S. R. Kandel, B. B. Dumre, D. Gall, S. V. Khare, Computational Materials Science 221, 112084, Supplementary Material (2023)

Mechanical and electronic properties of transition metal hexa-nitrides in hexagonal structure from density functional theory calculations

S. R. Kandel[a*], B. B. Dumre[a], D. Gall[b], S. V. Khare[a]

[a]Department of Physics and Astronomy, University of Toledo, Toledo, OH 43606, USA

[b]Department of Materials Science and Engineering, Rensselaer Polytechnic Institute, Troy, NY 12180, USA

*Corresponding Author: shreedhar.kandel@rockets.utoledo.edu

S. R. Kandel, B. B. Dumre, D. Gall, S. V. Khare, Computational Materials Science 221, 112084, Supplementary Material (2023)

Table S1: Wyckoff positions for M (3a) and N (18h) atoms in MN_6 compounds. x and z are the fractional internal free parameters denoting the coordinates for M and N atoms in unit cell respectively.

Multiplicity	Wyckoff letter	Coordinates
		(0, 0, 0) + (2/3, 1/3, 1/3) + (1/3, 2/3, 2/3)
18	h	(x, -x, z), (x, 2x, z), (-2x, -x, z), (-x, x, -z), (2x, x, -z), (-x, -2x, -z)
3	a	(0, 0, 0)

Table S2: Total magnetic moment found in the atomic orbitals. Only 8 MN_6 compounds possess the magnetic moment calculated in terms of Bohr magneton (μ_B).

Material	Magnetic Moment (μ_B)							
	Transition Metal				Nitrogen			Total in the Unit Cell
	s-orbital	p-orbital	d-orbital	Total	s-orbital	p-orbital	Total	
ScN_6	-0.001	0.003	0.022	0.024	0.003	0.069	0.072	1.368
VN_6	0.014	0.013	1.446	1.473	-0.005	-0.075	-0.08	2.979
CrN_6	0.02	0.022	2.281	2.323	-0.006	-0.052	-0.058	5.925
MnN_6	0.00	0.00	0.029	0.029	0.00	0.00	0.00	0.087
FeN_6	0.004	0.012	1.285	1.301	0.002	0.049	0.051	4.821
CoN_6	0.003	0.006	0.821	0.83	0.004	0.017	0.021	2.868
YN_6	-0.002	0.015	0.019	0.032	0.004	0.109	0.113	2.13
AgN_6	0.005	0.003	0.024	0.032	0.003	0.056	0.059	1.158

Table S3: Electronegativity (χ) of transition metal M [1].

Group no.	M			χ		
3	Sc	Y	N/A	1.20	1.11	N/A
4	Ti	Zr	Hf	1.32	1.22	1.23
5	V	Nb	Ta	1.45	1.23	1.33
6	Cr	Mo	W	1.56	1.30	1.40
7	Mn	Tc	Re	1.60	1.36	1.46
8	Fe	Ru	Os	1.64	1.42	1.52
9	Co	Rh	Ir	1.70	1.45	1.55
10	Ni	Pd	Pt	1.75	1.35	1.44
11	Cu	Ag	Au	1.75	1.42	1.21
12	Zn	Cd	Hg	1.66	1.46	N/A

Figure S1: Variation of bond length as a function of hardness for mechanically stable MN_6.

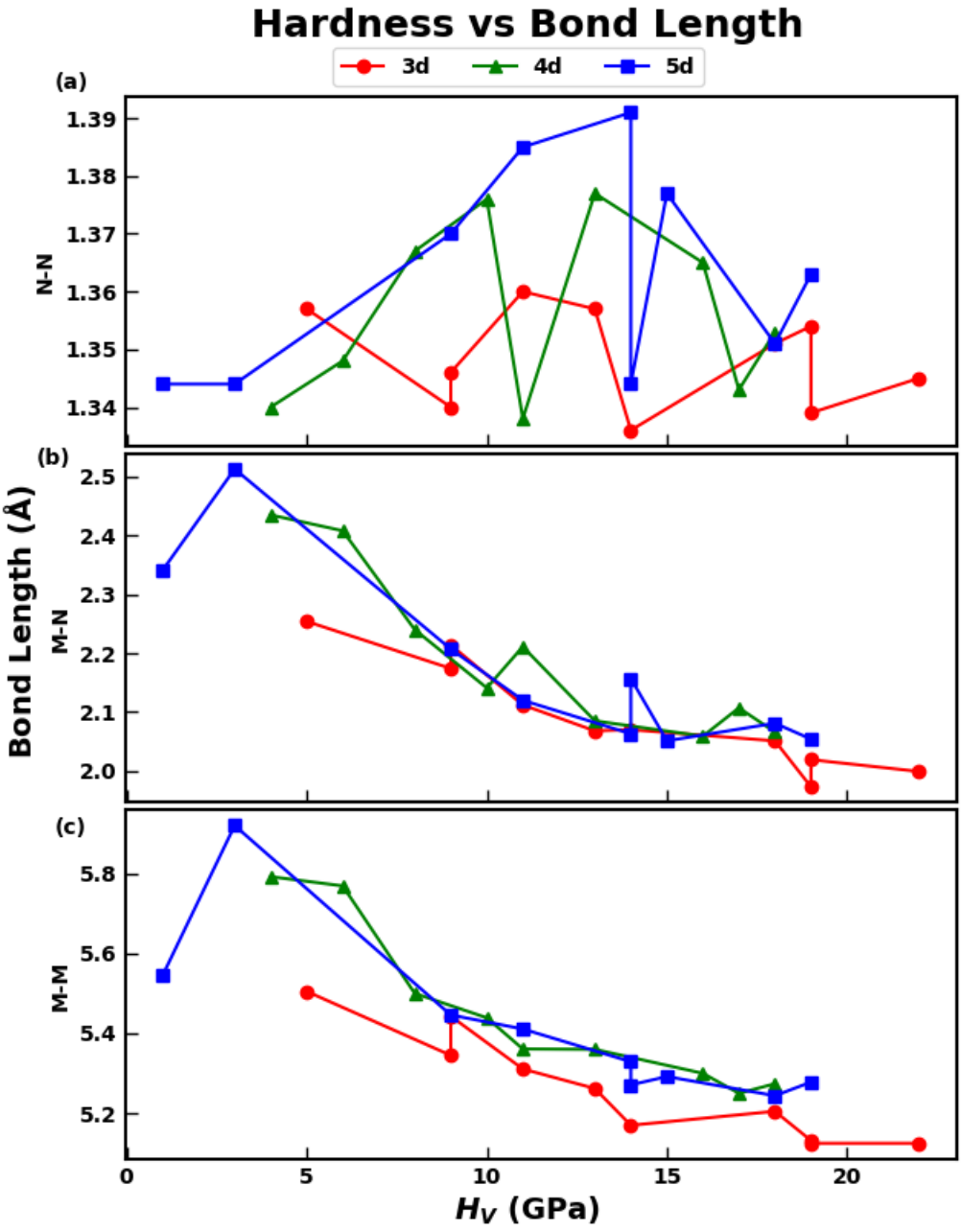


Figure S2: Phonon DOS for all mechanically stable 3d – MN_6. Presence of phonon DOS in imaginary frequency region shows vibrationally unstable compounds.

