0775	0.0854	0.0972	0.974
Ni_2B	0	0	0	0	0	0
Ni_4B_3	0	0	0.0026	0.0447	0.0448	0.0451
NiB	0.0053	0	0	0	0	0
Ni_2B_3	0.1629	0.0933	0.0459	0.0065	0	0

Table S2: Energies above hull of the considered iron carbides.

Compound	Energy above hull (eV/atom)					
	0 GPa	50 GPa	100 GPa	200 GPa	300 GPa	400 GPa
Ni_3C	0.0591	0.0082	0	0	0	0
Ni_7C_3	0.7493	0.0492	0.0417	0.0333	0.026	0.0213

Table S3: Energies above hull of the considered iron nitrides.

Compound	Energy above hull (eV/atom)					
	0 GPa	50 GPa	100 GPa	200 GPa	300 GPa	400 GPa
Ni_6N	0.3856	0.0375	0	0.0751	0.0509	0.053
Ni_3N	0.0319	0	0.0016	0.0331	0.0199	0
Ni_5N_2	0.3123	0.1525	0.0619	0.0663	0.0466	0.0482
Ni_7N_3	12.2958	0.0796	0	0	0	0
NiN	13.2809	0.1414	0.0685	0.0331	0.0398	0.0288
NiN_2	2.6114	0	0	0	0	0

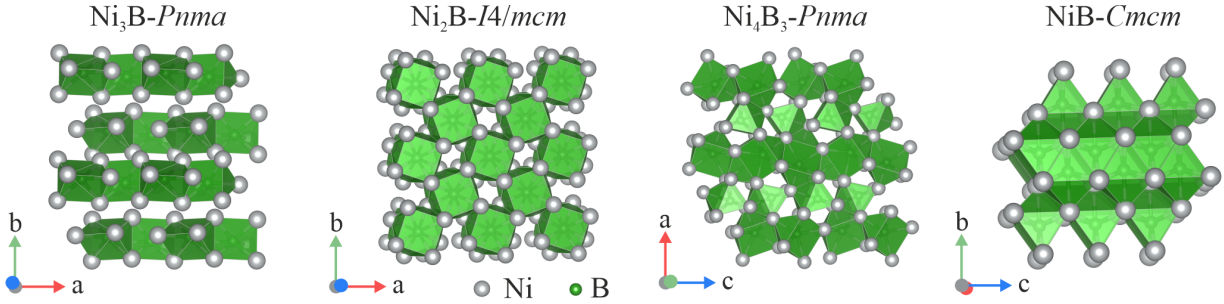

Figure S1: Crystal structures of predicted nickel borides.

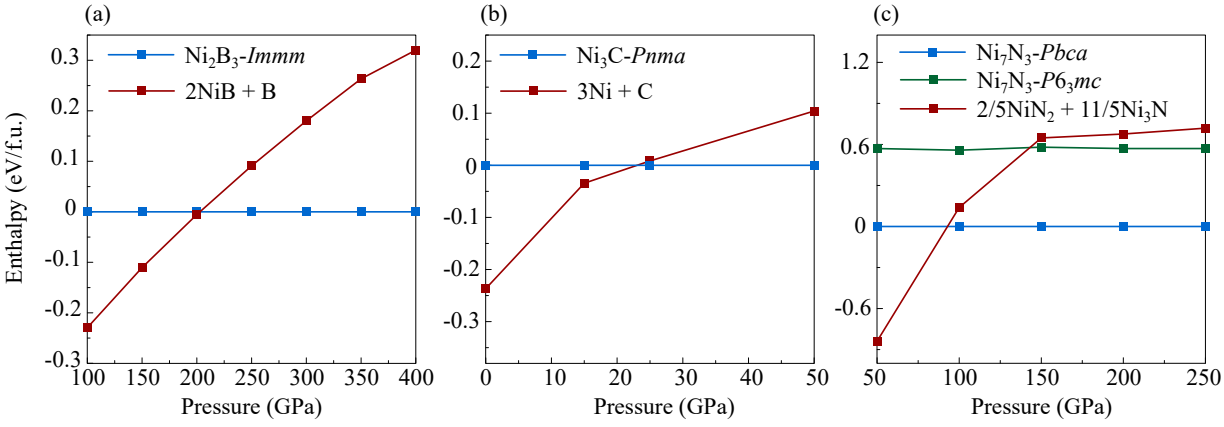

Figure S2: Enthalpy-pressure dependence for the reactions $2NiB + B = Ni_2B_3$ (a), $3Ni + C = Ni_3C$ (b), and $2NiN_2 + 11Ni_3N = 5Ni_7N_3$ (c).

