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Investigation of hardness in transition metal hexa-nitrides in cubic structure: A first-principles study

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Table S1: Total magnetic moment found in the atomic orbitals. Only in 8 MN_6 compounds possesses the magnetic moment calculated in terms of Bohr magneton.

Material	Magnetic Moment							
	Transition Metal				Nitrogen			Total in the Unit Cell
	s-orbital	p-orbital	d-orbital	Total	s-orbital	p-orbital	Total	
CoN_6	-0.006	-0.003	-1.531	-1.540	-0.003	0.036	0.033	-2.684
CuN_6	-0.001	0.003	0.044	0.046	0.002	0.062	0.064	0.860
TcN_6	-0.002	0.003	-0.052	-0.051	0.003	0.066	0.069	0.726
RhN_6	0.003	0.003	0.983	0.989	0.004	0.004	0.008	2.074
AgN_6	-0.001	0.006	0.022	0.027	0.002	0.088	0.090	1.134
ReN_6	-0.002	0.002	-0.037	-0.037	0.002	0.040	0.042	0.430
IrN_6	0.011	0.004	1.125	1.140	0.009	0.008	0.017	2.484
AuN_6	0.475	0.000	-0.020	0.455	0.002	0.004	0.006	0.982

Table S2: 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 lengths as functions of hardness for mechanically stable MN_6.

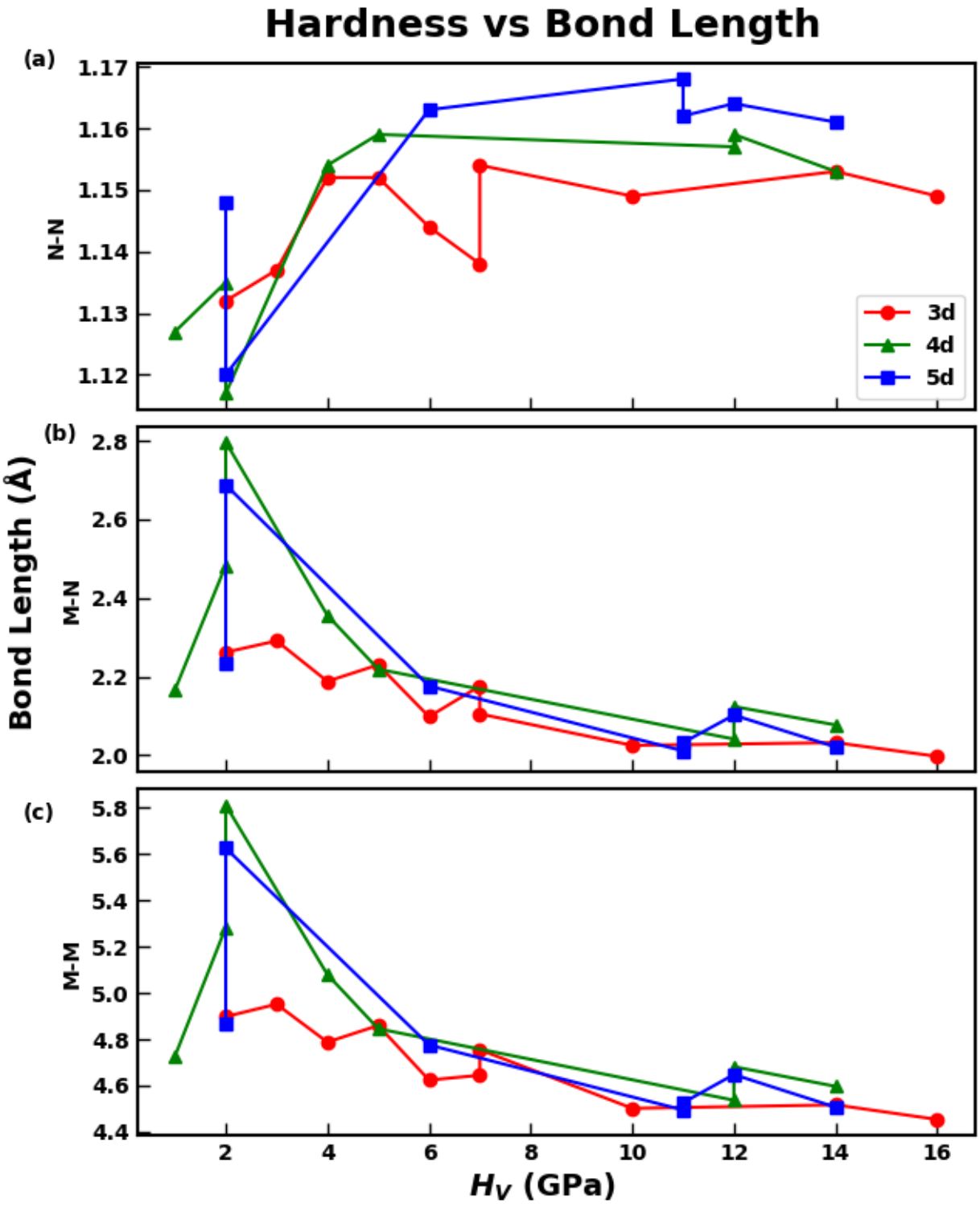


Figure S2-1: Comparison of phonon DOS for only mechanically stable MN_6 compounds in the order of increasing hardness from top to bottom in each column. ZrN_6 is harder than ScN_6.

