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First-principles study of mechanical and magnetic properties of transition metal (M) nitrides in the cubic M_4N structure

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SUPPLEMENTAL MATERIAL

Table S1. Calculated magnetic moments due to the electrons in s, p and d orbitals and total magnetic moments in Bohr magnetons (μ_B) of magnetic phases Mn_4N, Fe_4N, Co_4N, Ni_4N, and Sc_4N.

Mn_4N				
Atoms	**s**	**p**	**d**	**Total**
Mn1	0.042	0.053	3.145	3.24
Mn2	-0.01	0	-0.81	-0.82
Mn3	-0.004	-0.008	-0.744	-0.755
Mn4	-0.008	-0.009	-0.548	-0.565
N	0.009	0.08	0	0.089
Total	0.029	0.116	1.043	1.189

Fe_4N				
Atoms	**s**	**p**	**d**	**Total**
Fe1	-0.012	-0.023	2.982	2.948
Fe2	-0.016	0	2.316	2.3
Fe3	0.008	-0.013	2.264	2.259
Fe4	0.006	-0.033	2.341	2.314
N	-0.002	0.022	0	0.021
Total	-0.016	-0.047	9.903	9.842

Co_4N				
Atoms	**s**	**p**	**d**	**Total**
Co1	-0.012	-0.019	1.949	1.918
Co2	-0.01	0.01	1.227	1.227
Co3	0.014	-0.01	1.366	1.37
Co4	0.009	-0.026	1.773	1.756
N	0.001	0.086	0	0.088
Total	0.002	0.041	6.315	6.359

Ni_4N				
Atoms	**s**	**p**	**d**	**Total**
Ni1	-0.002	-0.002	0.659	0.655
Ni2	-0.006	0.004	0.133	0.132
Ni3	0.008	-0.004	0.247	0.251
Ni4	0.005	-0.007	0.419	0.417
N	0	0.031	0	0.031
Total	0.005	0.022	1.458	1.486

Sc_4N				
Atoms	**s**	**p**	**d**	**Total**
Sc1	0.011	0.061	0.434	0.507
Sc2	0.02	0.019	0.359	0.398
Sc3	0.007	0.028	0.302	0.337
Sc4	0.008	0.042	0.243	0.292
N	-0.001	-0.011	0	-0.012
Total	0.045	0.139	1.338	1.522

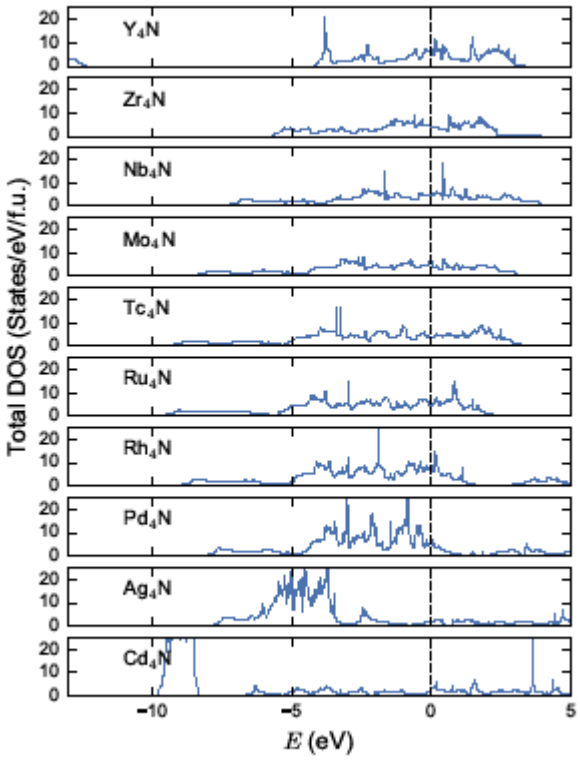

Fig. S1. Total Density of States (DOS) per formula unit (primitive cell) of the 10 4d M_4N-type transition metal nitrides. Fermi energy is set to zero in each panel.

