Supporting Information

Density Functional Theory Study of Bulk Properties of Transition Metal Nitrides

Michael Lynn,[1] Damilola Ologunagba,[1] Beni B. Dangi[2*], Shyam Kattel[1]*

[1] *Department of Physics, Florida Agricultural and Mechanical University, Tallahassee, FL 32307*

[2] *Department of Chemistry, Florida Agricultural and Mechanical University, Tallahassee, FL 32307*

Corresponding authors: beni.dangi@famu.edu; shyam.kattel@famu.edu

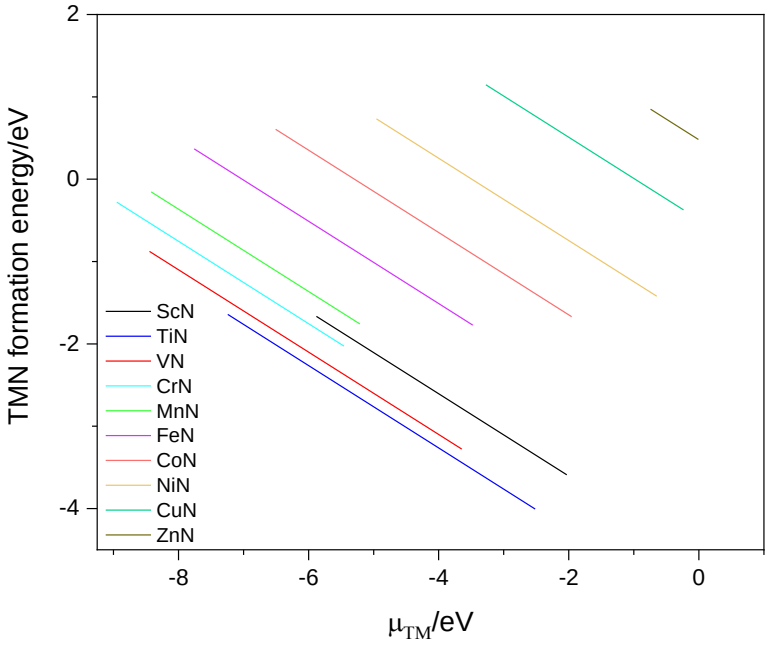

Figure S1. Variation of bulk TMN (TM = 3d series) formation energy with TM chemical potential (μ_{TM}).

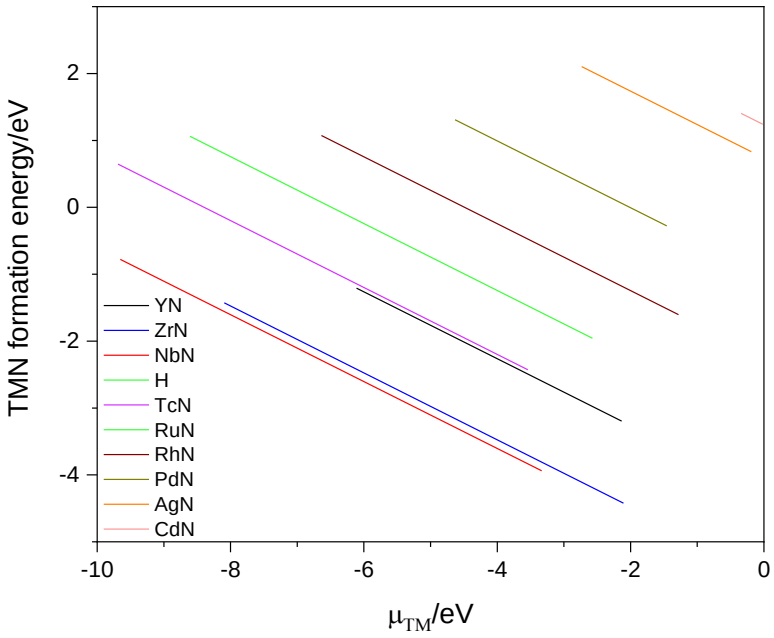

Figure S2. Variation of bulk TMN (TM = 4d series) formation energy with TM chemical potential (μ_{TM}).