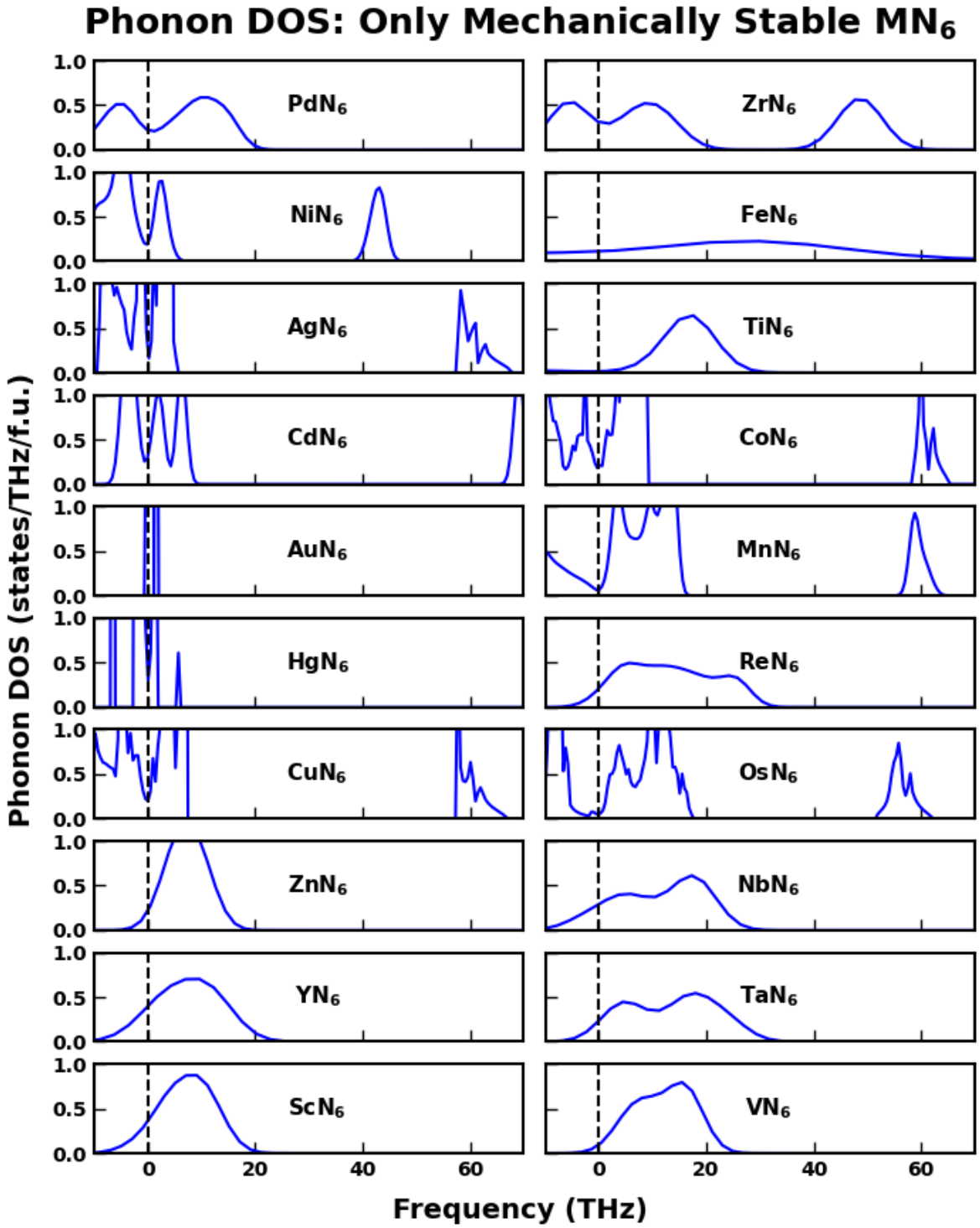


Figure S2-2: Comparison of phonon DOS for both mechanically and vibrationally unstable MN_6 compounds.