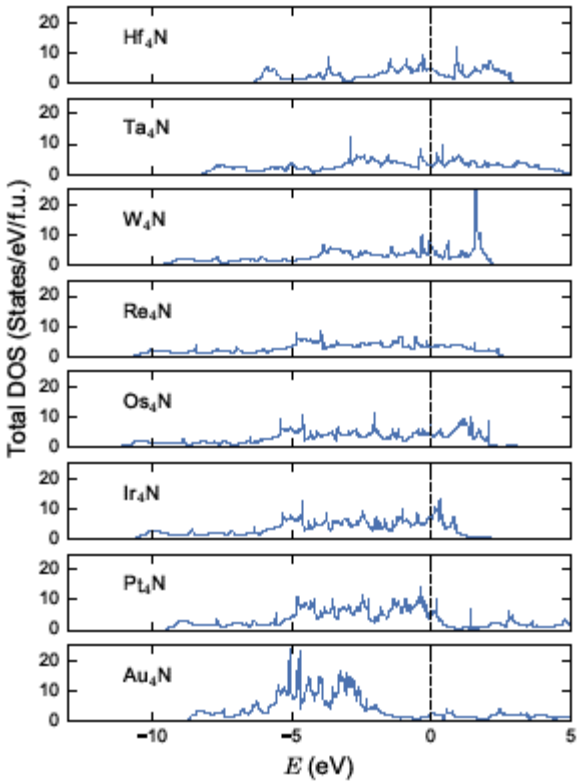

Fig. S2. Total Density of States (DOS) per formula unit (primitive cell) of the 8 5d M_4N-type transition metal nitrides. Fermi energy is set to zero in each panel.

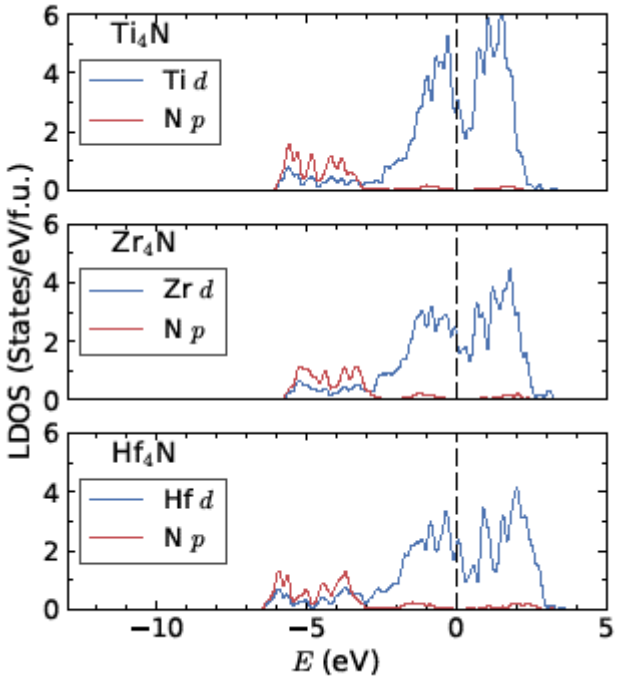

Fig. S3. Local density of states (LDOS) of M_4N-type group 4 nitrides Ti_4N, Zr_4N, and Hf_4N. Fermi energy is set to zero in each panel.

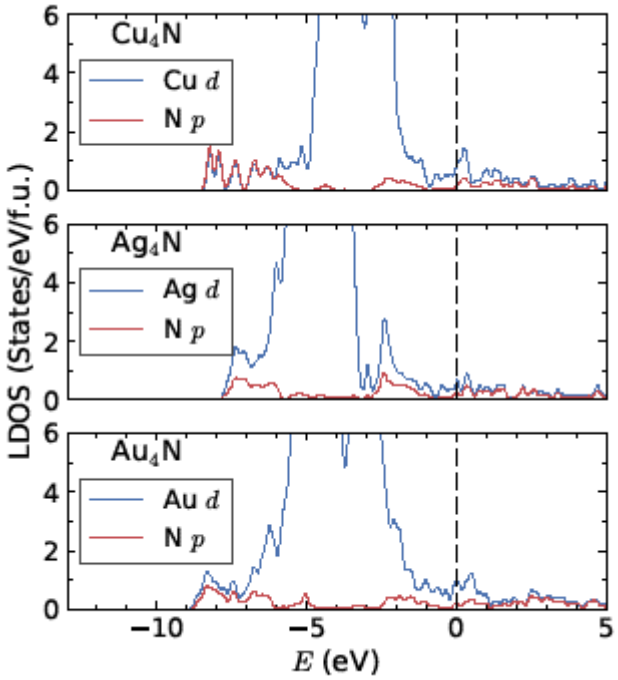

Fig. S4. Local density of states (LDOS) of M_4N-type group 11 nitrides Cu_4N, Ag_4N, and Au_4N. Fermi energy is set to zero in each panel.