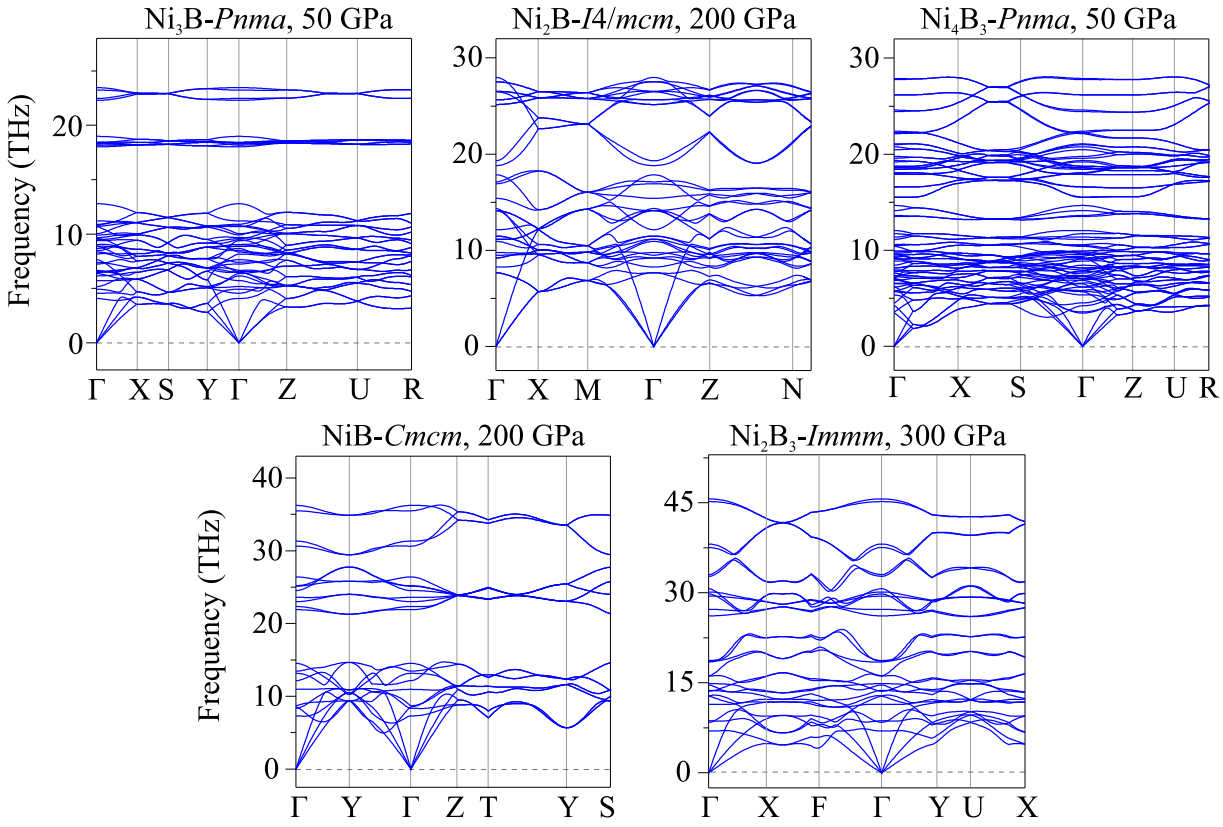

Figure S3: Phonon dispersion curves of predicted nickel borides.