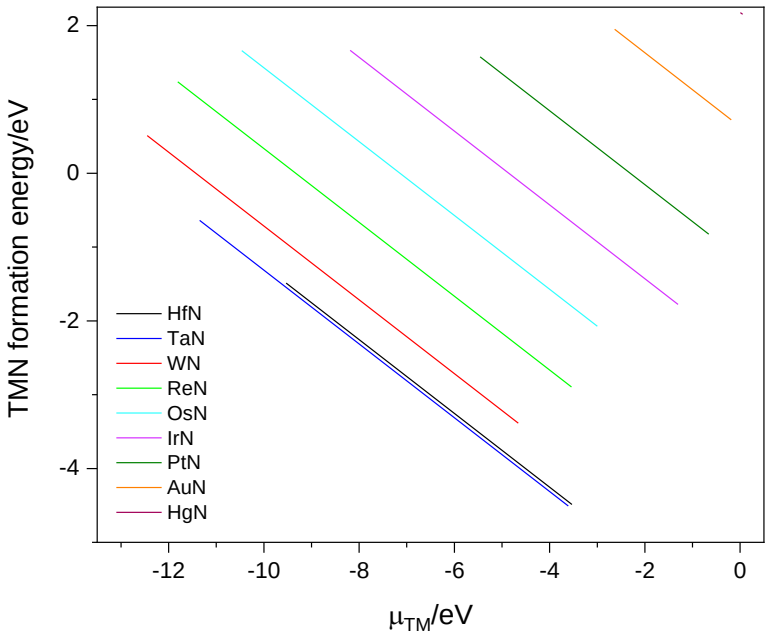

Figure S3. Variation of bulk TMN (TM = 5d series) formation energy with TM chemical potential (μ_{TM}).

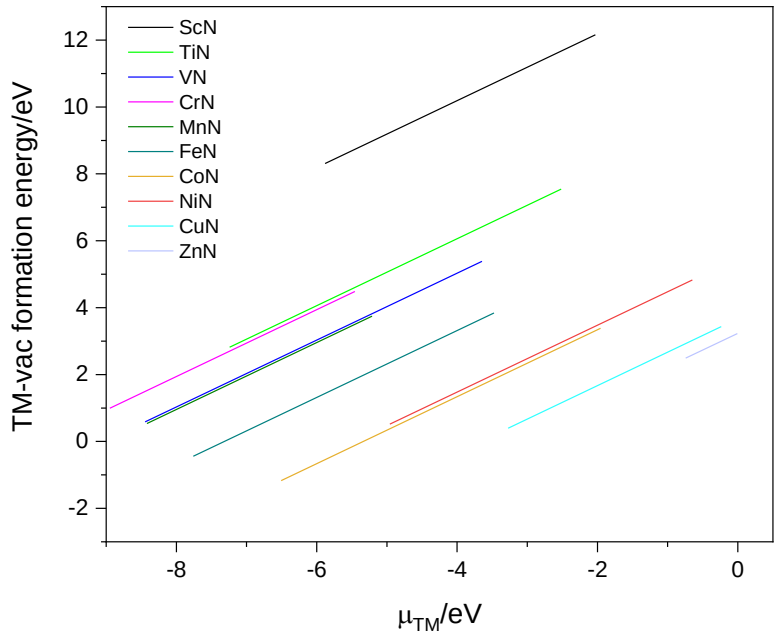

Figure S4. Variation of TM-vacancy (TM = 3d series) formation energy with TM chemical potential (μ_{TM}) .