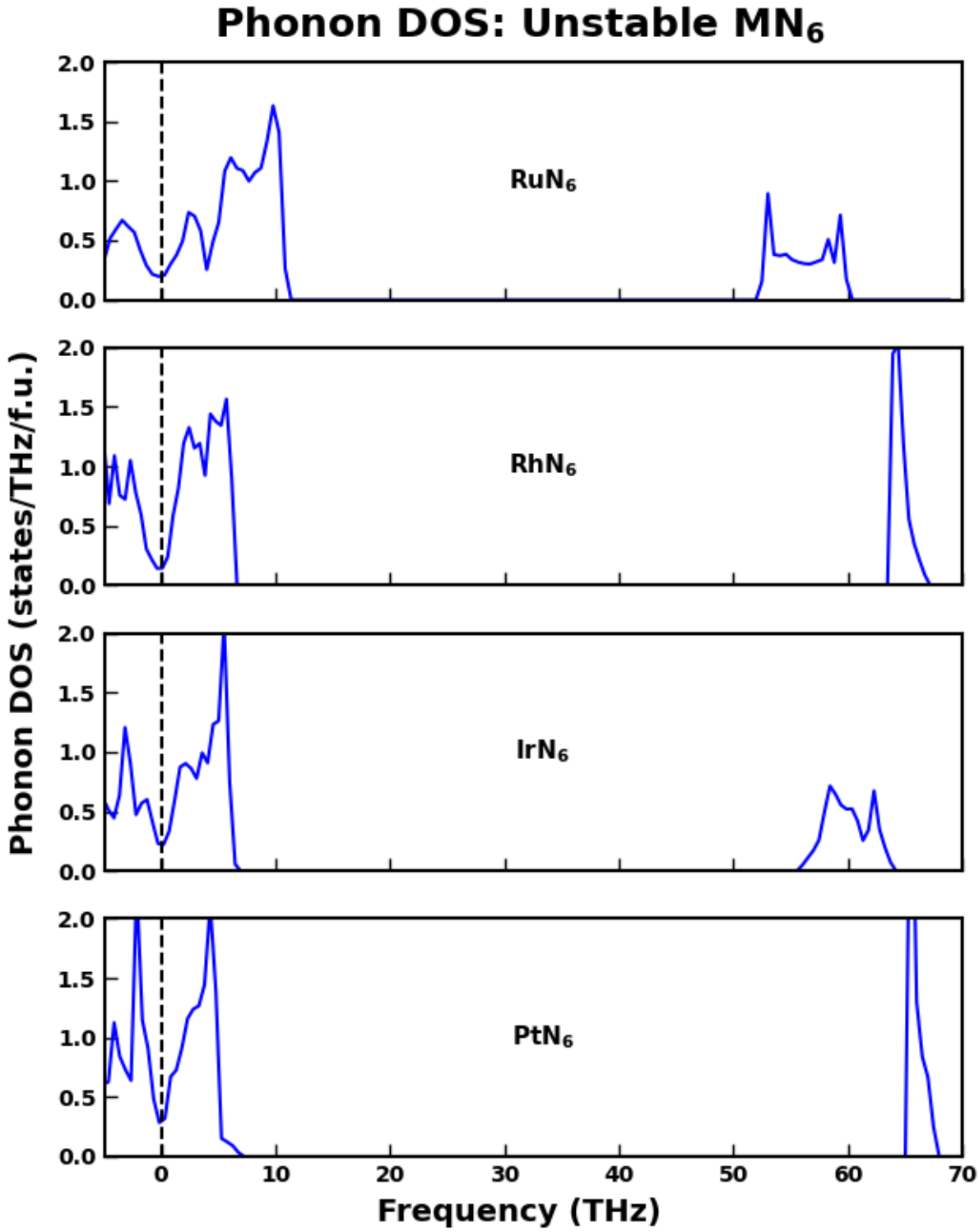


Figure S3-1: Comparison of LDOS for only mechanically stable MN_6 compounds in the order of increasing hardness from top to bottom in each column. ZrN_6 is harder than ScN_6. The Fermi level is set at 0 eV.