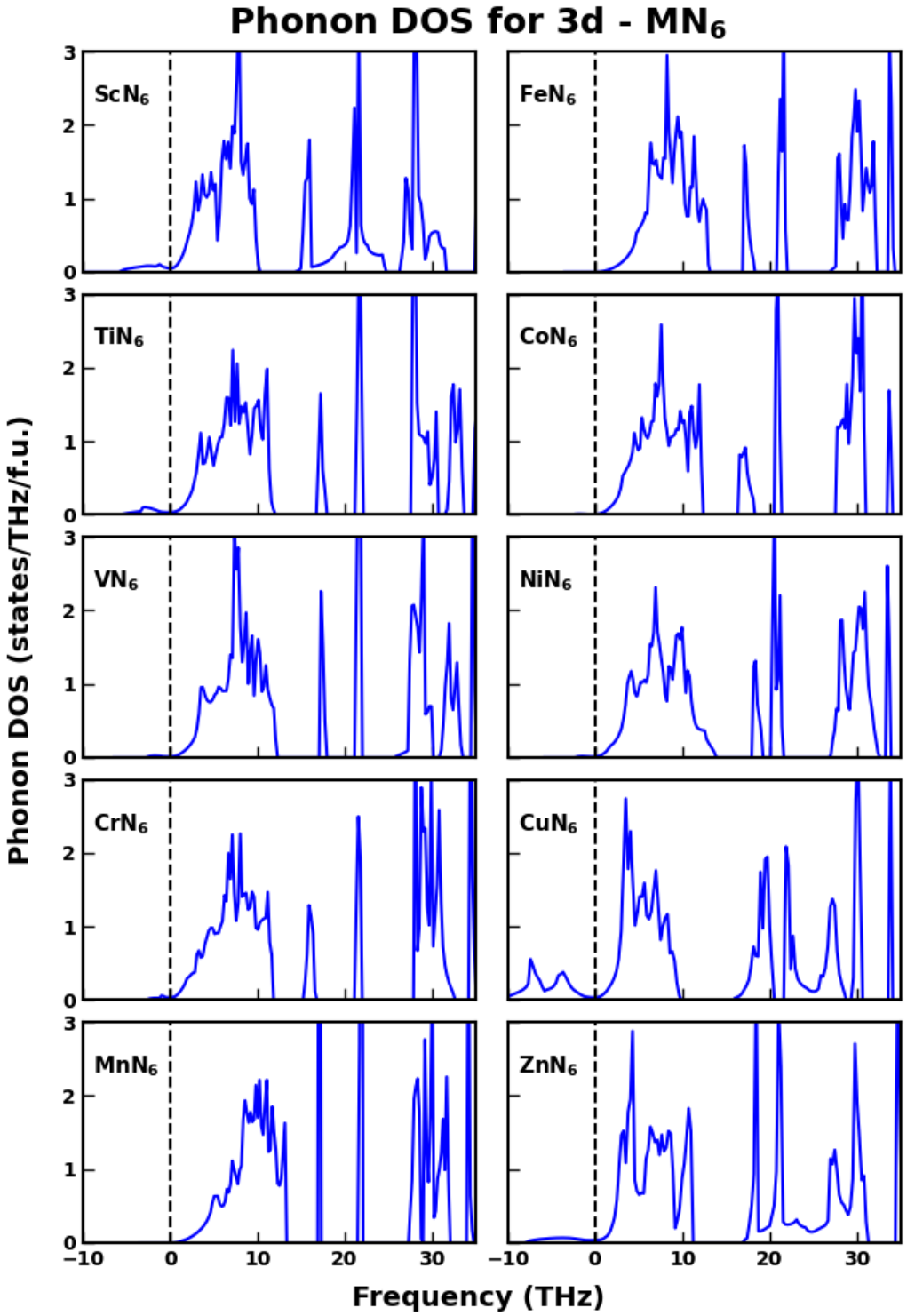


Figure S3: Phonon DOS for all mechanically stable 4d – MN_6. Presence of phonon DOS in imaginary frequency region shows vibrationally unstable compounds.

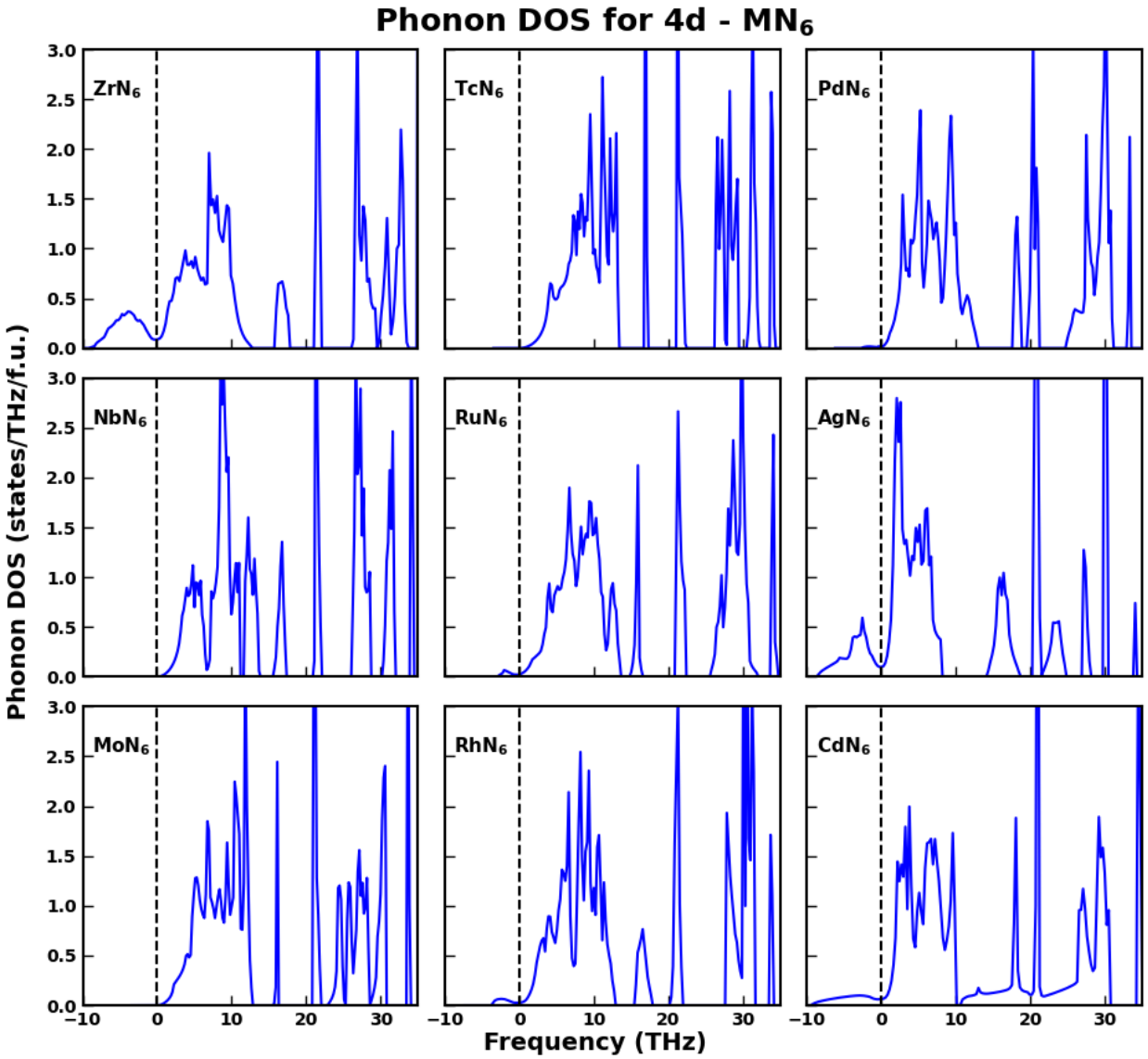


Figure S4: Phonon DOS for all mechanically stable 5d – MN_6. Presence of phonon DOS in imaginary frequency region shows vibrationally unstable compounds.