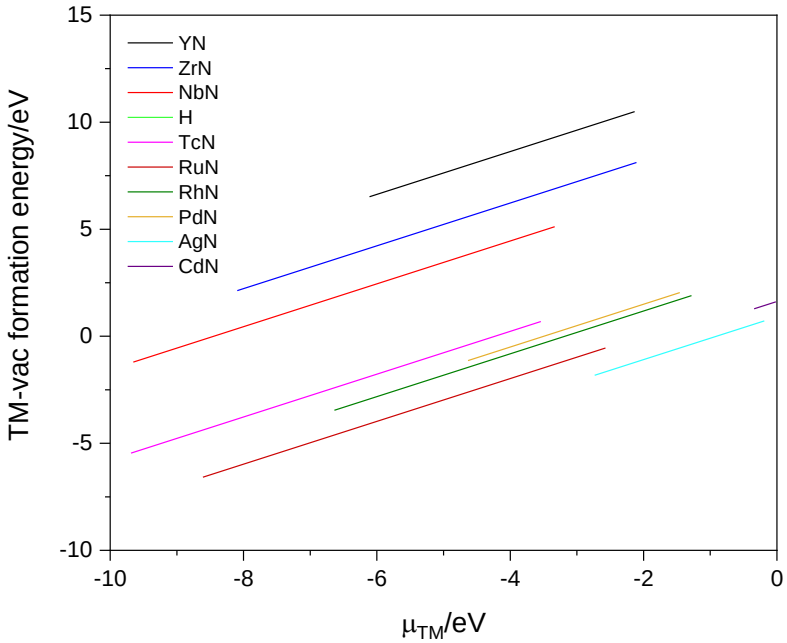

Figure S5. Variation of TM-vacancy (TM = 4d series) formation energy with TM chemical potential (μ_{TM}).

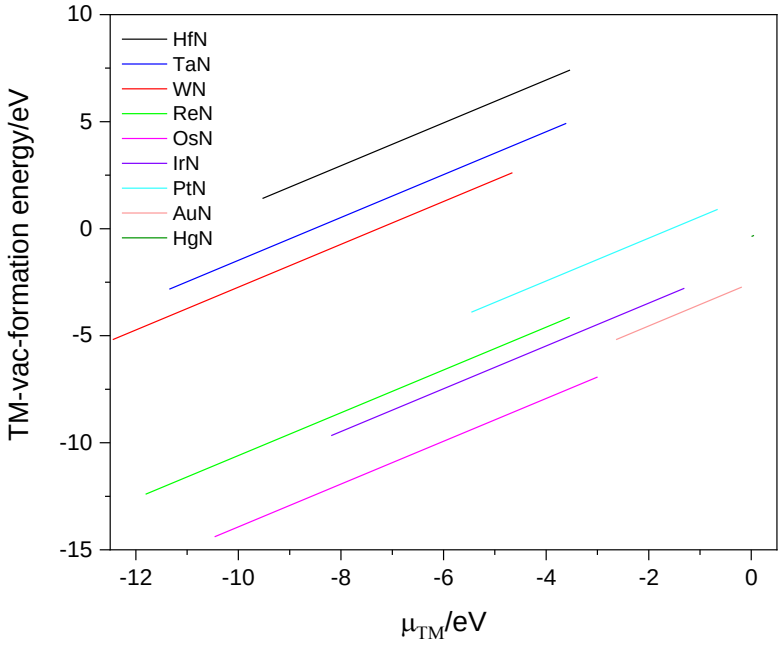

Figure S6. Variation of TM-vacancy (TM = 5d series) formation energy with TM chemical potential (μ_{TM}).

Table S1. Calculated lattice constants (in Å) using rPBE as a function of cutoff energy and van der Waal (vdW) and Tkatchenko and Scheffler (T-S) long range corrections.

