

Supplementary Information

Machine Learning Aided Design of Reversible MXene Electrocatalysts for Li-Air Batteries

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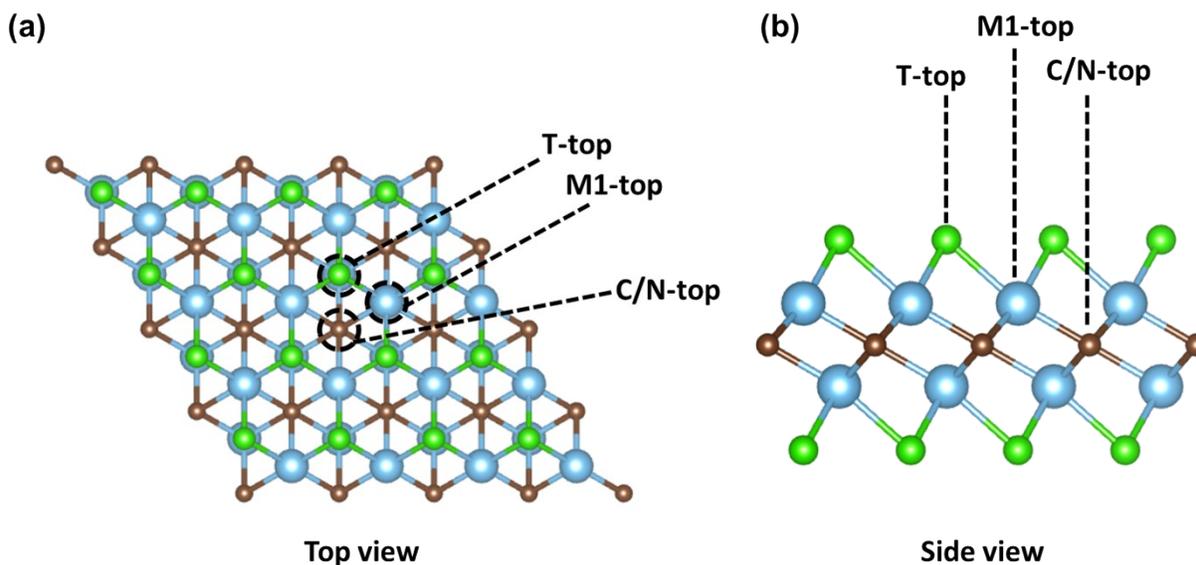


Fig. S1. Representation of the adsorption sites considered for adsorption site determination, (a) Top view, and (b) side view.

Table S1. Relative energies of Ti₂C MXene upon LiO₂ adsorption (through Li/O) at different sites (Ti/C/T). All the energies are in eV.

Material	Terminal group (T)	Ti-Li	C-Li	T-Li	Ti-O	C-O	T-O
Ti₂CBr₂	Br	0	0.02	0.18	0.43	0.43	36.28
Ti₂CCl₂	Cl	0	0.01	0.17	0.54	0.53	70.19
Ti₂C(CN)₂	CN	0	-0.07	0.38	1.29	1.40	1.39
Ti₂CF₂	F	0	-0.15	-0.08	-0.67	0.53	0.57
Ti₂C(NCO)₂	NCO	0	0.00	0.08	0.63	0.63	0.66
Ti₂C(NCS)₂	NCS	0	-0.01	0.35	0.31	0.32	0.36
Ti₂C(OCN)₂	OCN	0	-0.01	0.46	1.53	1.57	1.51
Ti₂CO₂	O	0	-0.11	-0.06	0.50	0.80	0.92
Ti₂C(PO)₂	PO	0	0.01	0.54	1.52	1.76	1.71
Ti₂C(SCN)₂	SCN	0	0.00	0.32	1.19	1.21	1.16

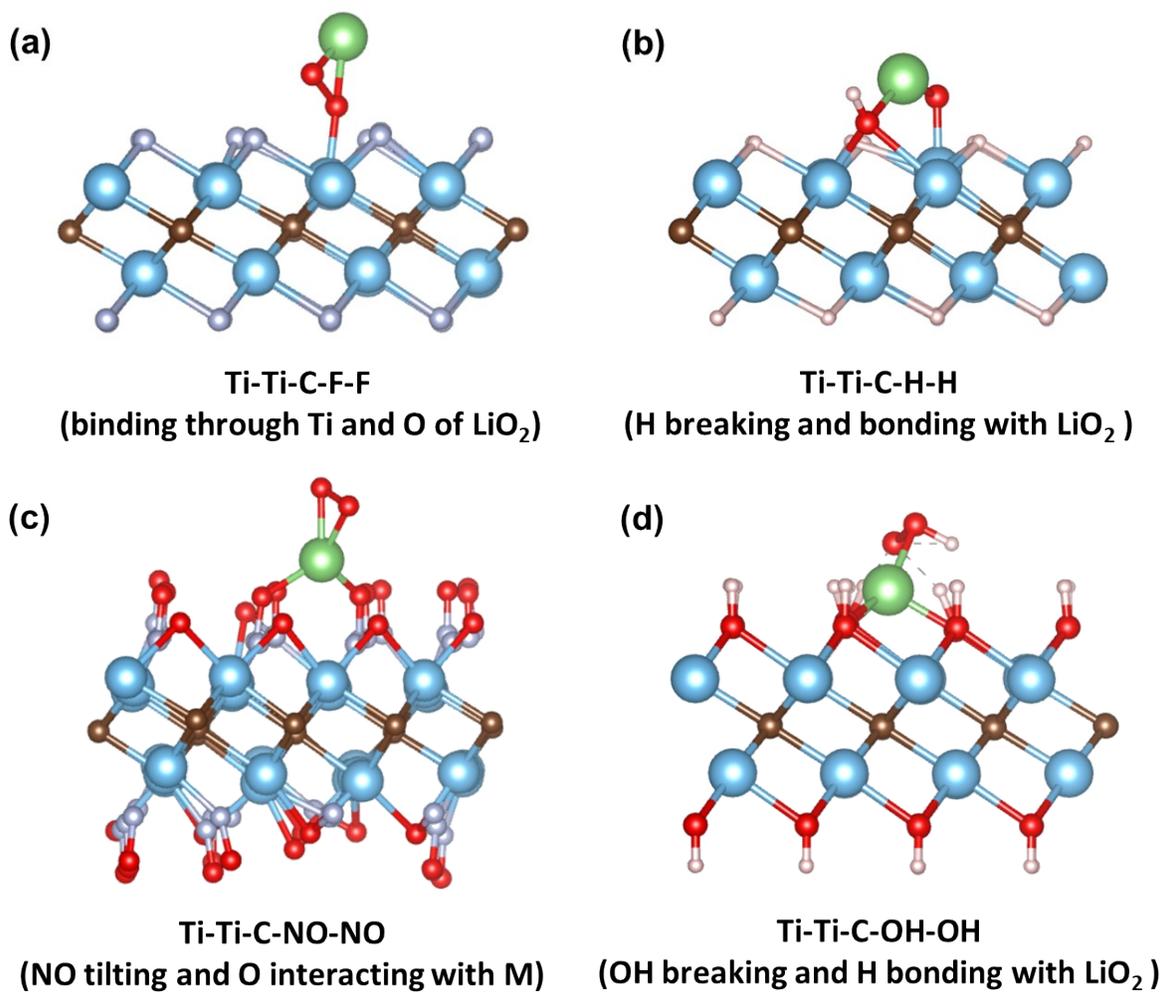


Fig. S2. Sample of distorted MXene structures with various terminal groups that have been excluded. (a) T=F, (b) T=H, (c) T=NO, and (d) T=OH. LiO_2 has been utilized as adsorbate.