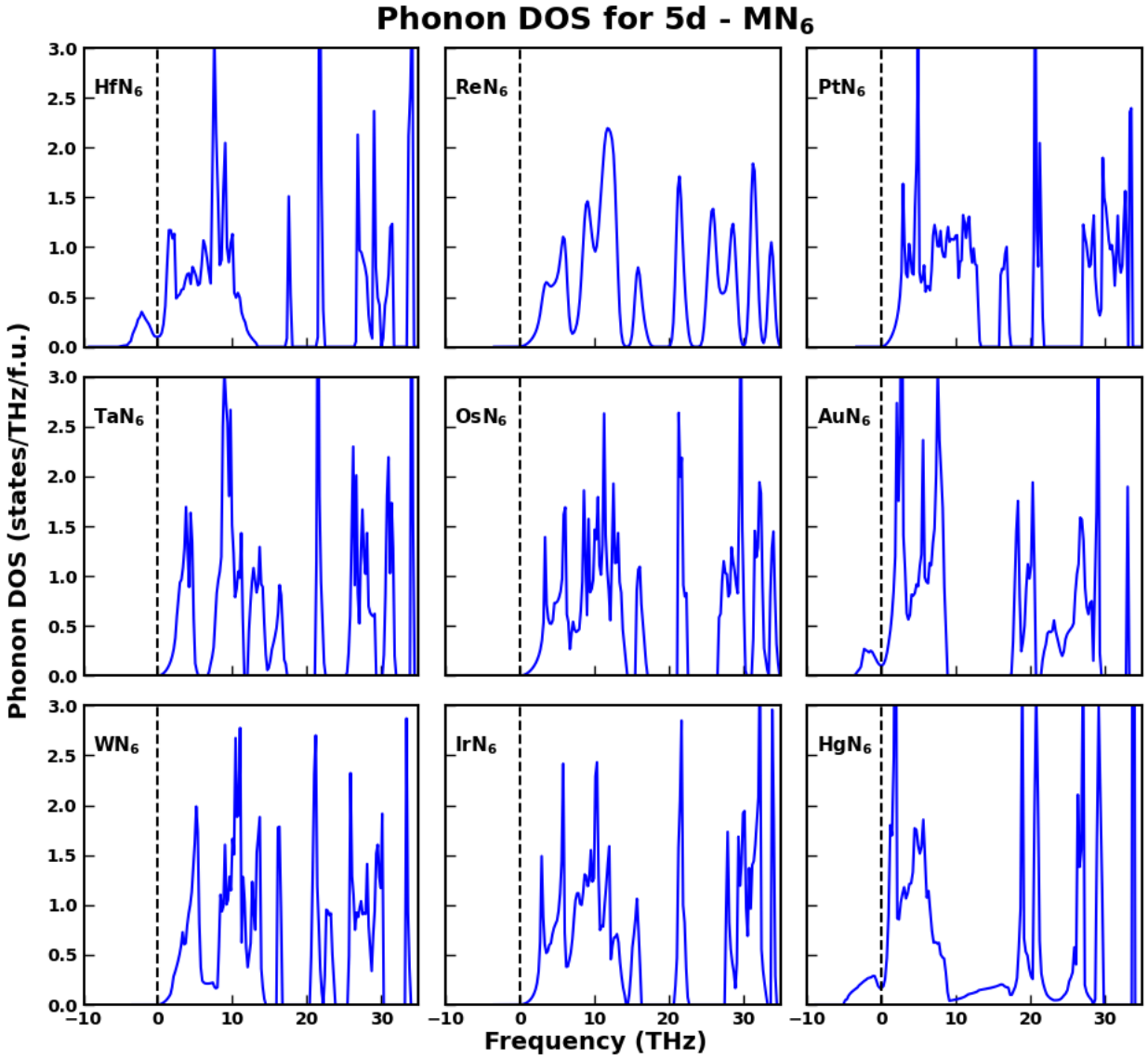


Figure S5: Variation of hardness with Pugh's ratio (k) showing brittle and ductile regions for all mechanically stable 3d, 4d, and 5d MN_6 compounds. All compounds having $H_V > 16$ GPa are mostly brittle.

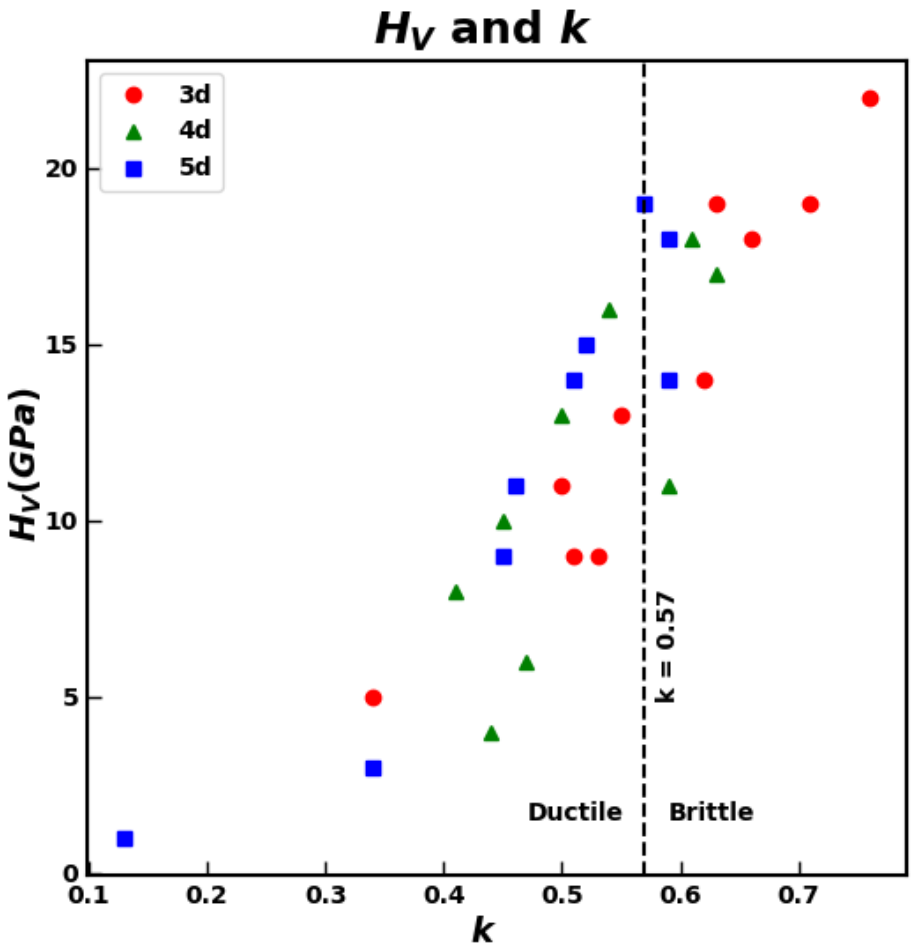


Figure S6: Variation of B, G, E, and H_V with C_{44} for all mechanically stable MN_6 compounds.