TMN	400 eV	500 eV	% diff 500 vs. 400 eV	600 eV	% diff 600 vs. 400 eV	vdW 400 eV	% diff vdW vs. no-vdW 400 eV	T-S 400 eV	% diff T-S vs. no T-S 400 eV
ScN	4.47	4.53	1.34	4.53	1.27	4.51	0.84	4.30	-3.81
TiN	4.24	4.28	0.94	4.28	0.93	4.28	0.88	4.17	-1.70
VN	4.12	4.14	0.53	4.14	0.54	4.15	0.61	4.06	-1.34
CrN	4.15	4.19	1.08	4.20	1.10	4.19	1.03	3.85	-7.24
MnN	4.15	4.20	1.32	4.21	1.35	4.14	-0.12	3.81	-8.31
FeN	4.10	4.14	0.93	4.14	0.95	4.09	-0.12	3.93	-4.17
CoN	4.02	4.03	0.28	4.03	0.28	4.03	0.25	3.89	-3.11
NiN	4.08	4.10	0.42	4.10	0.42	4.09	0.33	3.81	-6.50
CuN	4.18	4.22	0.85	4.22	0.90	4.21	0.67	4.02	-3.93
ZnN	4.29	4.35	1.49	4.36	1.52	4.34	1.07	4.17	-2.74
YN	4.79	4.94	3.03	4.94	3.09	4.91	2.56	4.62	-3.51
ZrN	4.55	4.62	1.55	4.62	1.56	4.62	1.45	4.34	-4.59
NbN	4.40	4.44	0.90	4.44	0.91	4.45	1.04	4.13	-6.03
MoN	4.32	4.37	1.10	4.37	1.12	4.38	1.35	4.08	-5.53
TcN	4.29	4.32	0.76	4.32	0.77	4.34	1.15	3.96	-7.76
RuN	4.29	4.33	0.95	4.33	0.97	4.35	1.36	4.10	-4.42
RhN	4.32	4.36	0.85	4.36	0.87	4.37	1.15	4.18	-3.31
PdN	4.40	4.46	1.39	4.46	1.39	4.46	1.46	4.39	-0.16
AgN	4.53	4.64	2.45	4.64	2.49	4.63	2.22	4.49	-0.82
CdN	4.66	4.81	3.19	4.81	3.30	4.78	2.53	4.62	-0.96
HfN	4.50	4.56	1.25	4.56	1.27	4.56	1.26	4.24	-5.73
TaN	4.40	4.43	0.78	4.43	0.79	4.44	0.95	4.18	-5.02
WN	4.34	4.37	0.66	4.37	0.67	4.38	1.01	4.14	-4.68
ReN	4.34	4.37	0.69	4.37	0.70	4.39	1.07	4.16	-4.03
OsN	4.35	4.38	0.79	4.38	0.80	4.40	1.23	--	--
IrN	4.38	4.43	1.08	4.43	1.10	4.45	1.52	4.33	-1.19
PtN	4.45	4.51	1.38	4.51	1.40	4.53	1.77	4.41	-0.82
AuN	4.59	4.69	2.16	4.69	2.20	4.70	2.32	4.58	-0.32
HgN	4.74	4.91	3.49	4.91	3.58	4.89	3.22	4.72	-0.35

% difference (% diff) are calculated with respect to the rPBE-400 eV lattice constants. A negative % diff indicates that the lattice constants are smaller than the rPBE-400 eV values. Missing values in the table correspond to TMNs that require different convergence criteria to converge the self-consistent calculations.

Table S2. Calculated bulk TMN formation energies/atom (in eV) using rPBE as a function of cutoff energy and van der Waal and Tkatchenko and Scheffler long-range corrections. Sign changes are calculated with respect to rPBE-400 eV values.

TMN	400 eV	500 eV	Sign change	600 eV	Sign change	vdW rPBE	Sign change	T-S rPBE	Sign change
ScN	-1.64	-1.77	No	-1.77	No	-2.01	No	--	--
TiN	-1.62	-1.55	No	-1.55	No	--	--	-2.07	No
VN	-0.85	-0.79	No	-0.79	No	-0.94	No	-1.35	No
CrN	-0.25	-0.23	No	-0.23	No	-0.41	No	-0.17	No
MnN	-0.13	-0.12	No	--	--	--	--	--	--
FeN	0.39	0.40	No	0.40	No	0.24	No	-0.05	Yes
CoN	0.63	0.65	No	0.65	No	0.42	No	0.12	No
NiN	0.76	0.77	No	0.77	No	0.59	No	1.10	No
CuN	1.17	1.16	No	1.16	No	1.01	No	1.58	No
ZnN	0.88	0.83	No	0.83	No	0.69	No	0.94	No
YN	-1.18	-1.58	No	-1.57	No	-1.82	No	-1.68	No
ZrN	-1.40	-1.59	No	-1.59	No	-1.75	No	-1.58	No
NbN	-0.75	-0.82	No	-0.82	No	-0.96	No	-0.61	No
MoN	0.19	0.18	No	0.18	No	0.05	No	0.68	No
TcN	0.67	0.62	No	0.62	No	0.49	No	1.39	No
RuN	1.09	1.03	No	1.03	No	0.88	No	1.74	No
RhN	1.10	1.05	No	1.05	No	0.90	No	1.65	No
PdN	1.33	1.24	No	1.24	No	1.12	No	1.11	No
AgN	2.13	1.68	No	1.68	No	1.56	No	1.98	No
CdN	1.43	1.16	No	1.16	No	1.02	No	1.22	No
HfN	-1.46	-1.60	No	-1.60	No	-2.01	No	--	--
TaN	-0.61	-0.69	No	-0.69	No	-0.80	No	-0.40	No
WN	0.54	0.48	No	0.48	No	0.37	No	0.88	No
ReN	1.26	1.21	No	1.21	No	1.08	No	1.92	No
OsN	1.69	1.62	No	1.63	No	1.47	No	--	--
IrN	1.69	1.62	No	1.62	No	1.45	No	1.93	No
PtN	1.60	1.49	No	1.49	No	1.36	No	1.78	No
AuN	1.97	1.78	No	1.78	No	1.67	No	1.79	No
HgN	2.18	--	--	--	--	--	--	--	

Missing values in the table correspond to TMNs that require different convergence criteria to converge the self-consistent calculations.