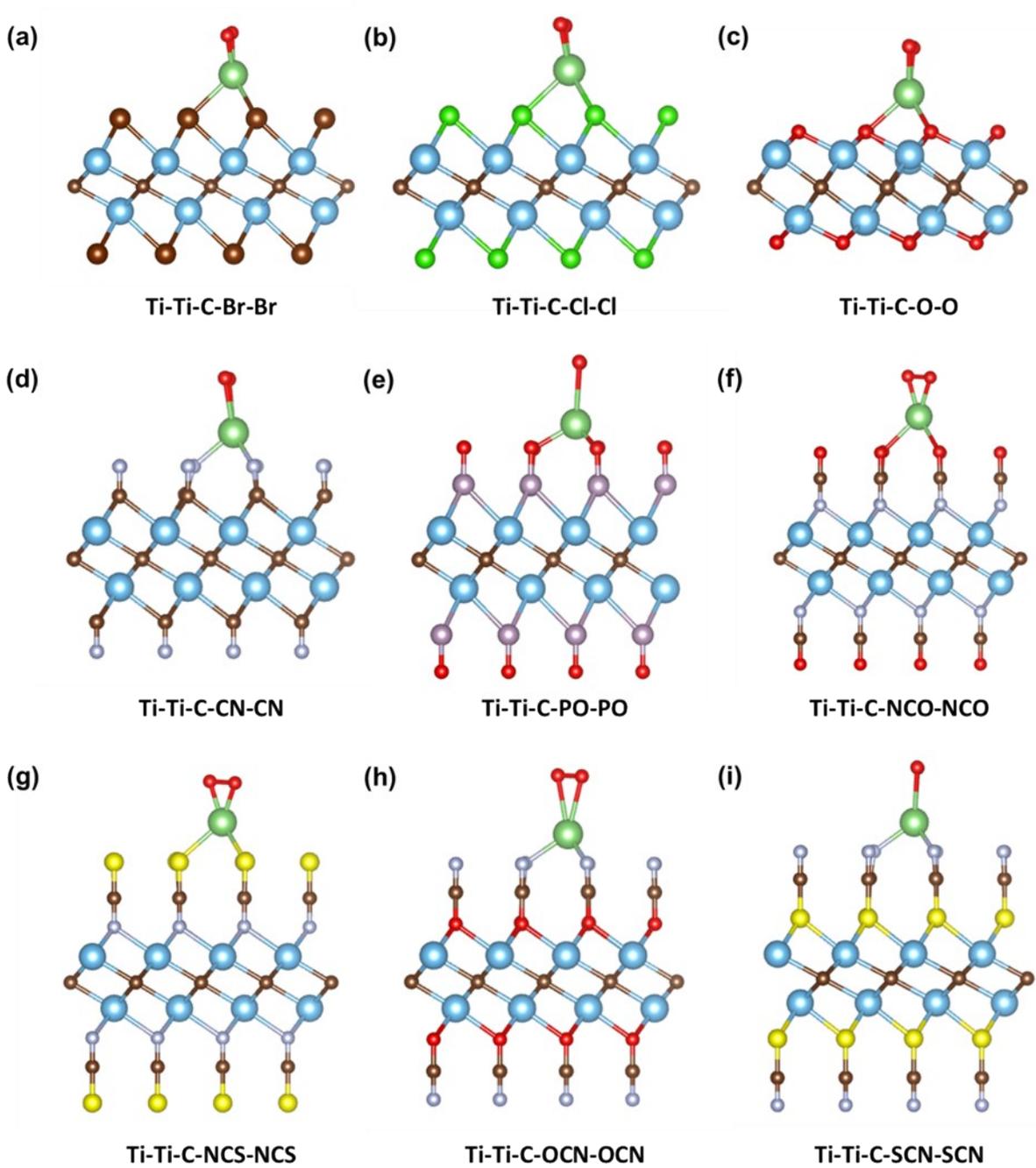


Fig. S3. Sample of undistorted MXene structures with various terminal groups that have been considered. (a) T=Br, (b) T=Cl, (c) T=O, (d) T=CN, (e) T=PO, (f) T=NCO, (g) T=NCS, (h) T=OCN, and (i) T=SCN. LiO_2 has been utilized as adsorbate.

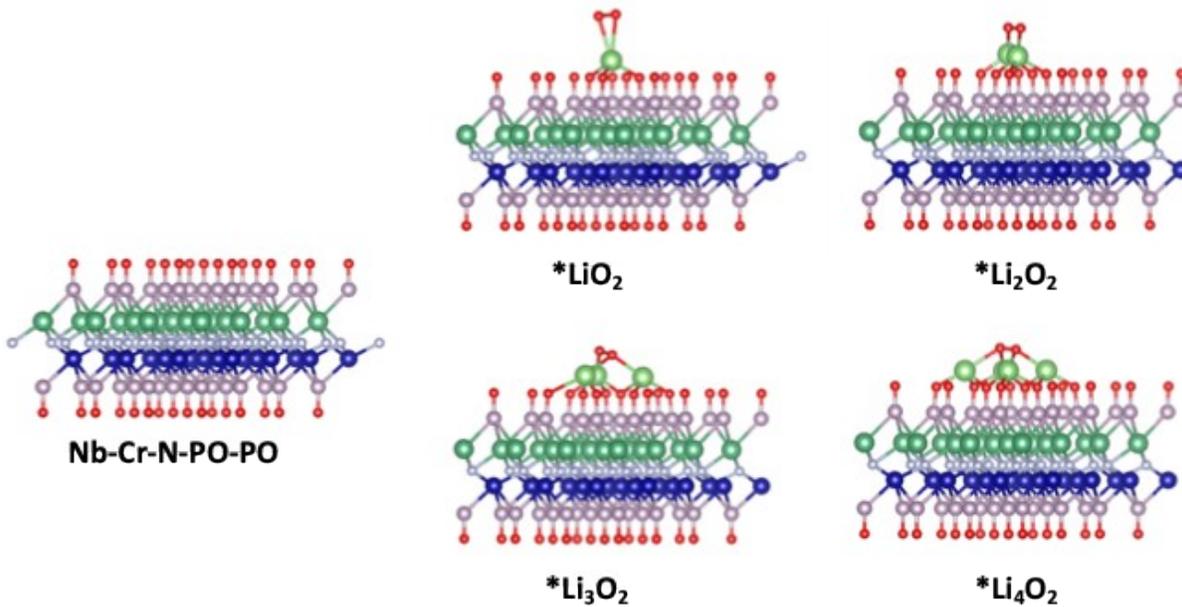


Fig. S4. Adsorption of various LAB intermediates on a representative MXene material.