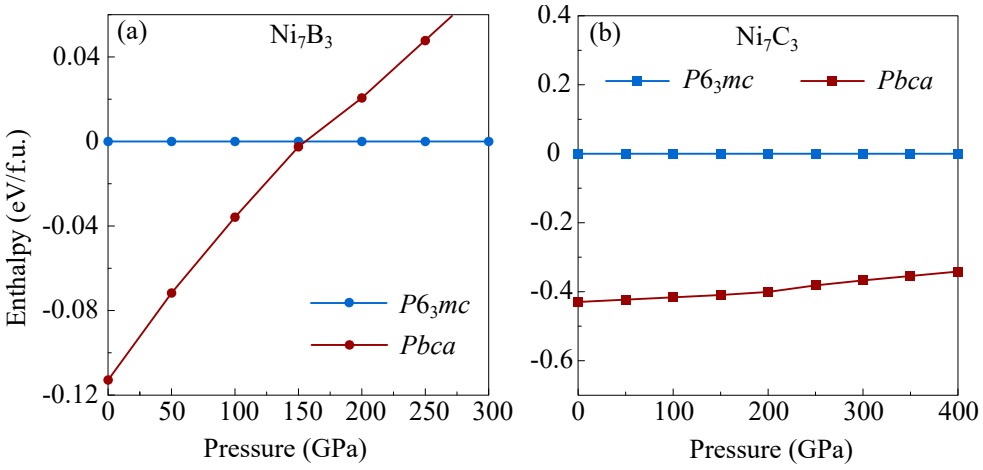

Figure S4: Enthalpy-pressure dependence for metastable phases Ni_7B_3 (a) and Ni_7C_3 (b).

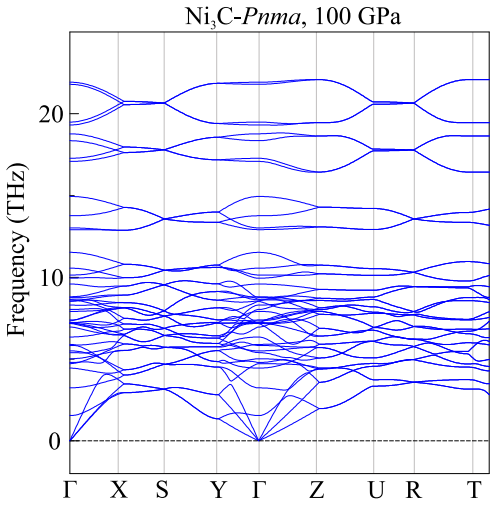

Figure S5: Phonon dispersion curves of Ni_3C-*Pnma*.