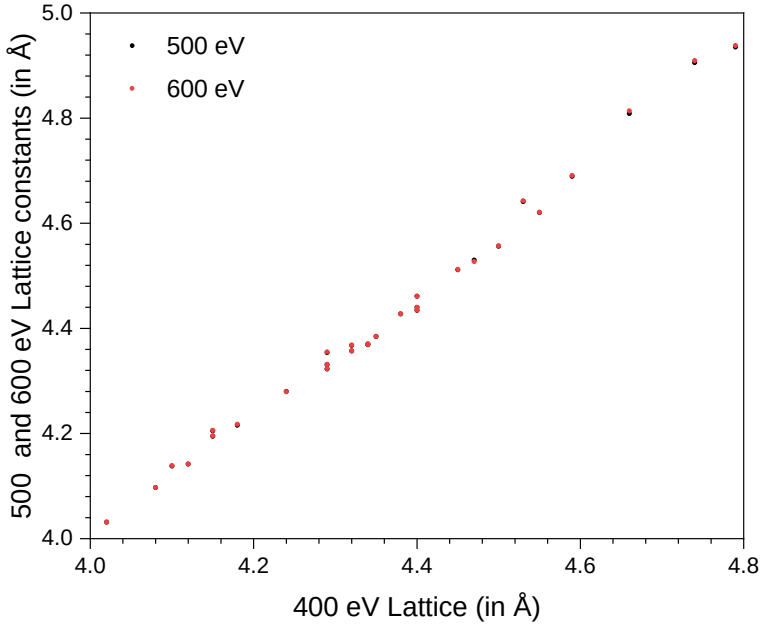

Figure S7. Comparison of calculated TMN lattice constants using rPBE: 500 eV and 600 eV cut off energy vs. 400 eV cutoff energy.

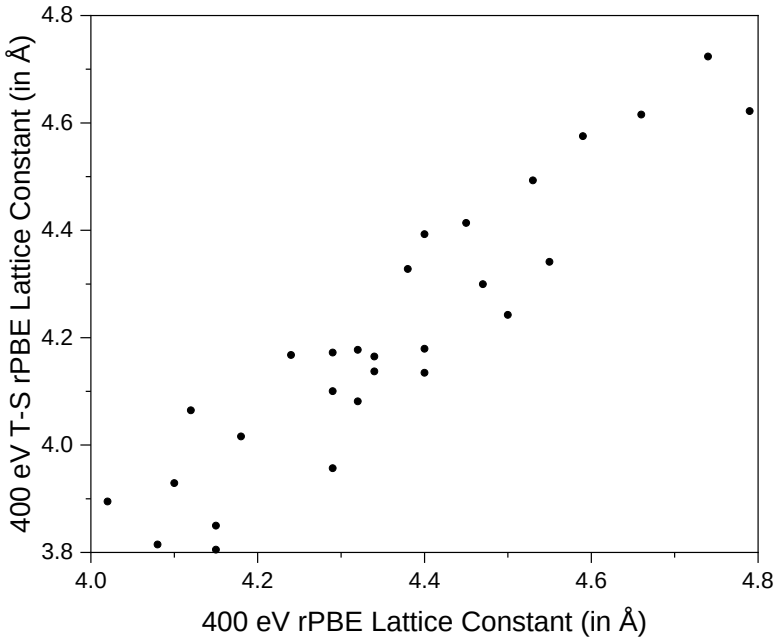

Figure S8. Comparison of calculated TMN lattice constants using rPBE and 400 eV with and without Tkatchenko and Scheffler (T-S) long range corrections.