Table S2. The abbreviation of the considered features and their symbols utilized for the prediction of reaction energy changes (ΔE).

Abbreviation
LC: Lattice constant, BG: Band Gap, MM: Magnetic Moment, M1,M2,X,T1,T2: Element names, TA: Terminal atom name, W: Atomic mass, AN: Atomic number, P: Period number, G: Group number, V: Valence electron, IE: First ionization potential, R: Atomic radius, MP: Melting point, BP: Boiling point, χ : Pauling electronegativity, CE: Cohesive energy, GVE: Gilmore number of valence electron, VS: Valence s electrons, VP: Valence p electrons, VD: valence d electrons, VF: Valence f electrons, USV: Number of unfilled s valence electrons, UPV: Number of unfilled p valence electrons, UDV: Number of unfilled d valence electrons, UFV: Number of unfilled f valence electrons, T1-M1, M1-X, X-M2, M2-T2: Distance between two components, SA: Surface area, SW: Surface weight, ΔIE : First ionization potential difference, $\Delta\chi$: Electronegativity difference
Symbols
M1, M2, X, T1, T2, TA, M1W, M1AN, M1P, M1G, M1V, M1IE, M1R, M1MP, M1BP, M1 χ , M2W, M2AN, M2P, M2G, M2V, M2IE, M2R, M2MP, M2BP, M2 χ , XW, XAN, XP, XG, XV, XIE, XR, XMP, XBP, X χ , T1W, T1AN, T1P, T1G, T1V, T1IE, T1R, T1MP, T1BP, T1 χ , M1CE, M1GVE, M1VS, M1VP, M1VD, M1VF, M1USV, M1UPV, M1UDV, M1UFV, M2CE, M2GVE, M2VS, M2VP, M2VD, M2VF, M2USV, M2UPV, M2UDV, M2UFV, XGVE, XVP, XUPV, T1GVE, T1VS, T1VP, T1UPV, T1UDV, T1UFV, T1-M1, M1-X, X-M2, M2-T2, SA, SW, M1 ΔIE , M1X ΔIE , M2X ΔIE , M2 ΔIE , M1 $\Delta\chi$, M1X $\Delta\chi$, M2X $\Delta\chi$, M2 $\Delta\chi$

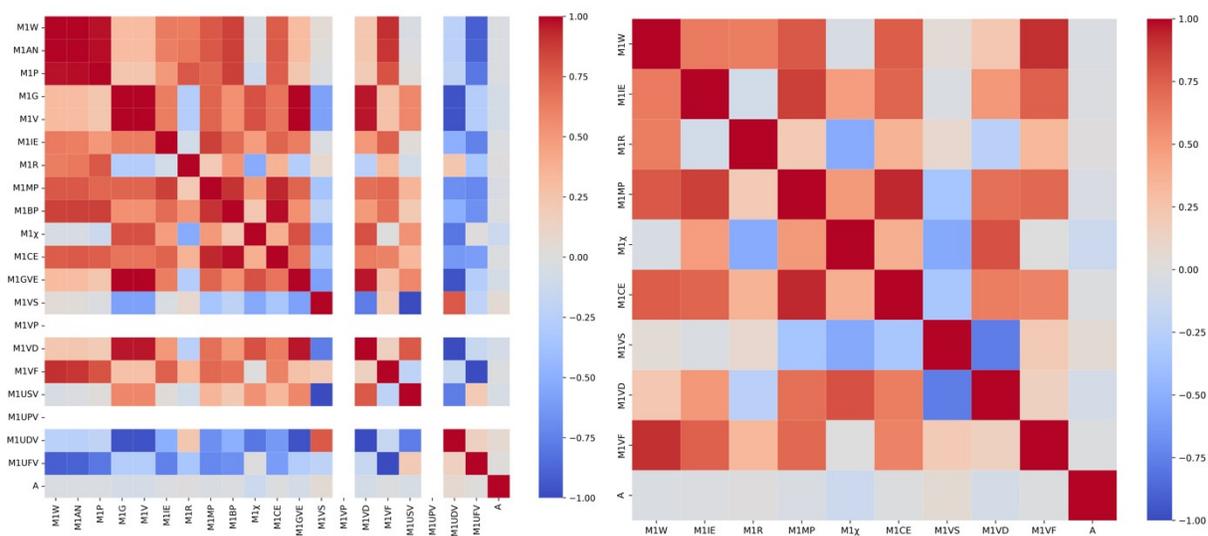


Fig. S5. Correlation plots before and after dropping of highly correlated features for M1 related features.

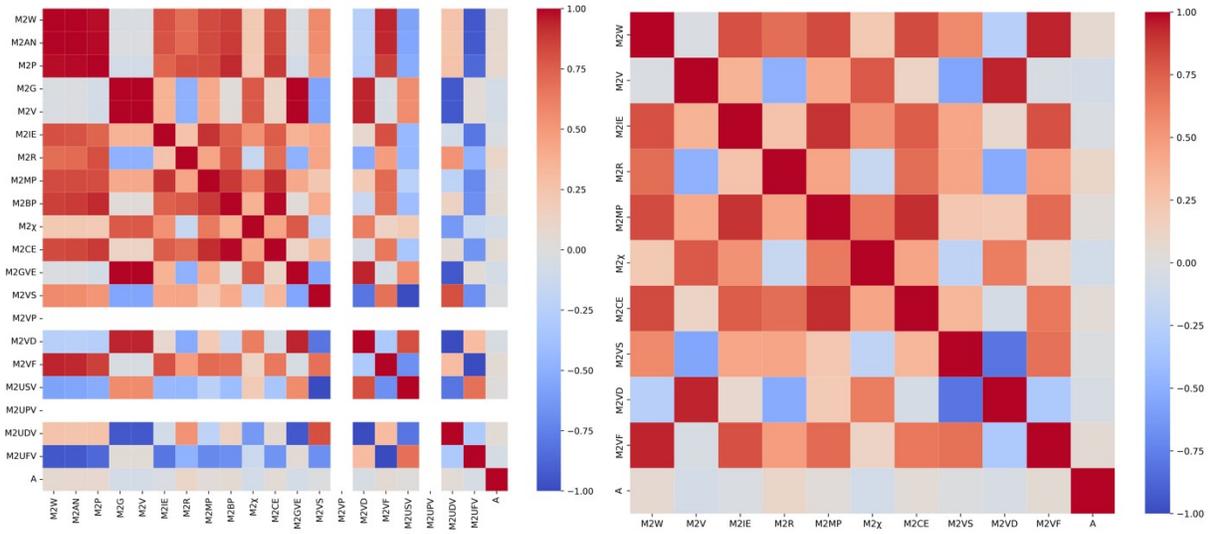


Fig. S6. Correlation plots before and after dropping of highly correlated features for M2 related features.