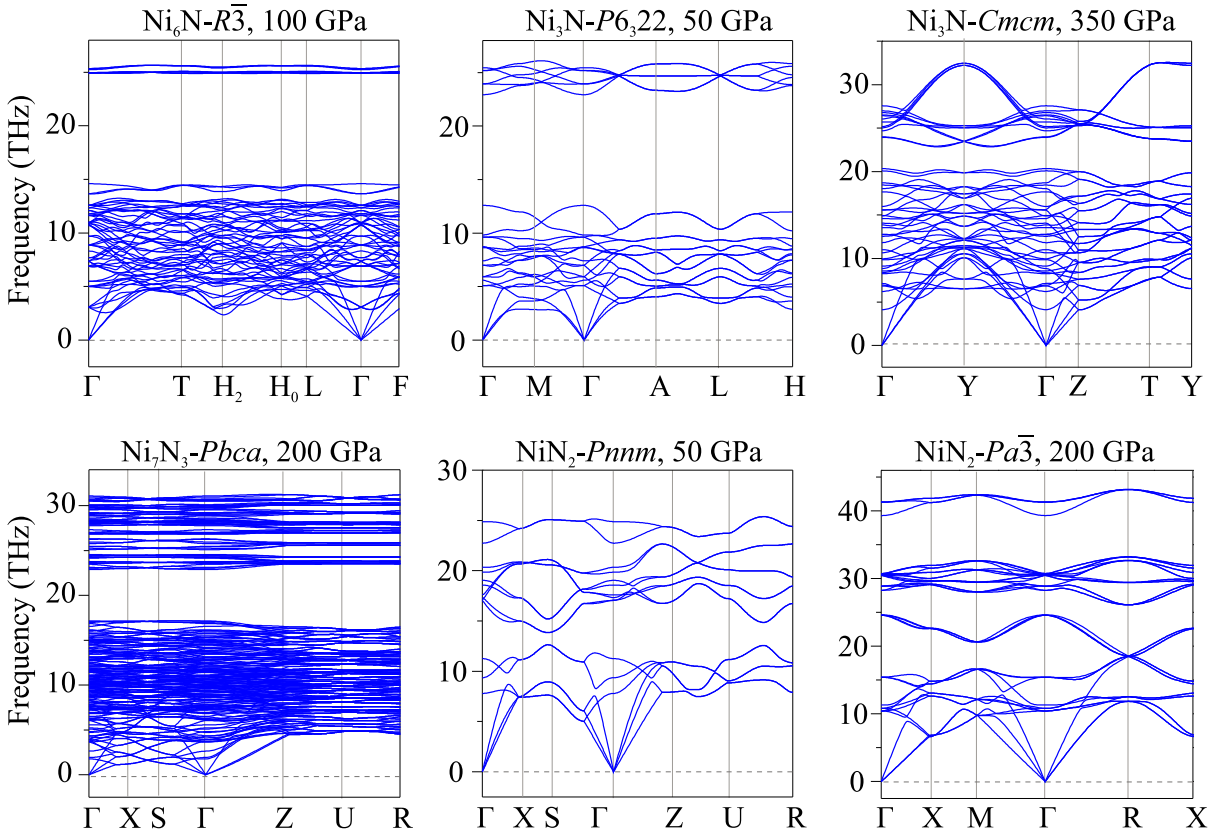

Figure S6: Phonon dispersion curves of predicted nickel nitrides.

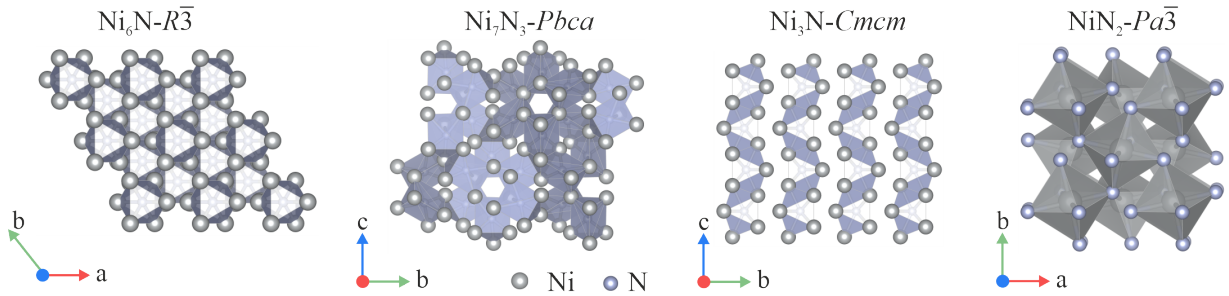

Figure S7: Crystal structures of predicted nickel nitrides.

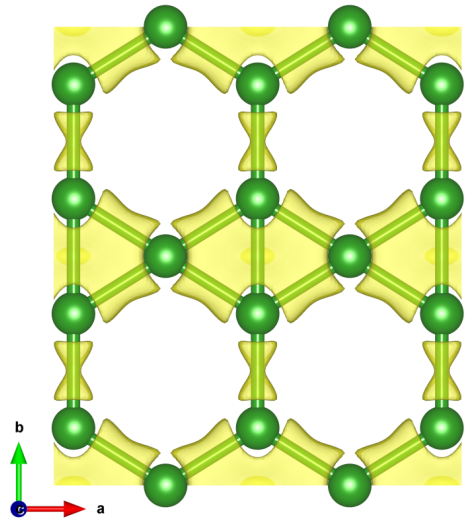

Figure S8: Electronic charge density distribution in infinite (001) layer of B atoms in the Ni_2B_3 structure.