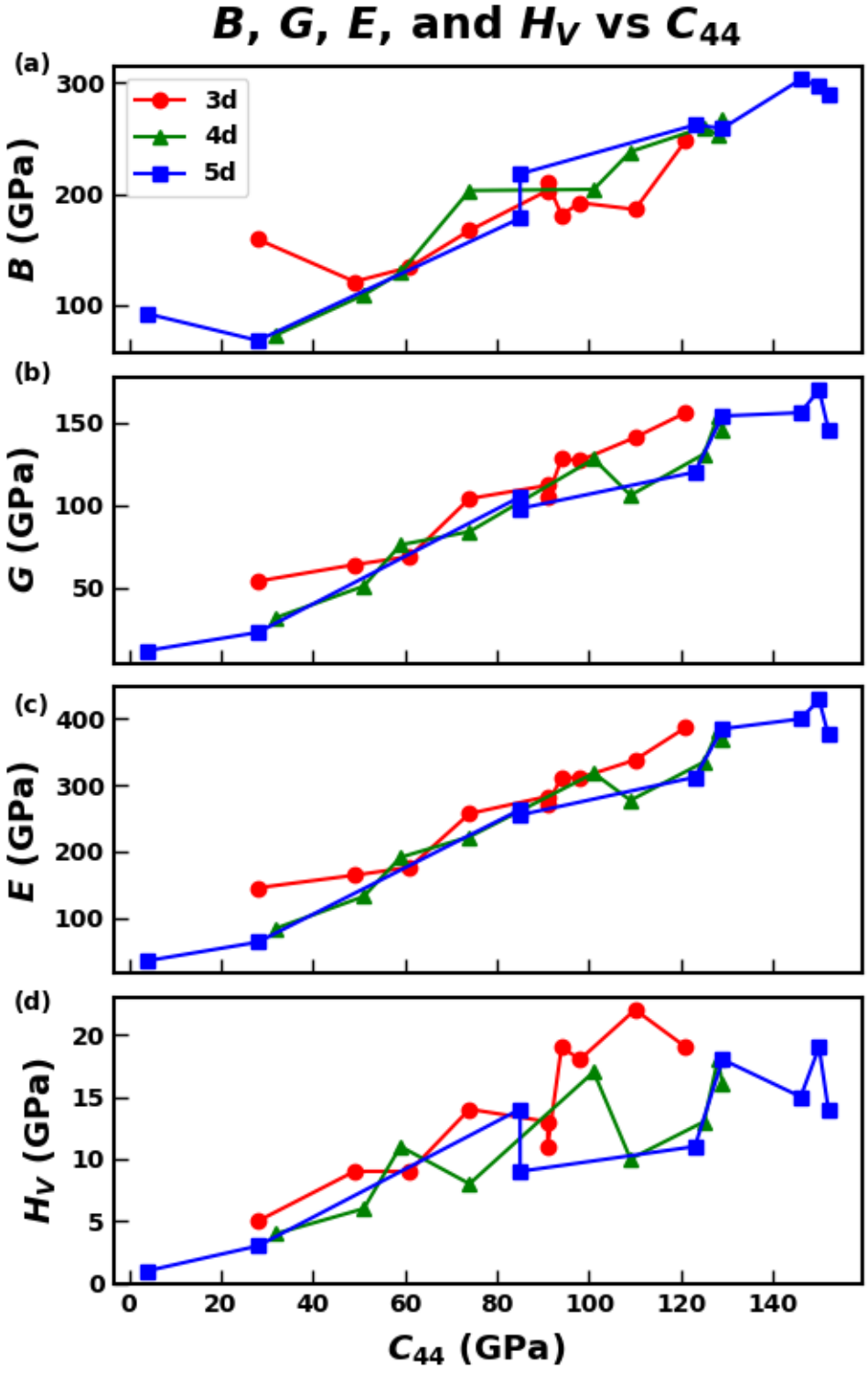


Figure S7: Variation of H_V and Q_t with VEC for all mechanically stable MN_6 compounds.

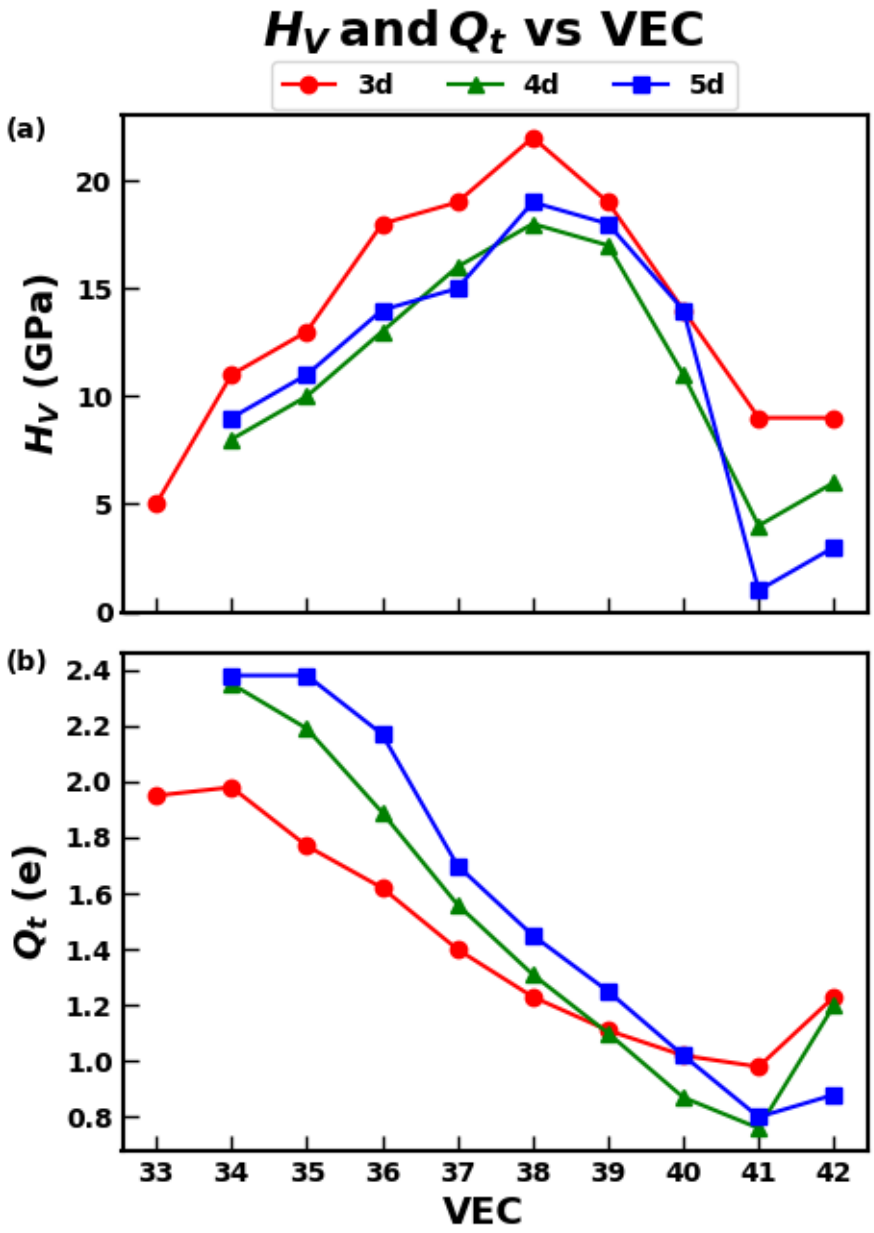


Figure S8: LDOS for mechanically stable 3d – MN_6. The Fermi level is set at 0 eV.

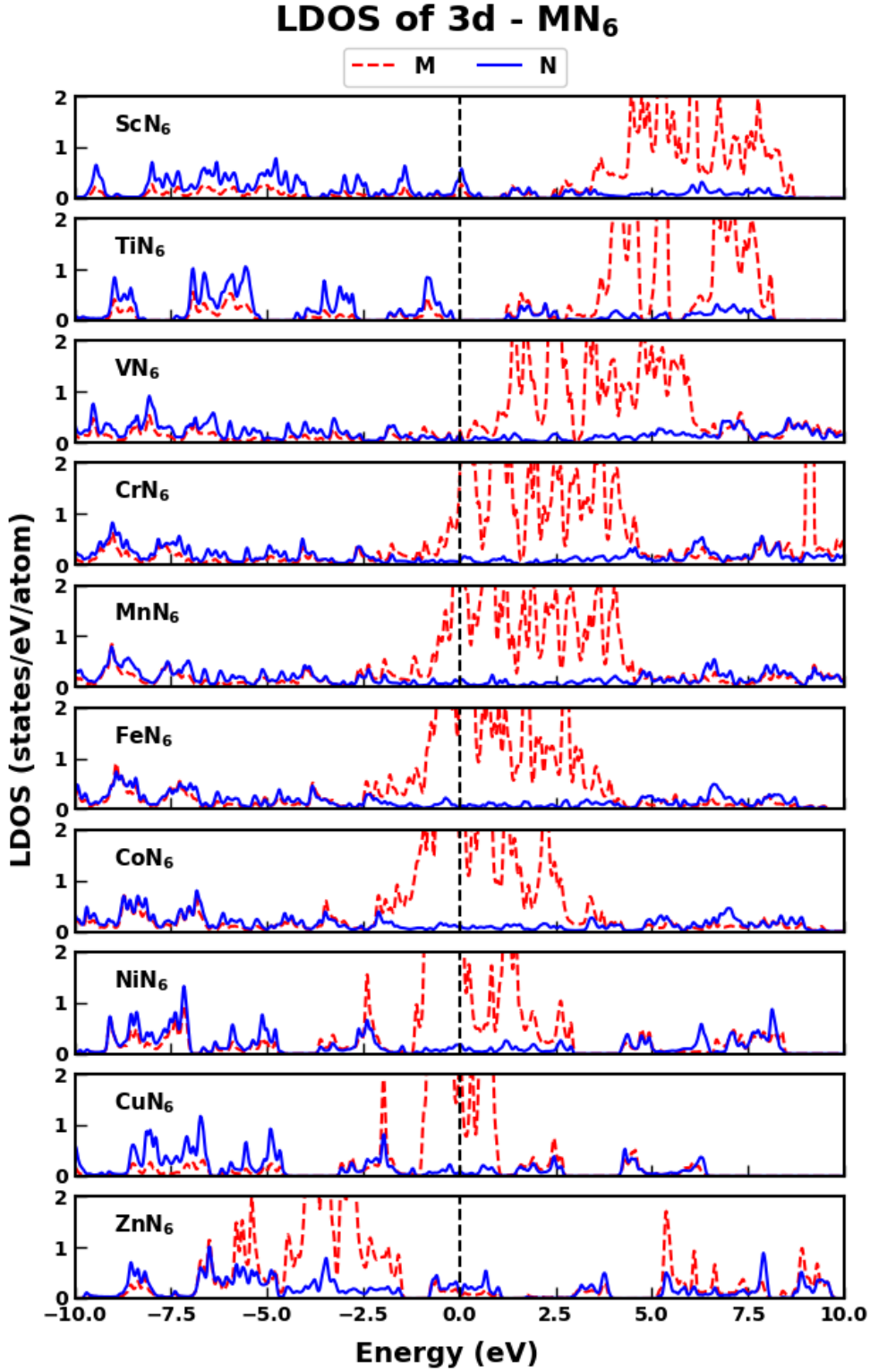


Figure S9: LDOS for mechanically stable 4d – MN_6. The Fermi level is set at 0 eV.