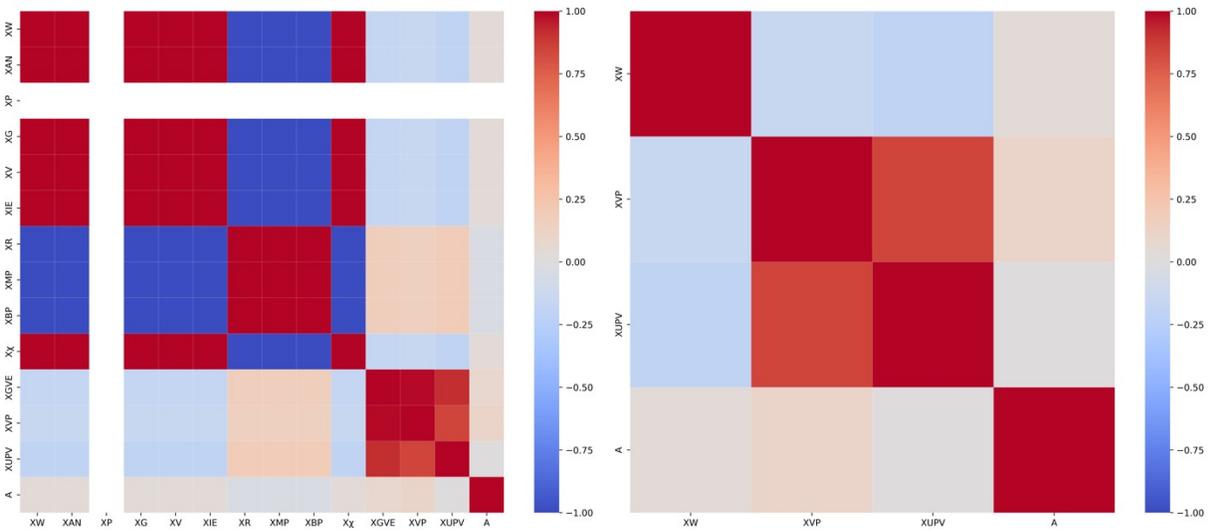


Fig. S7. Correlation plots before and after dropping of highly correlated features for X related features.

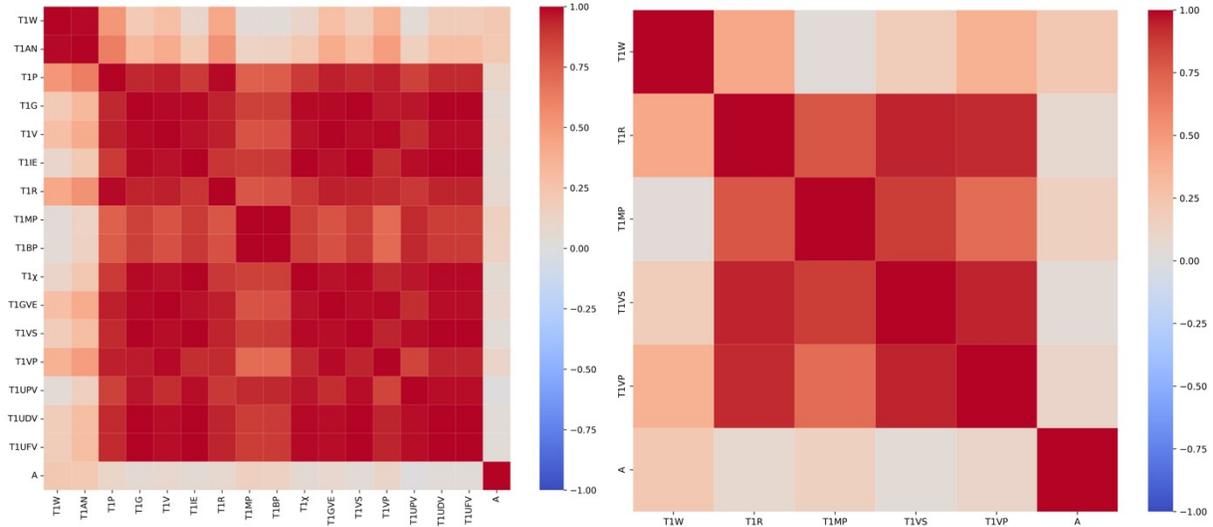


Fig. S8. Correlation plots before and after dropping of highly correlated features for T related features.

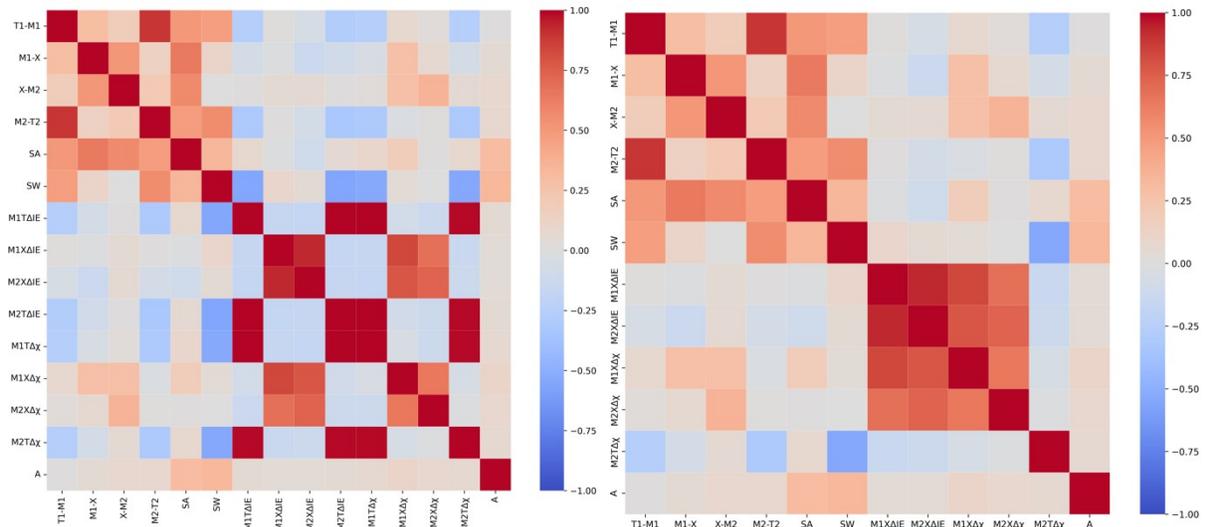


Fig. S9. Correlation plots before and after dropping of highly correlated features for MXene features which do not relate to any one single component of the MXene.