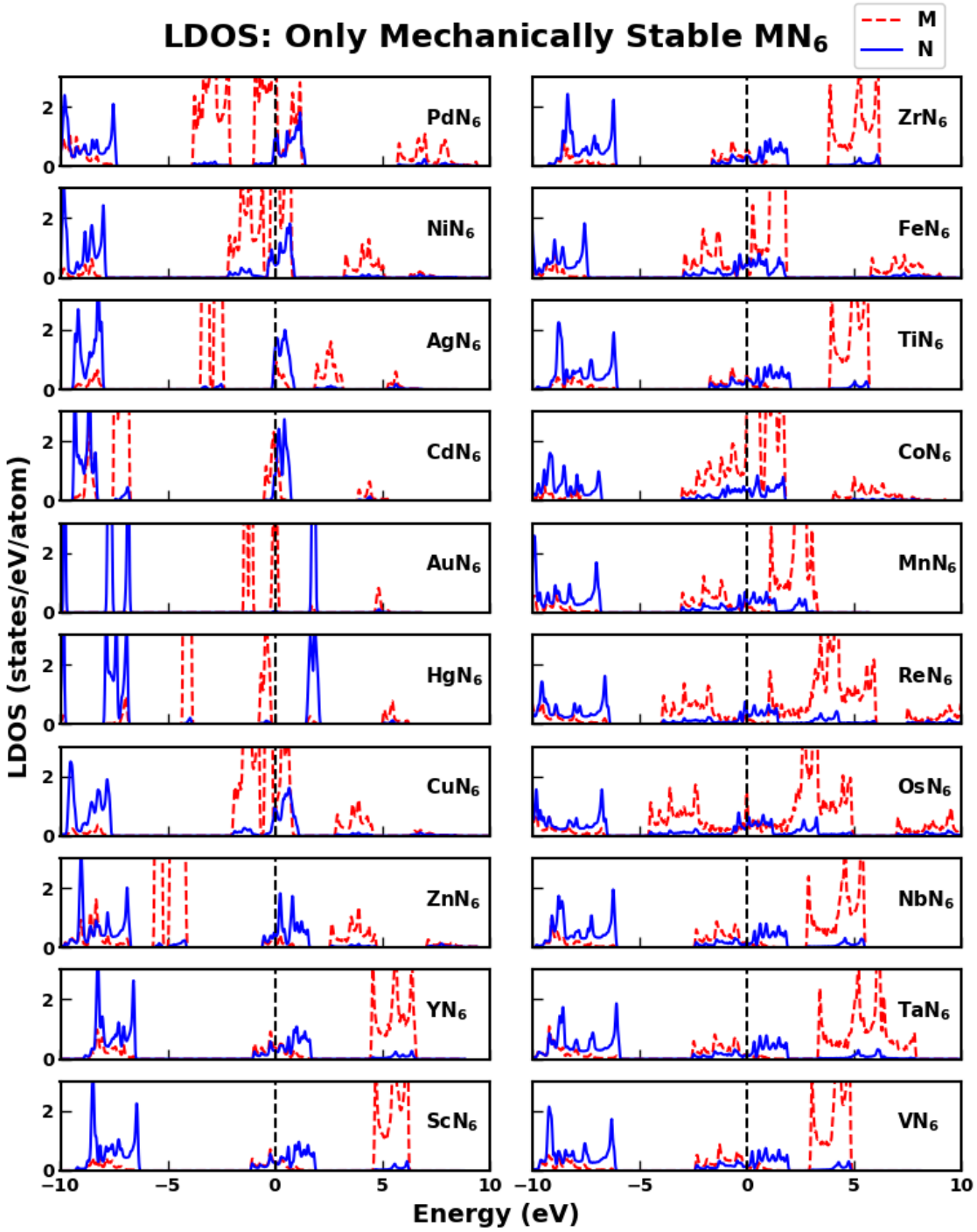


Figure S3-2: Comparison of LDOS for both mechanically and vibrationally unstable MN_6 compounds. The Fermi level is set at 0 eV.

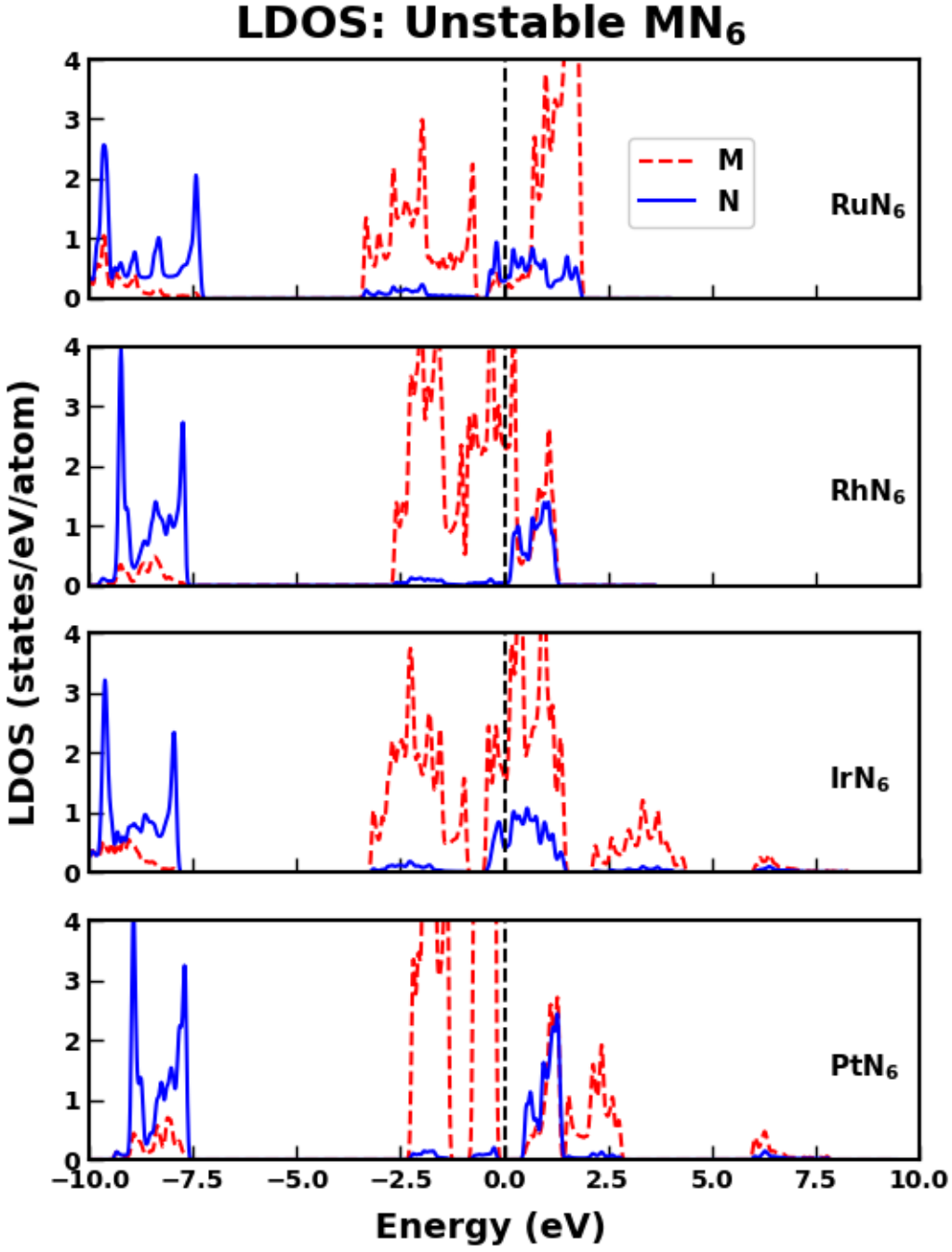


Figure S4-1: Comparison of -pCOHP for only mechanically stable MN_6 compounds in the order of increasing hardness from top to bottom in each column. ZrN_6 is harder than ScN_6. The Fermi level is set at 0 eV.