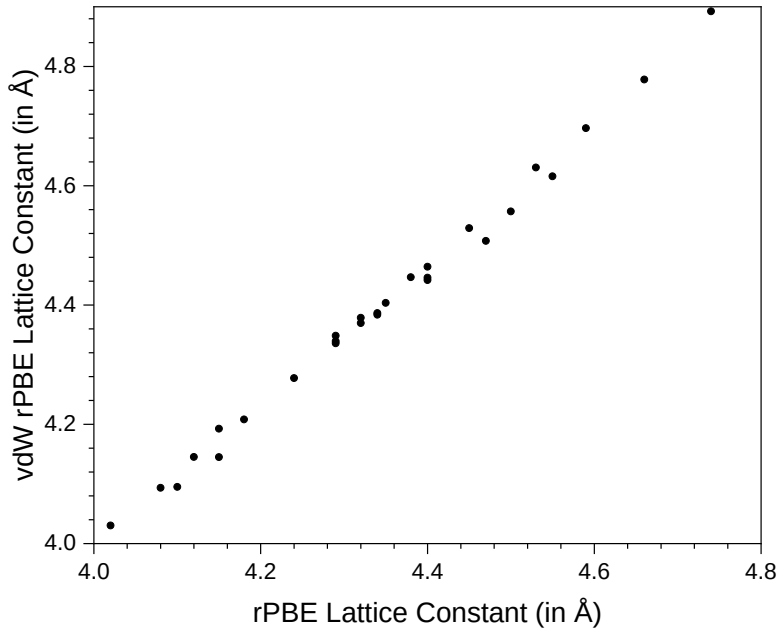

Figure S9. Comparison of calculated TMN lattice constants using rPBE and 400 eV with and without van der Waal's (vdW) long range corrections.

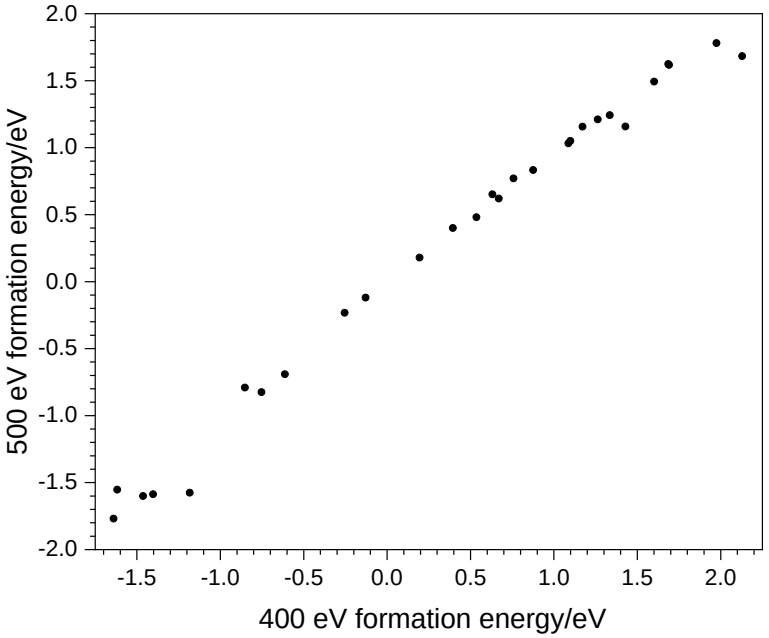

Figure S10. Comparison of calculated bulk TMN formation energies using rPBE: 500 eV vs. 400 eV cutoff energy.