All total and after dropped features

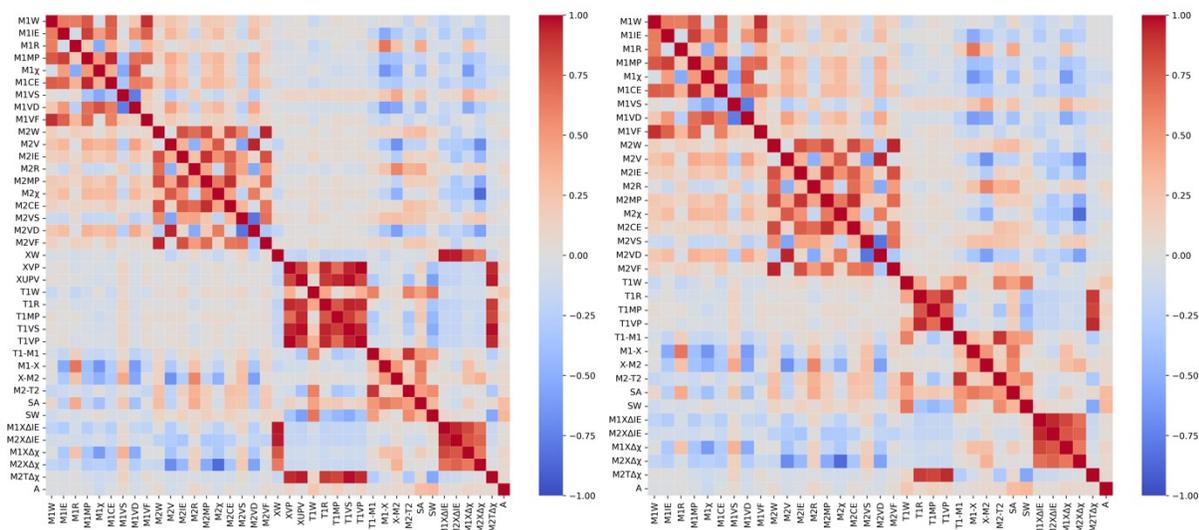


Fig. S10. Correlation plots before and after dropping of highly correlated features among the previously selected features from Fig.s S5-S9.

Table S3. Considered features after the exclusion of all highly correlated features, used further in the ML workflow.

Symbols
M1W, M1IE, M1R, M1MP, M1 χ , M1CE, M1VS, M1VD, M1VF, M2W, M2V, M2IE, M2R, M2MP, M2 χ , M2CE, M2VS, M2VD, M2VF, T1W, T1R, T1MP, T1VP, T1-M1, M1-X, X-M2, M2-T2, SA, SW, M1X Δ IE, M2X Δ IE, M1X Δ χ , M2X Δ χ , M2T Δ χ

Table S4. Optimized hyperparameters for all the four datasets using EXTR ML model for prediction of reaction energy (ΔE).

Dataset	ML Model	Optimized Hyperparameters
Dataset ΔE_A	EXTR	bootstrap=False, ccp_alpha=0.0, max_depth=7, max_leaf_nodes=None, min_impurity_decrease=0.0, min_samples_leaf=1, min_samples_split=2, min_weight_fraction_leaf=0.0, n_estimators=200, oob_score=False, random_state=42
Dataset ΔE_B	EXTR	bootstrap=False, ccp_alpha=0.0, max_depth=12, max_leaf_nodes=None, min_impurity_decrease=0.0, min_samples_leaf=4, min_samples_split=5, min_weight_fraction_leaf=0.0, n_estimators=100, oob_score=False, random_state=42
Dataset ΔE_C	EXTR	bootstrap=False, ccp_alpha=0.0, max_depth=5, max_leaf_nodes=None, min_impurity_decrease=0.0, min_samples_leaf=2, min_samples_split=2, min_weight_fraction_leaf=0.0, n_estimators=50, n_jobs=None, oob_score=False, random_state=42
Dataset ΔE_D	EXTR	bootstrap=False, ccp_alpha=0.0, max_depth=30, max_leaf_nodes=None, min_impurity_decrease=0.0, min_samples_leaf=1, min_samples_split=5, min_weight_fraction_leaf=0.0, n_estimators=400, n_jobs=None, oob_score=False, random_state=42

Table S5. Selected optimum features from SelectKBest method for the prediction of ΔE_A using EXTR model. The abbreviations of the following symbols are provided in Table S1.

Top ranked 28 features selected based on SelectKBest to fit the data on EXTR model
M1IE, M1R, M1 χ , M1CE, M1VS, M2W, M2V, M2IE, M2R, M2MP, M2 χ , M2CE, M2VS, M2VD, M2VF, T1W, T1MP, T1-M1, M1-X, X-M2, M2-T2, SA, SW, M1X Δ IE, M2X Δ IE, M1X Δ χ , M2X Δ χ , M2T Δ χ

Table S6. Selected optimum features from SelectKBest method for the prediction of ΔE_B using EXTR model. The abbreviations of the following symbols are provided in Table S1.

Top ranked 34 features selected based on SelectKBest to fit the data on EXTR model
M1W, M1IE, M1R, M1MP, M1 χ , M1CE, M1VS, M1VD, M1VF, M2W, M2V, M2IE, M2R, M2MP, M2 χ , M2CE, M2VS, M2VD, M2VF, T1W, T1R, T1MP, T1VP, T1-M1, M1-X, X-M2, M2-T2, SA, SW, M1X Δ IE, M2X Δ IE, M1X Δ χ , M2X Δ χ , M2T Δ χ

Table S7. Selected optimum features from SelectKBest method for the prediction of ΔE_C using EXTR model. The abbreviations of the following symbols are provided in Table S1.

Top ranked 25 features selected based on SelectKBest to fit the data on EXTR model
M1W, M1IE, M1R, M1MP, M1 χ , M1CE, M1VF, M2W, M2IE, M2R, M2MP, M2CE, M2VS, M2VF, T1W, T1R, T1VP, M1-X, SA, SW, M1X Δ IE, M2X Δ IE, M1X Δ χ , M2X Δ χ , M2T Δ χ

Table S8. Selected optimum features from SelectKBest method for the prediction of ΔE_D using EXTR model. The abbreviations of the following symbols are provided in Table S1.

Top ranked 16 features selected based on SelectKBest to fit the data on XGBR model
M1W, M1IE, M1MP, M1 χ , M1CE, M1VD, M1VF, T1W, T1R, M1-X, SA, SW, M1X Δ IE, M2X Δ IE, M1X Δ χ , M2T Δ χ

Table S9. ML predicted reaction energies for the four steps of the reaction (ΔE_A , ΔE_B , ΔE_C , and ΔE_D). All reaction energies are in eV.