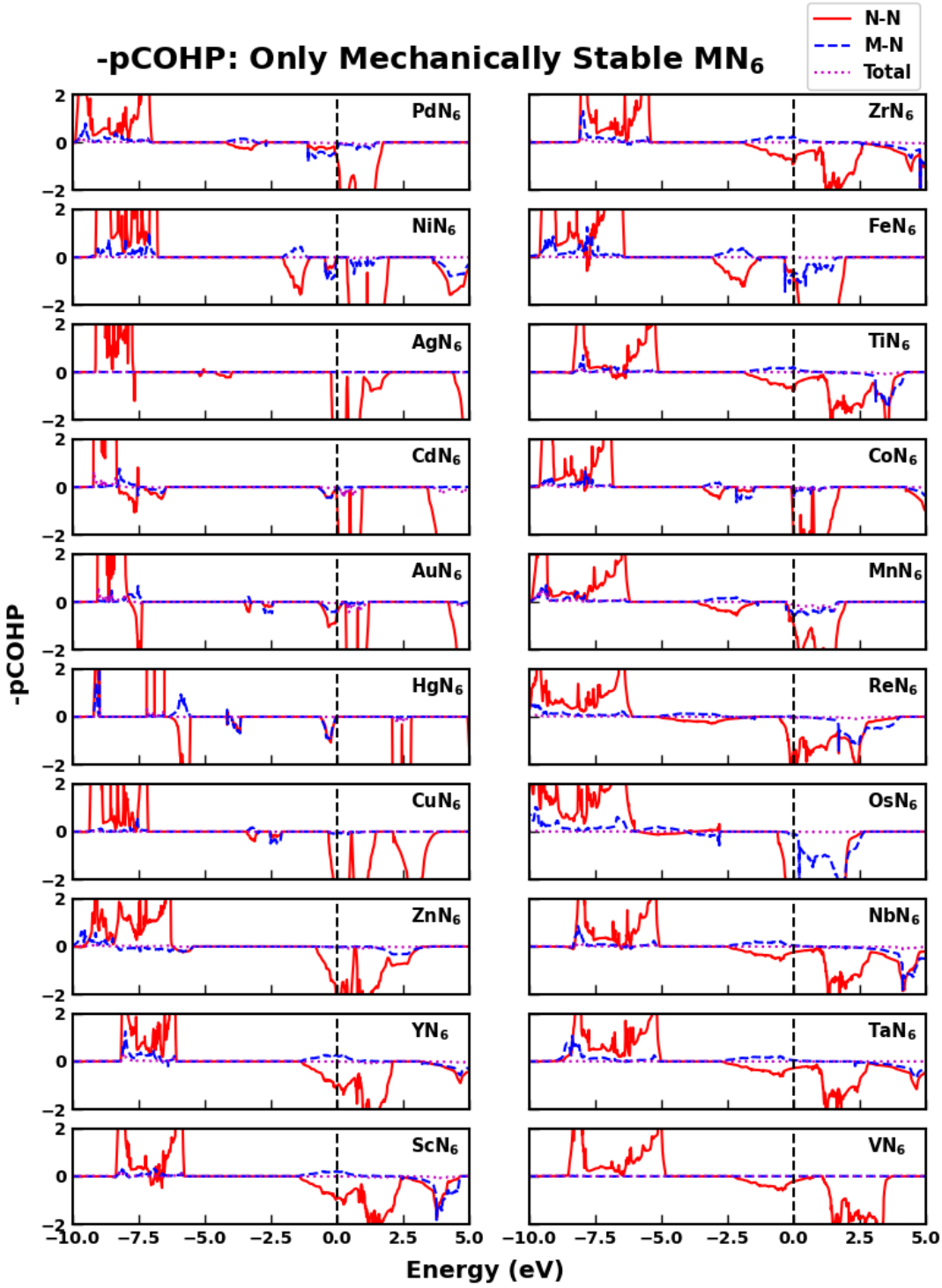


Figure S4-2: Comparison of -pCOHP for both mechanically and vibrationally unstable MN_6 compounds. The Fermi level is set at 0 eV.