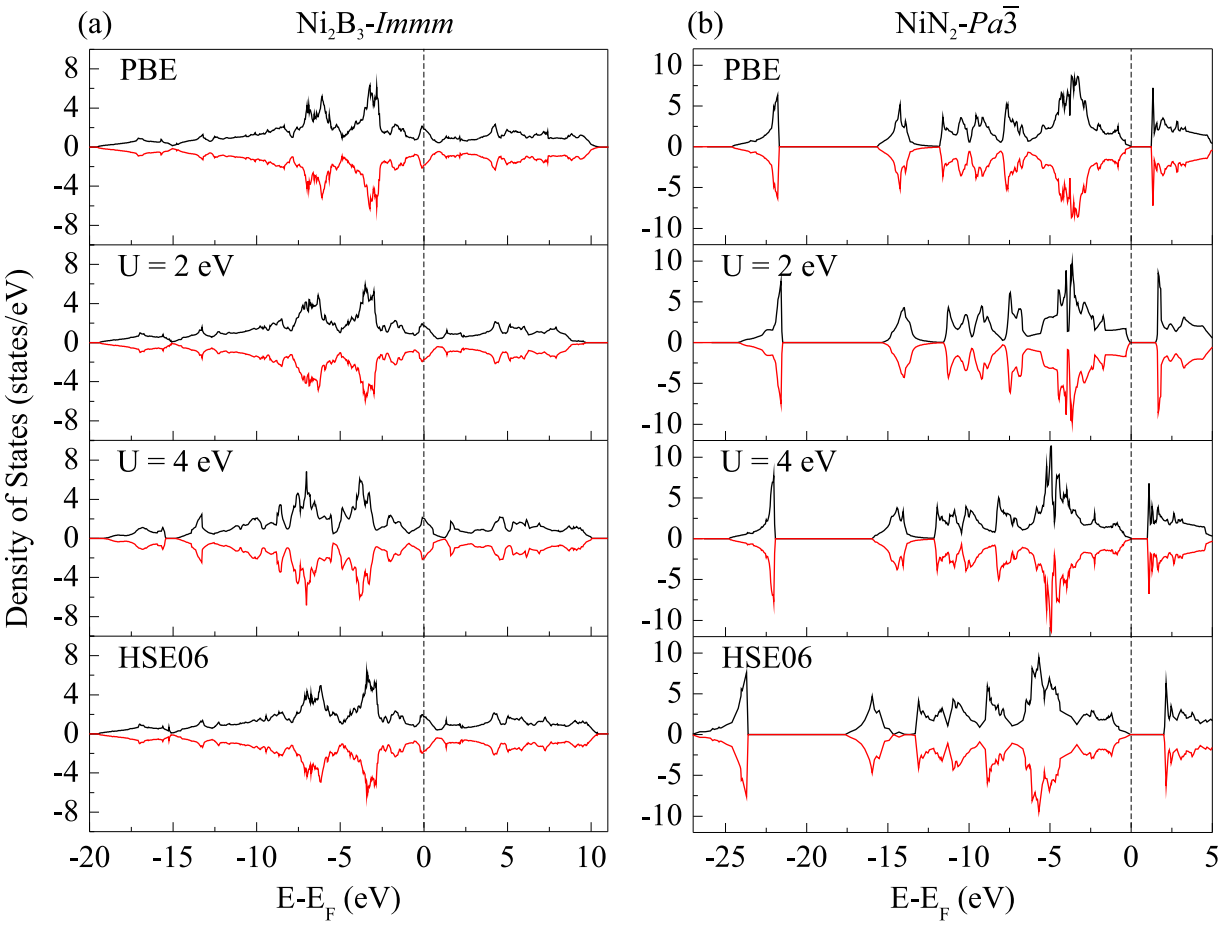

Figure S9: Total DOS of Ni_2B_3-*Immm* (a) and NiN_2-$Pa\bar{3}$ (b) calculated with PBE, GGA+U (U = 2, 4 eV), and HSE06.