MXene	ΔE_A	ΔE_B	ΔE_C	ΔE_D
Cr-Cr-N-Br-Br	-1.18725	-2.12111	-1.66262	-1.18244
Cr-Mo-C-Br-Br	-1.2006	-2.28703	-1.6185	-1.27411
Cr-Mo-N-Br-Br	-1.14964	-2.26624	-1.64489	-1.16203
Cr-W-C-Br-Br	-1.21047	-2.14333	-1.59956	-1.26907
Cr-W-N-Br-Br	-1.19199	-2.20149	-1.65393	-1.17767
Hf-Cr-C-Br-Br	-1.28879	-2.13159	-1.01209	-0.57108
Hf-Cr-N-Br-Br	-1.25163	-2.1292	-0.84804	-0.55785
Hf-Hf-C-Br-Br	-1.26963	-1.99826	-0.96853	-0.54051

Hf-Hf-N-Br-Br	-1.24213	-2.00766	-0.78875	-0.52077
Hf-Mo-C-Br-Br	-1.24863	-1.97841	-1.01983	-0.61055
Hf-Mo-N-Br-Br	-1.21962	-2.15033	-0.86865	-0.60421
Hf-Nb-C-Br-Br	-1.29029	-1.98489	-1.01504	-0.54556
Hf-Nb-N-Br-Br	-1.24129	-2.02971	-0.85531	-0.53791
Hf-Ta-C-Br-Br	-1.38519	-1.98	-1.00143	-0.53984
Hf-Ta-N-Br-Br	-1.37388	-1.99083	-0.85894	-0.5468
Hf-V-C-Br-Br	-1.29328	-2.00131	-1.00005	-0.56371
Hf-V-N-Br-Br	-1.25373	-2.02508	-0.84531	-0.53804
Hf-W-C-Br-Br	-1.35871	-1.96546	-1.00977	-0.61399
Hf-W-N-Br-Br	-1.34805	-2.04765	-0.88506	-0.63328
Mo-Mo-C-Br-Br	-1.10572	-2.06448	-1.38205	-2.01679
Mo-Mo-N-Br-Br	-1.09729	-2.05424	-1.36768	-2.06774
Mo-W-C-Br-Br	-1.13465	-2.02725	-1.42118	-2.01693
Mo-W-N-Br-Br	-1.13813	-2.08324	-1.44092	-2.20155
Nb-Cr-C-Br-Br	-1.10612	-2.18552	-1.3372	-0.74048
Nb-Cr-N-Br-Br	-1.09133	-2.01123	-1.19757	-0.65739
Nb-Mo-C-Br-Br	-1.07034	-1.97339	-1.3411	-0.73636
Nb-Mo-N-Br-Br	-1.06333	-1.96105	-1.24923	-0.66058
Nb-Nb-C-Br-Br	-1.0894	-1.9623	-1.33323	-0.7379
Nb-Nb-N-Br-Br	-1.08505	-1.96197	-1.21121	-0.65274
Nb-Ta-C-Br-Br	-1.13398	-1.95814	-1.35014	-0.73684
Nb-Ta-N-Br-Br	-1.14537	-1.95377	-1.26437	-0.69176
Nb-W-C-Br-Br	-1.11074	-1.96846	-1.38368	-0.74825
Nb-W-N-Br-Br	-1.12027	-2.02838	-1.33443	-0.82859
Sc-Cr-C-Br-Br	-1.34802	-2.77766	-1.74093	-0.9323
Sc-Cr-N-Br-Br	-1.28365	-2.70509	-1.68664	-0.93643
Sc-Hf-C-Br-Br	-1.32752	-2.04046	-1.69248	-0.95265
Sc-Hf-N-Br-Br	-1.27604	-2.02613	-1.6107	-0.90661
Sc-Mo-C-Br-Br	-1.33942	-2.63013	-1.73908	-0.99083
Sc-Mo-N-Br-Br	-1.27741	-2.77523	-1.72062	-0.97534
Sc-Nb-C-Br-Br	-1.36307	-2.17091	-1.71127	-0.93501
Sc-Nb-N-Br-Br	-1.28845	-2.19401	-1.66703	-0.93191
Sc-Sc-C-Br-Br	-1.3584	-2.1544	-1.71089	-0.96363
Sc-Sc-N-Br-Br	-1.29965	-2.04259	-1.63761	-0.89738
Sc-Ta-C-Br-Br	-1.33852	-2.02992	-1.68339	-0.92681
Sc-Ta-N-Br-Br	-1.31481	-2.014	-1.65325	-0.92545
Sc-Ti-C-Br-Br	-1.34188	-2.08817	-1.68509	-0.93295
Sc-Ti-N-Br-Br	-1.27726	-2.02551	-1.62834	-0.92437
Sc-V-C-Br-Br	-1.34651	-2.08785	-1.69364	-0.9292
Sc-V-N-Br-Br	-1.28237	-2.02952	-1.64894	-0.93176

Sc-W-C-Br-Br	-1.33279	-2.28144	-1.70841	-0.98959
Sc-W-N-Br-Br	-1.30936	-2.3418	-1.7422	-0.94826
Sc-Y-C-Br-Br	-1.34495	-2.09413	-1.7	-0.89559
Sc-Y-N-Br-Br	-1.29098	-2.03703	-1.63174	-0.82671
Sc-Zr-C-Br-Br	-1.34985	-2.08766	-1.70749	-0.95165
Sc-Zr-N-Br-Br	-1.29249	-2.03117	-1.62704	-0.90317
Ta-Cr-C-Br-Br	-1.10625	-2.1926	-1.04719	-0.29463
Ta-Cr-N-Br-Br	-1.13976	-2.0343	-0.90299	-0.24867
Ta-Mo-C-Br-Br	-1.01359	-1.95451	-1.05903	-0.07062
Ta-Mo-N-Br-Br	-1.08849	-2.00532	-0.91607	-0.12008
Ta-Ta-C-Br-Br	-1.51207	-1.96124	-1.04946	-0.12132
Ta-Ta-N-Br-Br	-1.55529	-1.96188	-0.91751	-0.17357
Ta-W-C-Br-Br	-1.47206	-1.96307	-1.06049	-0.08556
Ta-W-N-Br-Br	-1.50104	-1.98492	-0.93145	-0.16207
Ti-Cr-C-Br-Br	-1.38426	-2.44204	-1.61046	-0.88663
Ti-Cr-N-Br-Br	-1.30855	-2.16535	-1.64161	-0.93828
Ti-Hf-C-Br-Br	-1.34896	-1.99239	-1.56327	-0.87023
Ti-Hf-N-Br-Br	-1.28241	-1.98755	-1.56131	-0.88982
Ti-Mo-C-Br-Br	-1.35826	-2.26012	-1.56691	-0.9111
Ti-Mo-N-Br-Br	-1.28803	-2.27131	-1.61185	-0.95984
Ti-Nb-C-Br-Br	-1.38858	-1.96555	-1.5455	-0.86031
Ti-Nb-N-Br-Br	-1.29364	-2.00245	-1.59854	-0.91463
Ti-Ta-C-Br-Br	-1.35514	-1.97724	-1.55501	-0.86454
Ti-Ta-N-Br-Br	-1.31966	-1.99276	-1.59059	-0.90421
Ti-Ti-C-Br-Br	-1.37863	-2.10516	-1.56803	-0.87609
Ti-Ti-N-Br-Br	-1.30475	-2.02063	-1.59394	-0.91772
Ti-V-C-Br-Br	-1.38266	-2.07314	-1.57118	-0.88939
Ti-V-N-Br-Br	-1.30935	-2.02995	-1.60122	-0.93096
Ti-W-C-Br-Br	-1.34736	-2.10963	-1.55605	-0.91244
Ti-W-N-Br-Br	-1.31548	-2.13242	-1.6232	-0.94861
Ti-Zr-C-Br-Br	-1.38606	-2.04145	-1.56575	-0.87522
Ti-Zr-N-Br-Br	-1.32162	-2.01101	-1.57148	-0.89253
V-Cr-C-Br-Br	-1.37438	-2.38071	-1.63021	-1.05498
V-Cr-N-Br-Br	-1.30463	-2.11328	-1.66483	-1.03272
V-Mo-C-Br-Br	-1.3511	-2.18658	-1.59343	-1.05917
V-Mo-N-Br-Br	-1.28422	-2.18858	-1.63352	-1.032
V-Nb-C-Br-Br	-1.38151	-1.99361	-1.57843	-1.02848
V-Nb-N-Br-Br	-1.28758	-2.0111	-1.63102	-1.01652
V-Ta-C-Br-Br	-1.34595	-1.99681	-1.57731	-1.02564
V-Ta-N-Br-Br	-1.3017	-2.00172	-1.6033	-0.9951
V-V-C-Br-Br	-1.37826	-2.08238	-1.58763	-1.06058