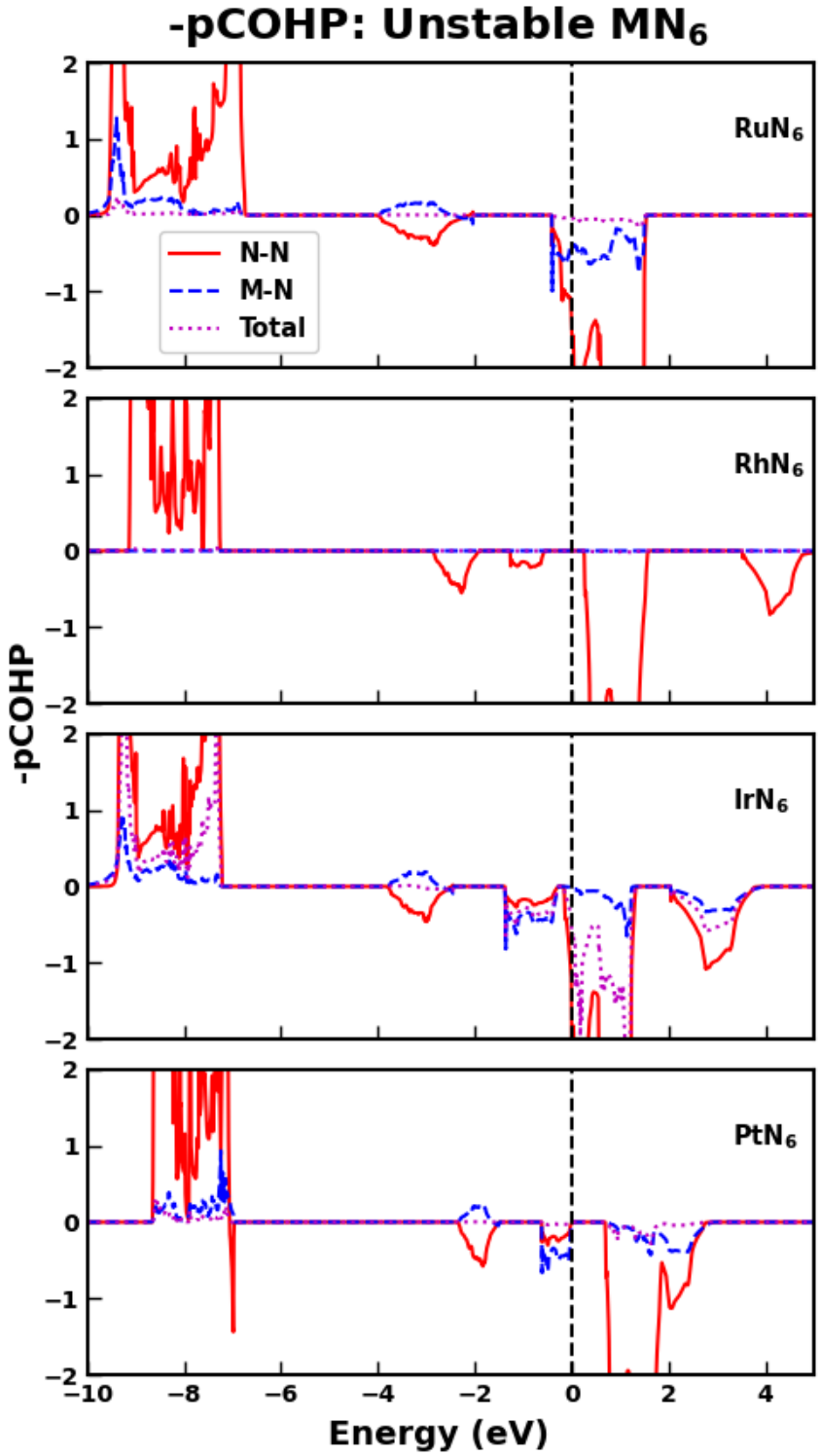


Figure S5-1(a): Electronic band structure curves for only mechanically stable MN_6 compounds in the order of increasing hardness from top to bottom in each column. HgN_6 is harder than AuN_6. The Fermi level is set at 0 eV.