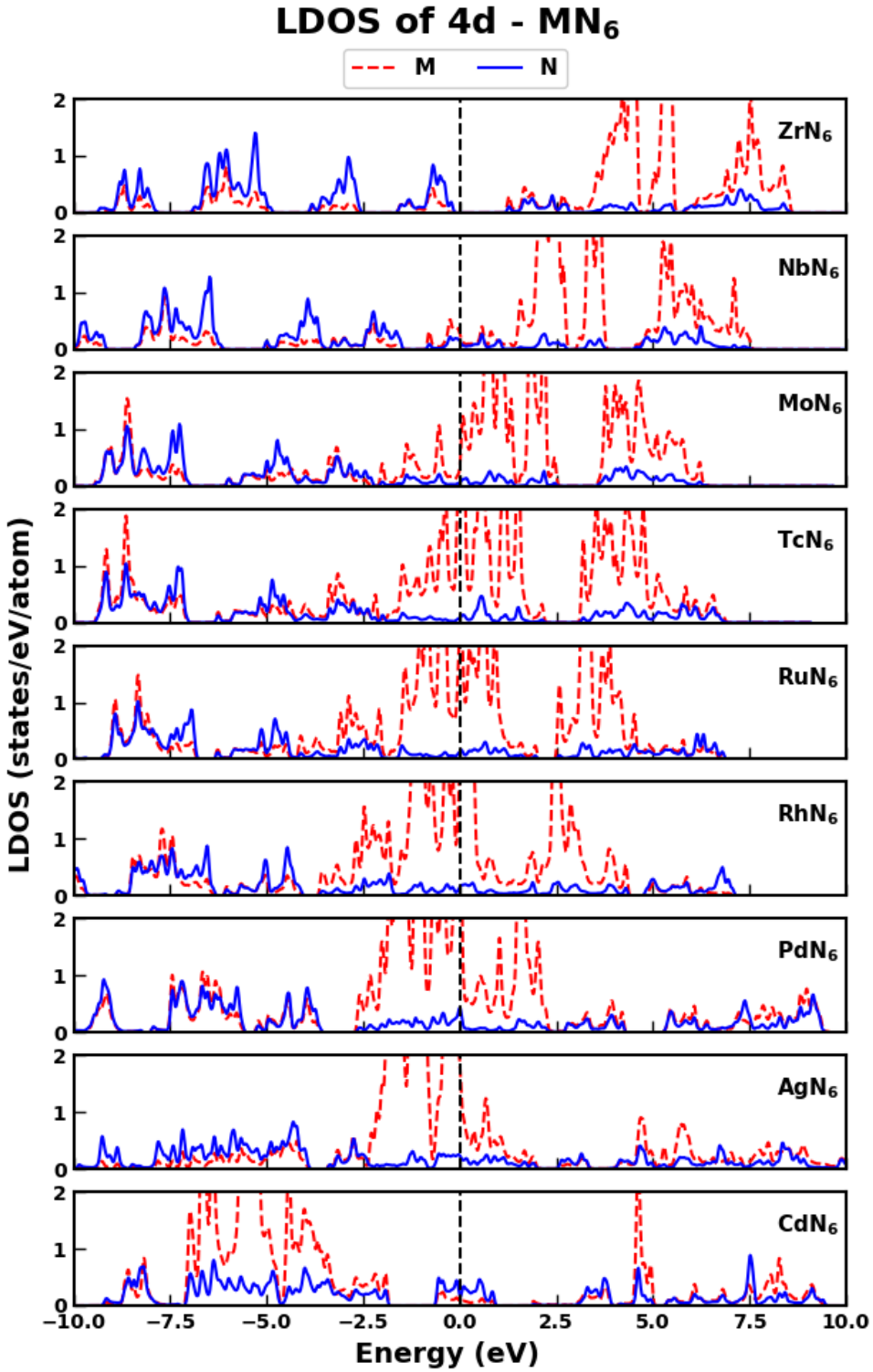


Figure S10: LDOS for mechanically stable 5d – MN_6. The Fermi level is set at 0 eV.

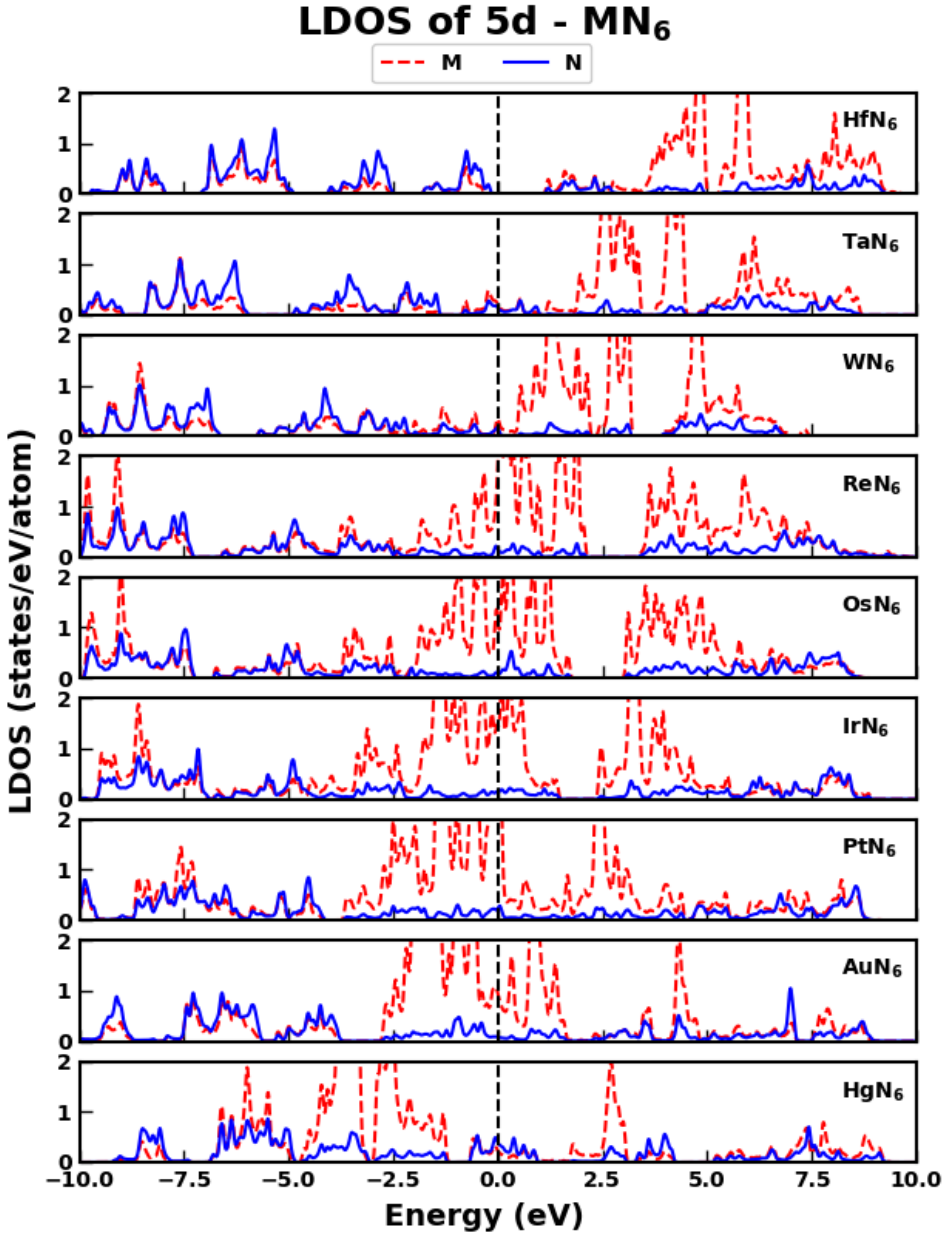


Figure S11: -pCOHP for mechanically stable 3d – MN_6. The Fermi level is set at 0 eV.