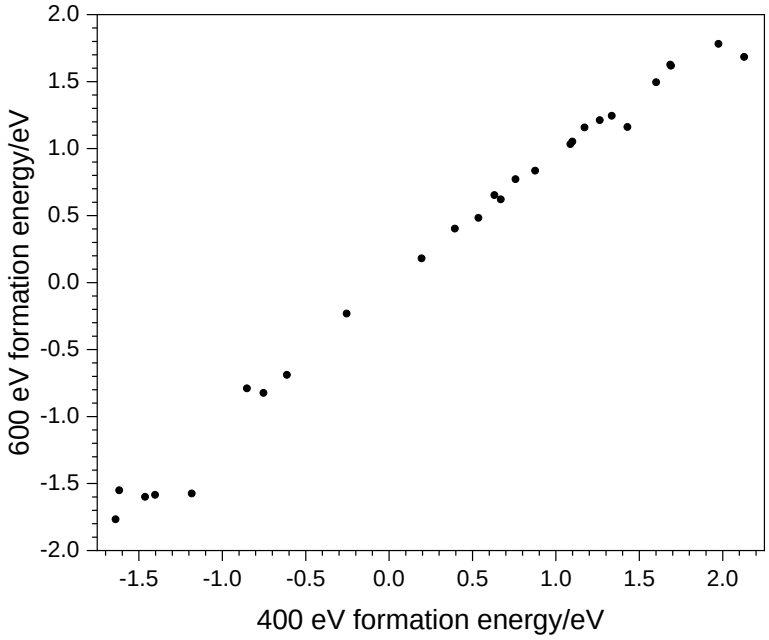

Figure S11. Comparison of calculated bulk TMN formation energies using rPBE: 600 eV vs. 400 eV cutoff energy.

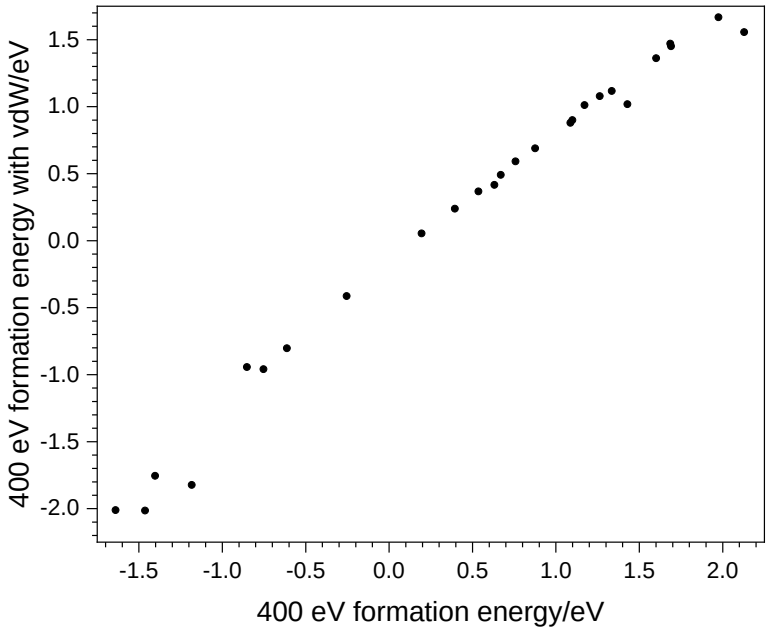

Figure S12. Comparison of calculated bulk TMN formation energies using rPBE at 400 eV cut off energy with and without vdW correction.

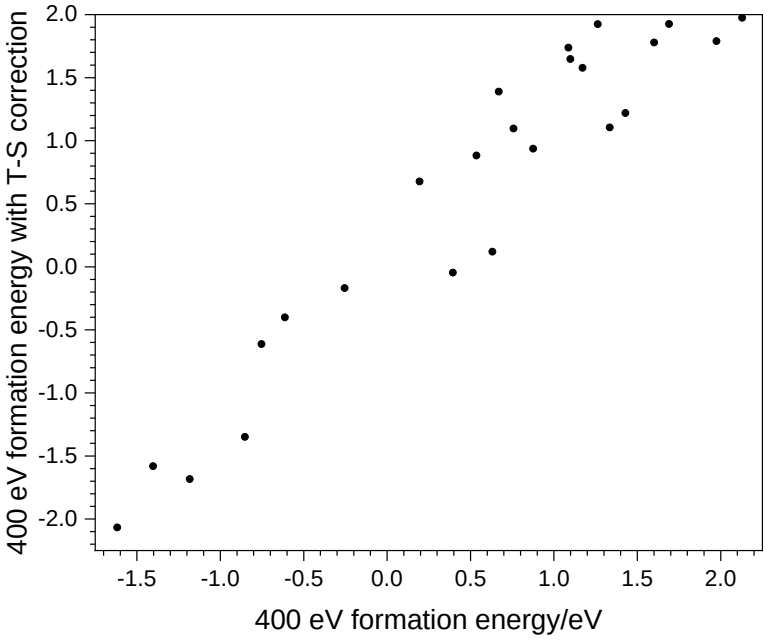

Figure S13. Comparison of calculated bulk TMN formation energies using rPBE at 400 eV cut off energy with and without T-S correction.