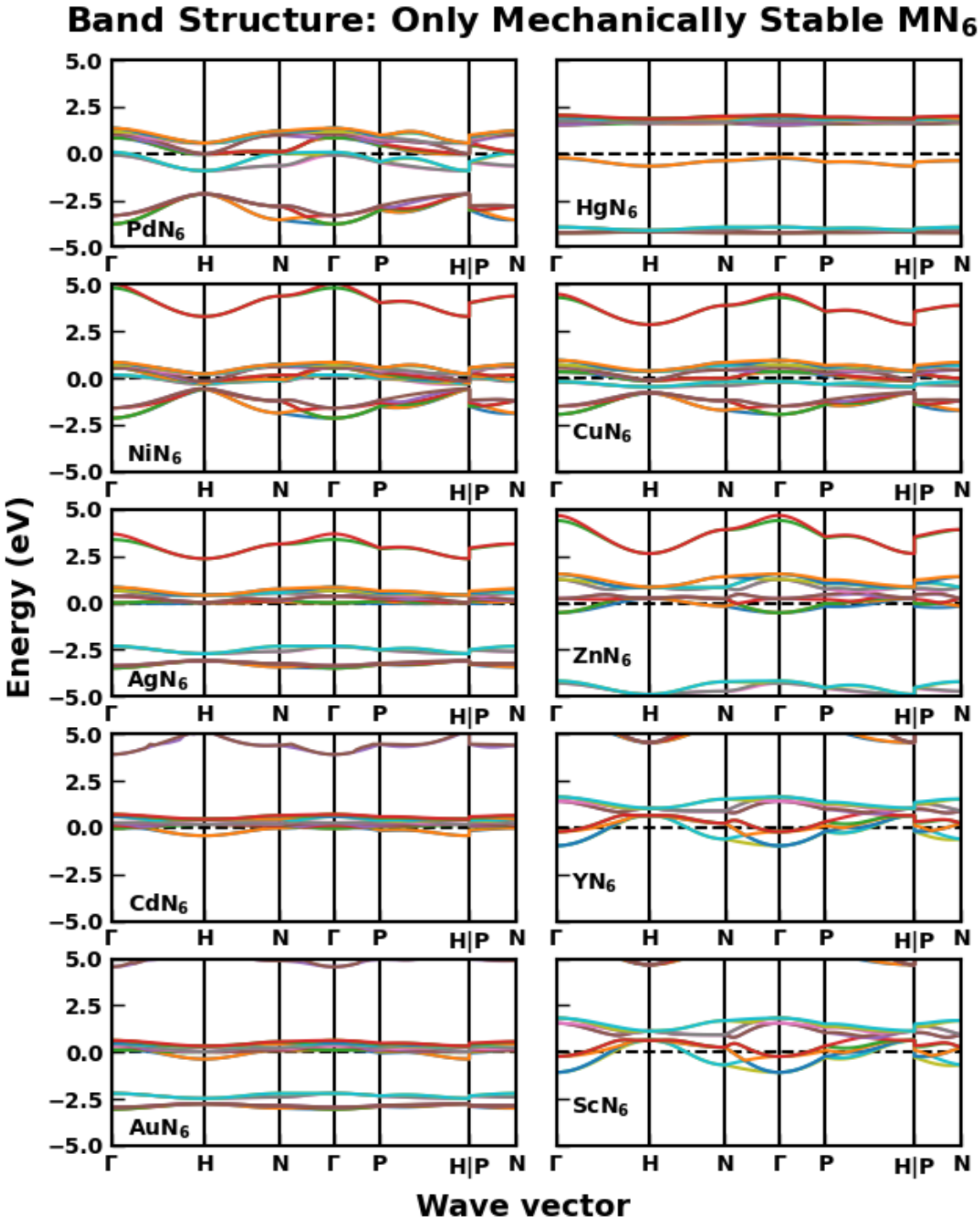


Figure S5-1(b): Electronic band structure curves for only mechanically stable MN_6 compounds in the order of increasing hardness from top to bottom in each column. ReN_6 is harder than MnN_6. The Fermi level is set at 0 eV.