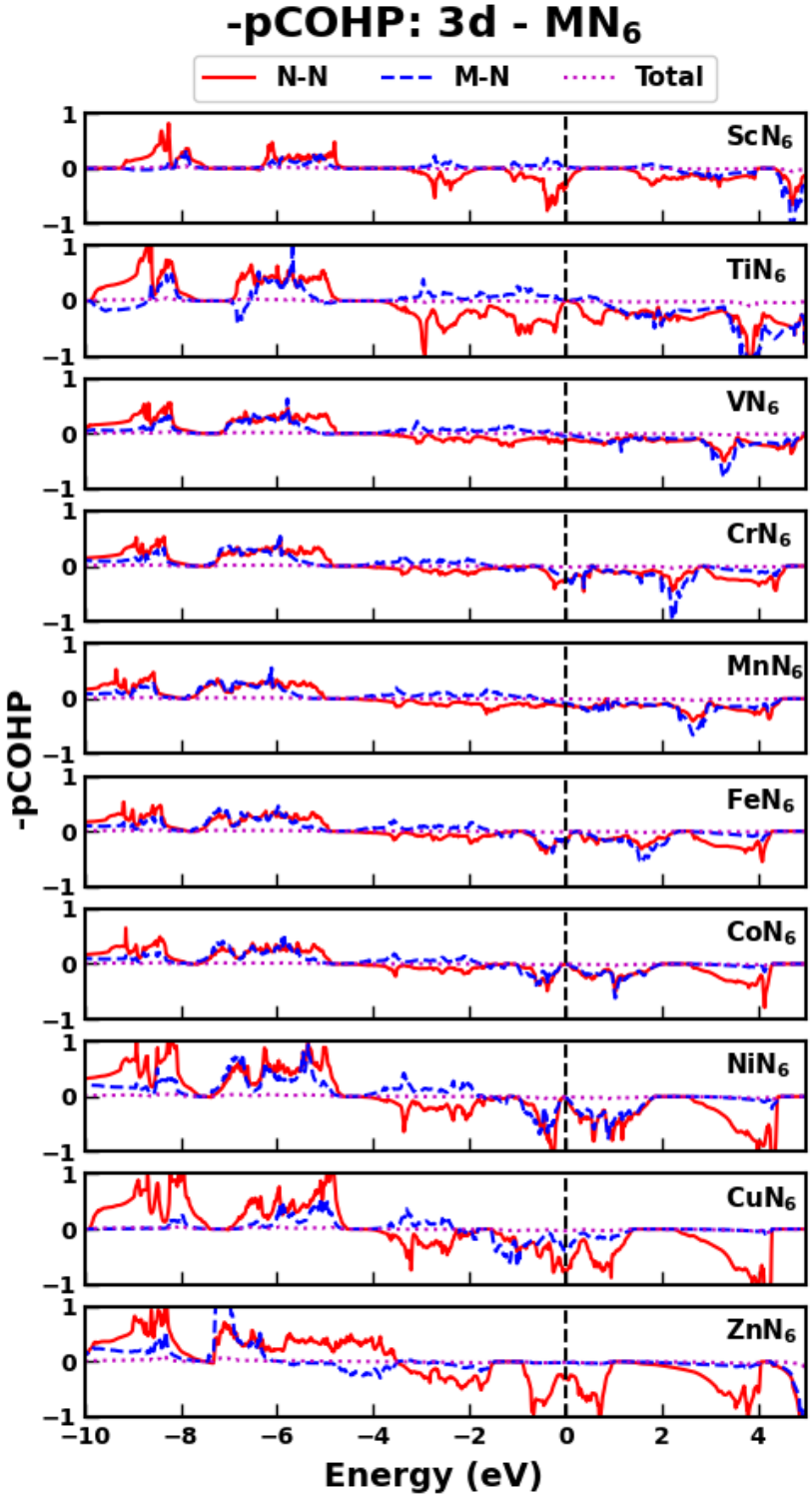


Figure S12: -pCOHP for mechanically stable 4d – MN_6. The Fermi level is set at 0 eV.

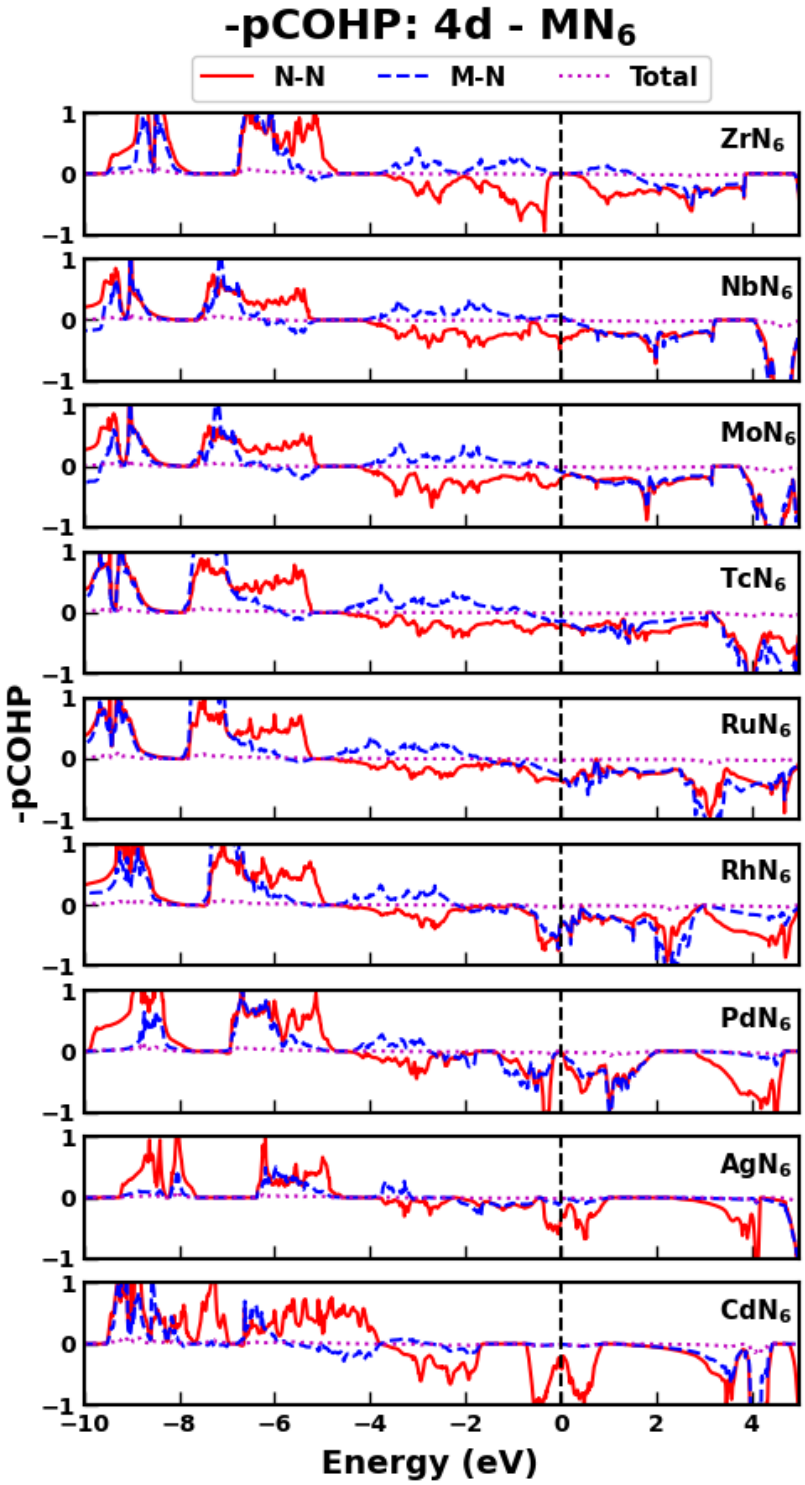


Figure S13: -pCOHP for mechanically stable 5d – MN_6. The Fermi level is set at 0 eV.