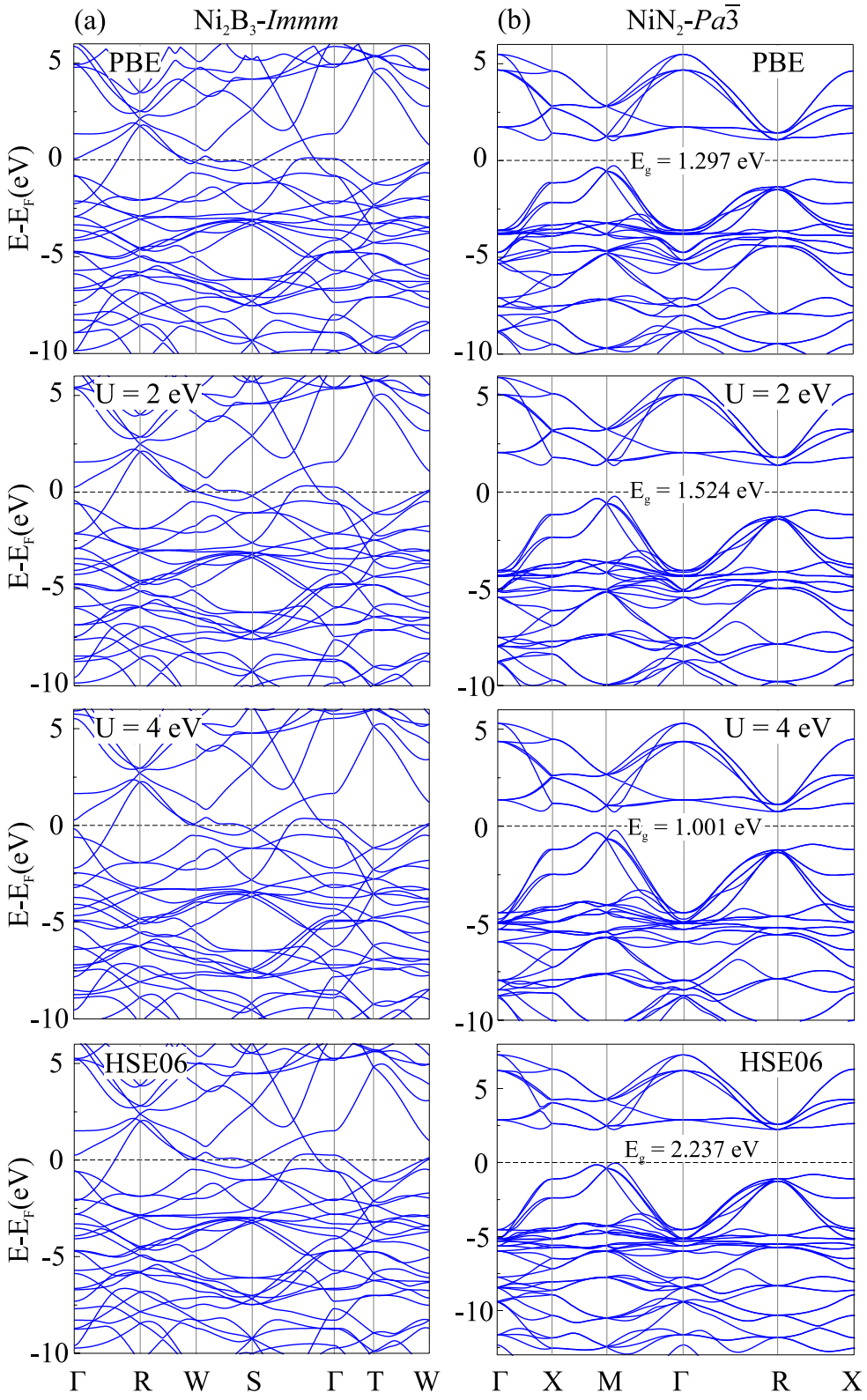

Figure S10: Band structures of Ni_2B_3-*Immm* (a) and NiN_2-$Pa\bar{3}$ (b) calculated with PBE, GGA+U (U = 2, 4 eV), and HSE06.