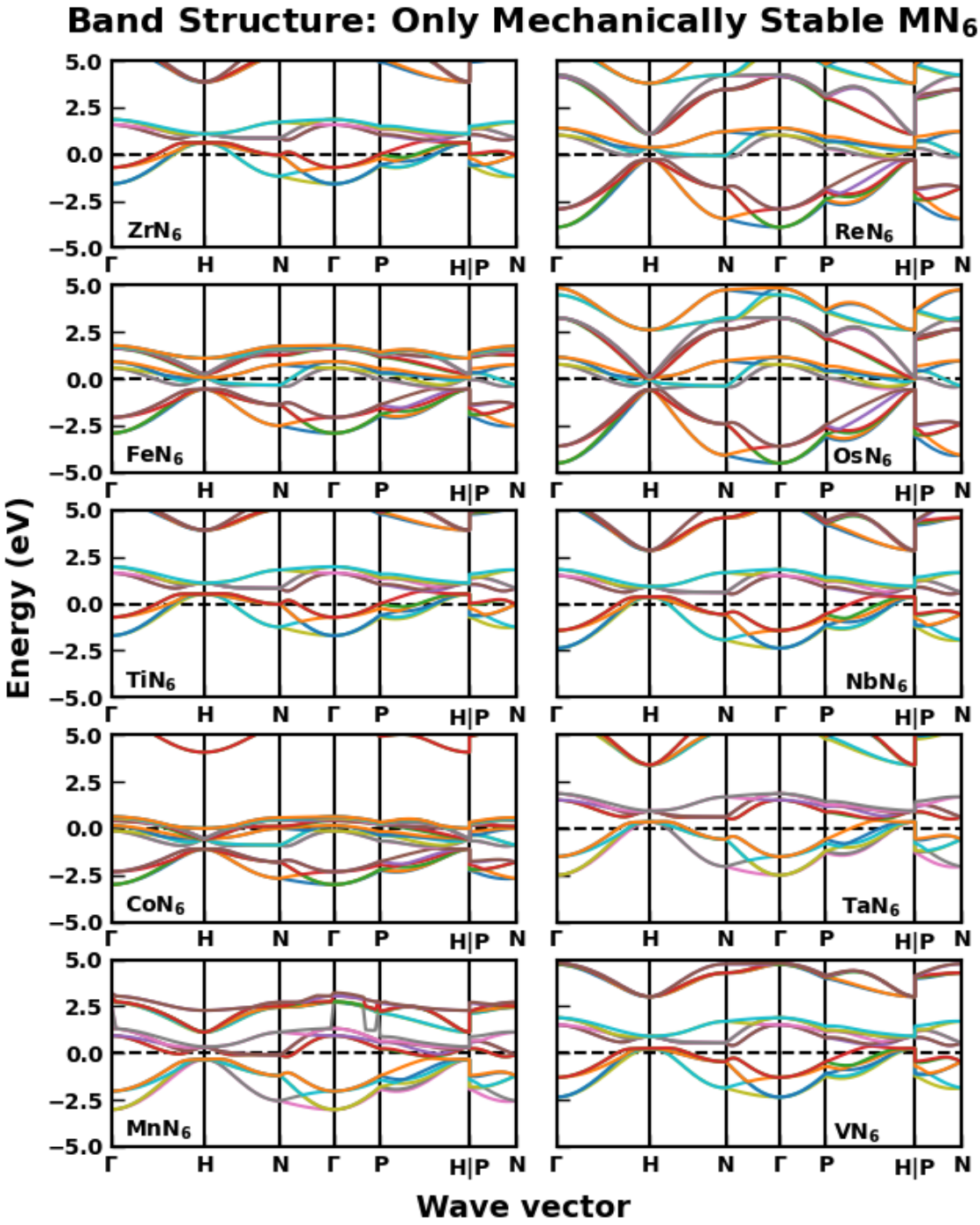
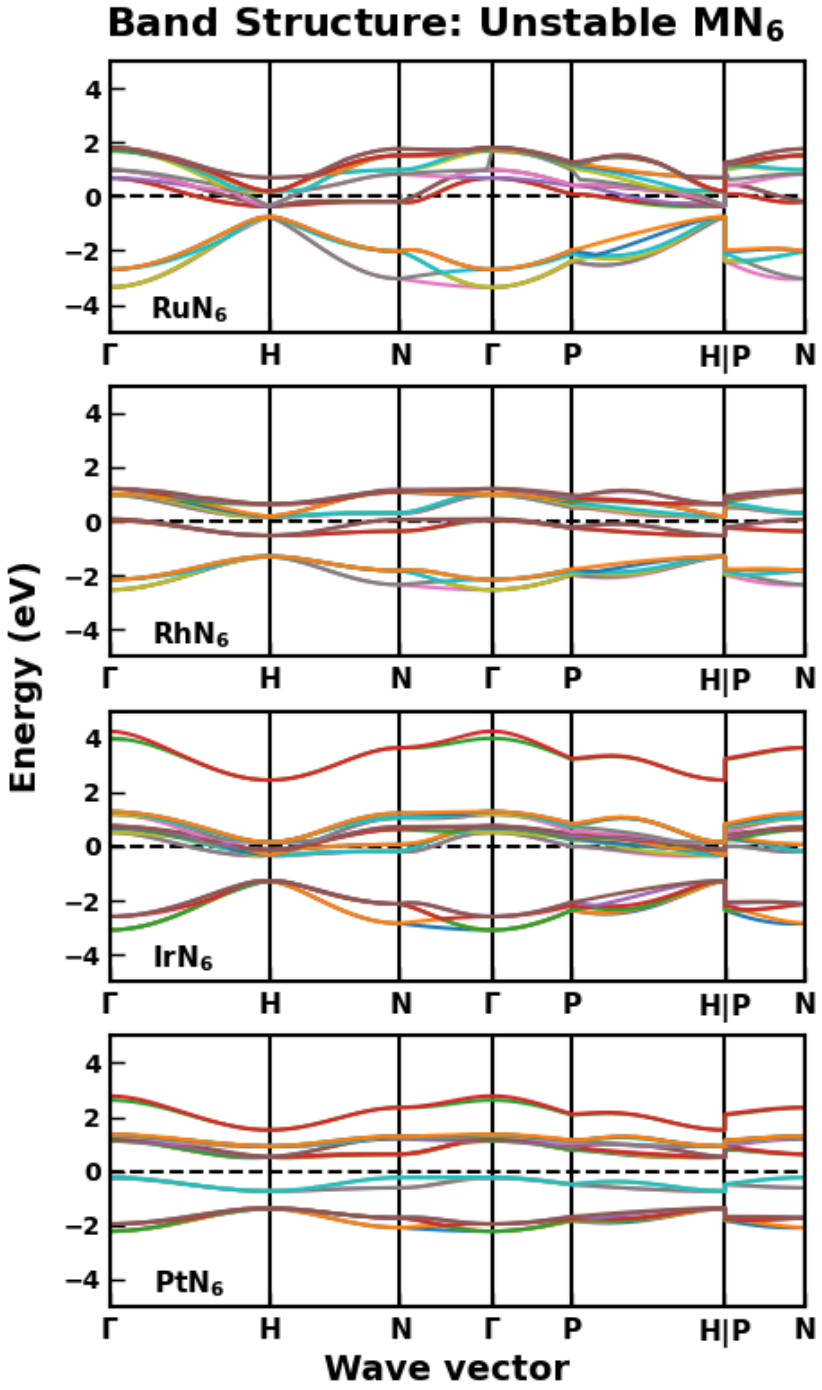


Figure S5-2: Electronic band structure curves for both mechanically and vibrationally unstable MN_6 compounds. The Fermi level is set at 0 eV.



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.