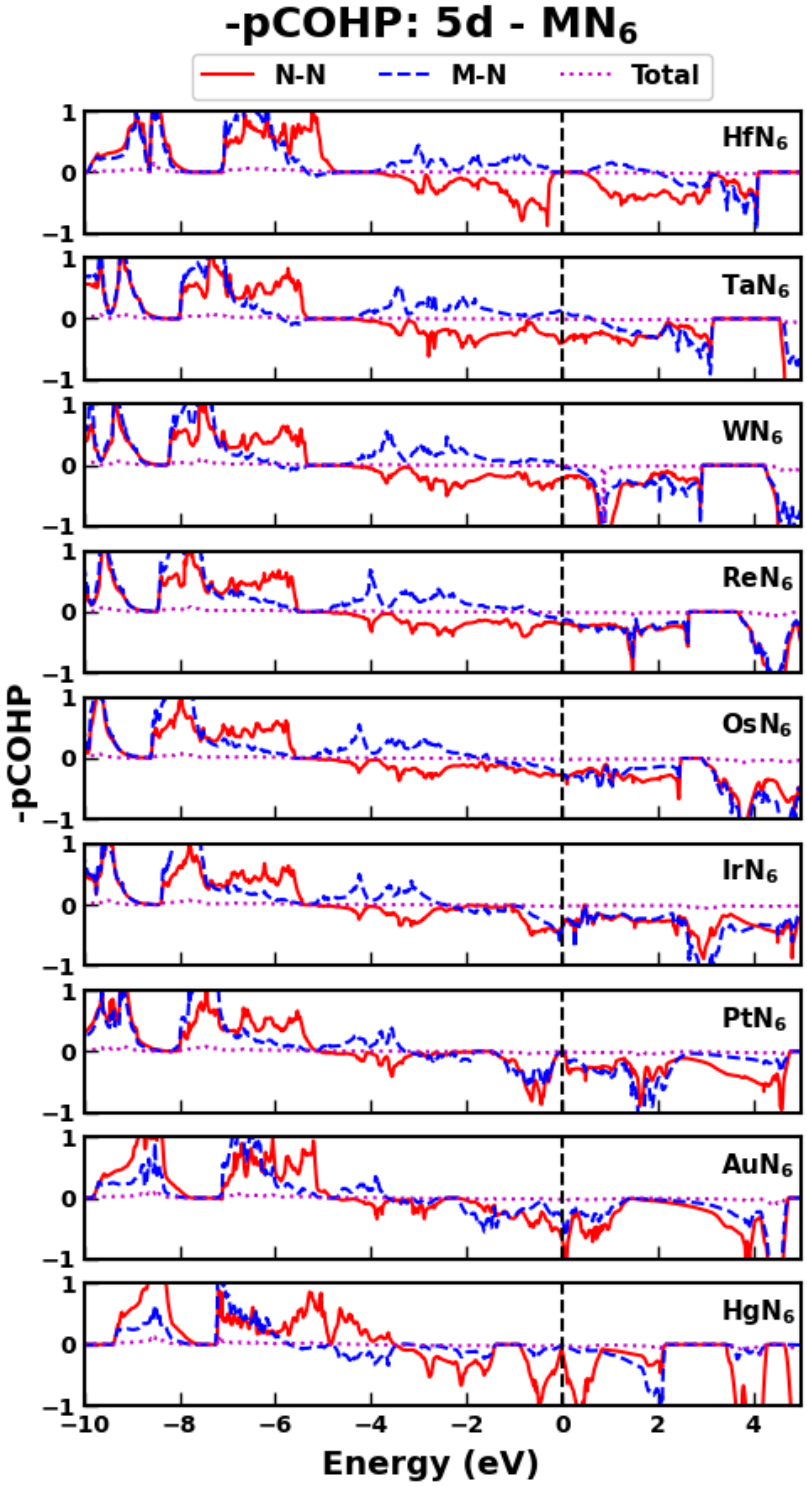


Figure S14: Electronic band structure curves for mechanically stable 3d – MN_6. The Fermi level is set at 0 eV.

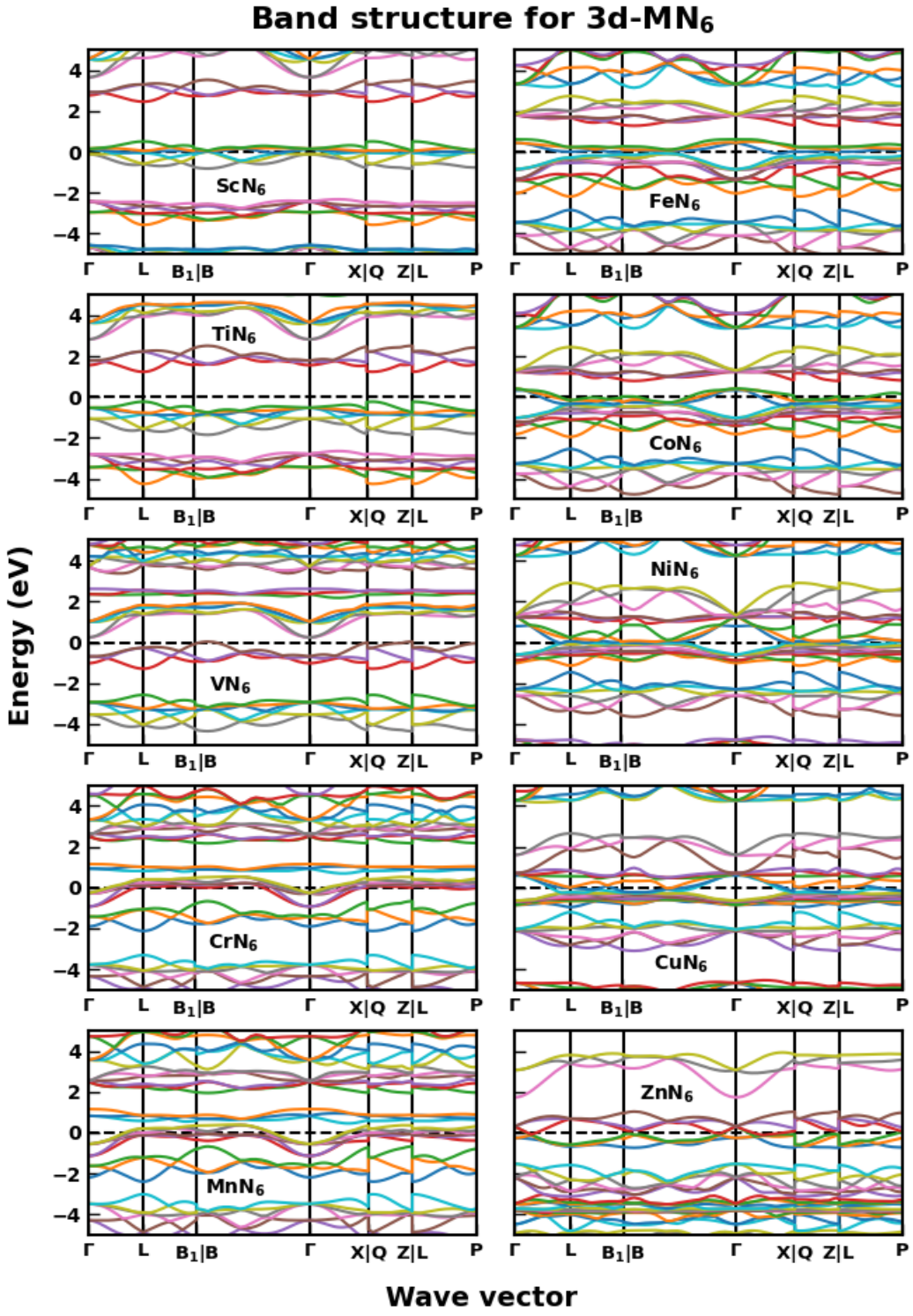


Figure S15: Electronic band structure curves for mechanically stable 4d – MN_6. The Fermi level is set at 0 eV.