V-V-N-Br-Br	-1.30613	-2.03469	-1.6151	-1.04803
V-W-C-Br-Br	-1.33819	-2.07024	-1.57087	-1.06208
V-W-N-Br-Br	-1.30019	-2.13425	-1.62729	-1.01445
W-W-C-Br-Br	-1.45652	-2.01711	-1.07179	-0.97964
W-W-N-Br-Br	-1.47258	-2.01544	-0.99116	-0.99924
Y-Cr-C-Br-Br	-1.33959	-2.12315	-1.80669	-1.17515
Y-Cr-N-Br-Br	-1.28582	-2.23893	-1.68636	-1.18967
Y-Hf-C-Br-Br	-1.40493	-2.0834	-1.72037	-0.99947
Y-Hf-N-Br-Br	-1.31657	-2.10065	-1.61357	-1.10639
Y-Mo-C-Br-Br	-1.34621	-2.10811	-1.77306	-1.3555
Y-Mo-N-Br-Br	-1.28193	-2.29603	-1.72538	-1.51483
Y-Nb-C-Br-Br	-1.36889	-2.09233	-1.7526	-1.12349
Y-Nb-N-Br-Br	-1.28753	-2.12558	-1.65887	-1.21661
Y-Ta-C-Br-Br	-1.4382	-2.07599	-1.71485	-1.10611
Y-Ta-N-Br-Br	-1.38379	-2.10022	-1.63959	-1.20617
Y-Ti-C-Br-Br	-1.3551	-2.10742	-1.72745	-1.09145
Y-Ti-N-Br-Br	-1.27996	-2.10867	-1.59724	-1.1786
Y-V-C-Br-Br	-1.33527	-2.10325	-1.73095	-1.11486
Y-V-N-Br-Br	-1.2841	-2.11783	-1.645	-1.19198
Y-W-C-Br-Br	-1.43379	-2.10341	-1.73918	-1.35453
Y-W-N-Br-Br	-1.37935	-2.1806	-1.72836	-1.47386
Y-Y-C-Br-Br	-1.42436	-2.08728	-1.71303	-0.93906
Y-Y-N-Br-Br	-1.31278	-2.09788	-1.62651	-0.93329
Y-Zr-C-Br-Br	-1.38496	-2.08841	-1.73043	-0.99483
Y-Zr-N-Br-Br	-1.29267	-2.11634	-1.6283	-1.08058
Zr-Cr-C-Br-Br	-1.29355	-2.17173	-1.43209	-0.88194
Zr-Cr-N-Br-Br	-1.24775	-2.12379	-1.33743	-0.88868
Zr-Hf-C-Br-Br	-1.27548	-1.99635	-1.4194	-0.82749
Zr-Hf-N-Br-Br	-1.23443	-1.9957	-1.33562	-0.81674
Zr-Mo-C-Br-Br	-1.2553	-1.97611	-1.42691	-0.96674
Zr-Mo-N-Br-Br	-1.22157	-2.15469	-1.37451	-1.00299
Zr-Nb-C-Br-Br	-1.29246	-1.98018	-1.4247	-0.87313
Zr-Nb-N-Br-Br	-1.23408	-2.03018	-1.35338	-0.88559
Zr-Ta-C-Br-Br	-1.37393	-1.9701	-1.43228	-0.86128
Zr-Ta-N-Br-Br	-1.35874	-1.97635	-1.36698	-0.87737
Zr-V-C-Br-Br	-1.29774	-1.99804	-1.43019	-0.87443
Zr-V-N-Br-Br	-1.25054	-1.99875	-1.33567	-0.88582
Zr-W-C-Br-Br	-1.34833	-1.95924	-1.42722	-0.99728
Zr-W-N-Br-Br	-1.33832	-2.06824	-1.41796	-1.06007
Zr-Zr-C-Br-Br	-1.30591	-2.02706	-1.41941	-0.85196
Zr-Zr-N-Br-Br	-1.26819	-2.0054	-1.33067	-0.83286

Cr-Cr-N-Cl-Cl	-1.37775	-2.22536	-1.78429	-1.28987
Cr-Mo-C-Cl-Cl	-1.283	-2.59645	-1.71895	-1.26483
Cr-Mo-N-Cl-Cl	-1.02972	-2.46288	-1.7473	-1.15515
Cr-W-C-Cl-Cl	-1.34905	-2.36964	-1.70086	-1.2618
Cr-W-N-Cl-Cl	-1.06766	-2.32541	-1.73595	-1.09985
Hf-Cr-C-Cl-Cl	-1.32708	-2.66298	-0.90461	-0.98929
Hf-Cr-N-Cl-Cl	-1.34364	-2.32779	-0.73702	-0.92663
Hf-Hf-C-Cl-Cl	-1.36947	-2.00406	-0.8075	-0.90248
Hf-Hf-N-Cl-Cl	-1.30746	-2.00312	-0.59422	-0.82623
Hf-Mo-C-Cl-Cl	-1.33313	-2.02419	-0.90142	-1.04315
Hf-Mo-N-Cl-Cl	-1.37054	-2.26855	-0.73998	-0.95322
Hf-Nb-C-Cl-Cl	-1.36774	-2.04579	-0.88433	-0.97162
Hf-Nb-N-Cl-Cl	-1.38925	-2.13691	-0.72635	-0.92823
Hf-Ta-C-Cl-Cl	-1.61658	-2.00989	-0.84738	-0.96117
Hf-Ta-N-Cl-Cl	-1.68771	-2.02462	-0.69927	-0.90669
Hf-V-C-Cl-Cl	-1.33384	-2.2423	-0.89465	-0.98719
Hf-V-N-Cl-Cl	-1.35145	-2.05434	-0.72161	-0.91701
Hf-W-C-Cl-Cl	-1.61602	-1.99048	-0.87526	-1.04157
Hf-W-N-Cl-Cl	-1.68072	-2.09373	-0.73178	-0.96943
Mo-Mo-C-Cl-Cl	-1.09935	-2.11701	-1.42056	-1.81601
Mo-Mo-N-Cl-Cl	-1.07342	-2.10542	-1.39502	-1.78232
Mo-W-C-Cl-Cl	-1.12819	-2.04856	-1.42245	-1.81642
Mo-W-N-Cl-Cl	-1.1039	-2.06797	-1.42598	-1.8131
Nb-Cr-C-Cl-Cl	-1.05684	-2.65264	-1.37661	-0.68205
Nb-Cr-N-Cl-Cl	-0.98574	-1.99736	-1.14056	-0.44209
Nb-Mo-C-Cl-Cl	-1.06768	-2.01254	-1.38282	-0.67716
Nb-Mo-N-Cl-Cl	-1.01283	-1.96424	-1.25856	-0.44348
Nb-Nb-C-Cl-Cl	-1.07662	-2.05796	-1.36946	-0.67529
Nb-Nb-N-Cl-Cl	-1.06772	-2.00791	-1.21621	-0.49472
Nb-Ta-C-Cl-Cl	-1.12083	-1.99132	-1.35991	-0.67299
Nb-Ta-N-Cl-Cl	-1.08995	-1.98768	-1.24379	-0.51495
Nb-W-C-Cl-Cl	-1.09369	-1.97417	-1.38926	-0.67719
Nb-W-N-Cl-Cl	-1.05533	-2.0181	-1.30892	-0.55081
Sc-Cr-C-Cl-Cl	-1.31513	-3.62213	-1.72791	-0.97334
Sc-Cr-N-Cl-Cl	-1.32828	-3.09048	-1.69537	-0.74815
Sc-Hf-C-Cl-Cl	-1.31383	-2.01898	-1.68013	-0.85436
Sc-Hf-N-Cl-Cl	-1.25218	-1.98144	-1.55054	-0.6179
Sc-Mo-C-Cl-Cl	-1.30677	-3.09702	-1.74492	-1.09978
Sc-Mo-N-Cl-Cl	-1.36133	-3.55825	-1.71013	-0.82716
Sc-Nb-C-Cl-Cl	-1.35254	-2.40368	-1.73001	-0.95949
Sc-Nb-N-Cl-Cl	-1.34549	-2.43811	-1.69858	-0.74823