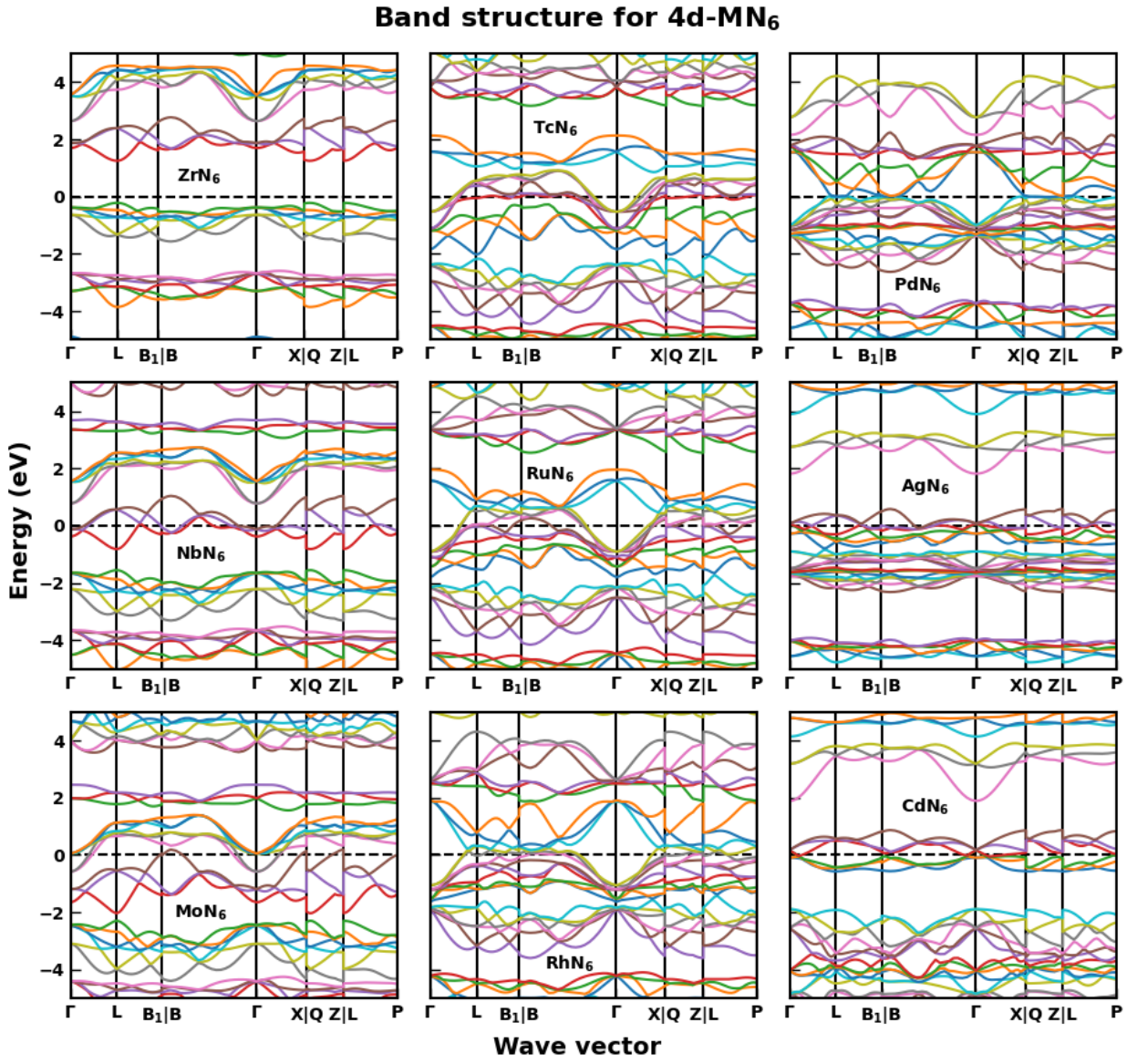
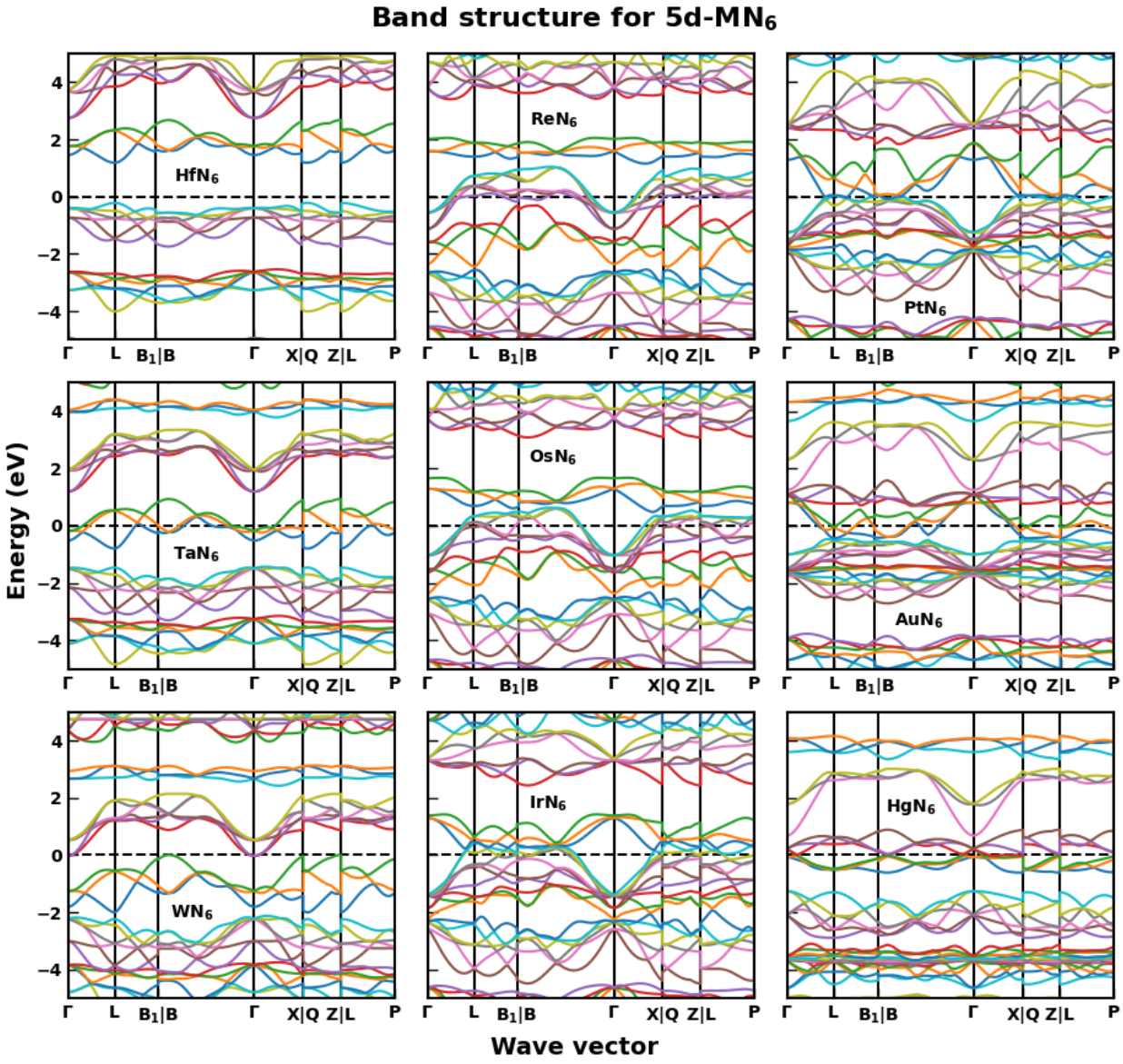


Figure S16: Electronic band structure curves for mechanically stable 5d – MN_6. The Fermi level is set at 0 eV.



References

1. A. L. Allred and E. G. Rochow, *A scale of electronegativity based on electrostatic force.* J. Inorg. Nucl. Chem., 1958. **5**: p. 264-268.