Sc-Sc-C-Cl-Cl	-1.34236	-2.29529	-1.70274	-0.86985
Sc-Sc-N-Cl-Cl	-1.31358	-2.03133	-1.61732	-0.60639
Sc-Ta-C-Cl-Cl	-1.39482	-2.08283	-1.69737	-0.98276
Sc-Ta-N-Cl-Cl	-1.40093	-2.20008	-1.66266	-0.72229
Sc-Ti-C-Cl-Cl	-1.30069	-2.40704	-1.71095	-0.98046
Sc-Ti-N-Cl-Cl	-1.2906	-2.28038	-1.67445	-0.71153
Sc-V-C-Cl-Cl	-1.34485	-2.49802	-1.71634	-0.96807
Sc-V-N-Cl-Cl	-1.31434	-2.33668	-1.69101	-0.75091
Sc-W-C-Cl-Cl	-1.35973	-2.51461	-1.70032	-1.09441
Sc-W-N-Cl-Cl	-1.48555	-2.95971	-1.70657	-0.82087
Sc-Y-C-Cl-Cl	-1.39062	-2.14156	-1.71083	-0.7044
Sc-Y-N-Cl-Cl	-1.37747	-2.04499	-1.58882	-0.45258
Sc-Zr-C-Cl-Cl	-1.39422	-2.0867	-1.69973	-0.85812
Sc-Zr-N-Cl-Cl	-1.3482	-2.01838	-1.59327	-0.60928
Ta-Cr-C-Cl-Cl	-1.39789	-2.71936	-0.98634	-1.17288
Ta-Cr-N-Cl-Cl	-1.43505	-2.09946	-0.82307	-1.16858
Ta-Mo-C-Cl-Cl	-1.41686	-2.0113	-0.98341	-1.07672
Ta-Mo-N-Cl-Cl	-1.46597	-2.0596	-0.82135	-1.06644
Ta-Ta-C-Cl-Cl	-2.09772	-2.01088	-0.94171	-1.18533
Ta-Ta-N-Cl-Cl	-2.23625	-2.02388	-0.78905	-1.13386
Ta-W-C-Cl-Cl	-2.0879	-1.97825	-0.95811	-1.06753
Ta-W-N-Cl-Cl	-2.08384	-2.01276	-0.81184	-1.15003
Ti-Cr-C-Cl-Cl	-1.45327	-2.99448	-1.69621	-1.04901
Ti-Cr-N-Cl-Cl	-1.38391	-2.32246	-1.73768	-0.99885
Ti-Hf-C-Cl-Cl	-1.29358	-2.08538	-1.6594	-0.8549
Ti-Hf-N-Cl-Cl	-1.24713	-2.05547	-1.61215	-0.79679
Ti-Mo-C-Cl-Cl	-1.45481	-2.62062	-1.70293	-1.05213
Ti-Mo-N-Cl-Cl	-1.30833	-2.50356	-1.7173	-1.00595
Ti-Nb-C-Cl-Cl	-1.35327	-2.25733	-1.68247	-0.9832
Ti-Nb-N-Cl-Cl	-1.35314	-2.10255	-1.72011	-0.99033
Ti-Ta-C-Cl-Cl	-1.38234	-2.16364	-1.67663	-0.97857
Ti-Ta-N-Cl-Cl	-1.40119	-2.07414	-1.70299	-0.91154
Ti-Ti-C-Cl-Cl	-1.35716	-2.32487	-1.671	-0.9841
Ti-Ti-N-Cl-Cl	-1.3137	-2.07944	-1.70941	-0.94915
Ti-V-C-Cl-Cl	-1.44986	-2.34553	-1.6885	-1.06755
Ti-V-N-Cl-Cl	-1.35285	-2.06647	-1.72807	-0.98523
Ti-W-C-Cl-Cl	-1.37114	-2.32868	-1.66055	-1.05023
Ti-W-N-Cl-Cl	-1.40032	-2.30235	-1.71333	-0.97751
Ti-Zr-C-Cl-Cl	-1.35606	-2.13013	-1.66698	-0.85519
Ti-Zr-N-Cl-Cl	-1.31144	-2.0697	-1.62718	-0.80607
V-Cr-C-Cl-Cl	-1.46197	-2.93514	-1.73487	-1.17737

V-Cr-N-Cl-Cl	-1.44055	-2.27572	-1.76872	-1.16048
V-Mo-C-Cl-Cl	-1.36759	-2.51752	-1.72562	-1.0936
V-Mo-N-Cl-Cl	-1.31103	-2.42646	-1.76419	-1.13172
V-Nb-C-Cl-Cl	-1.36208	-2.20136	-1.72344	-1.08927
V-Nb-N-Cl-Cl	-1.35923	-2.09026	-1.77189	-1.15937
V-Ta-C-Cl-Cl	-1.37654	-2.13729	-1.71234	-1.06636
V-Ta-N-Cl-Cl	-1.37817	-2.06269	-1.74418	-1.05943
V-V-C-Cl-Cl	-1.4484	-2.32053	-1.71724	-1.15362
V-V-N-Cl-Cl	-1.46846	-2.09473	-1.74855	-1.16697
V-W-C-Cl-Cl	-1.37829	-2.31156	-1.69257	-1.08824
V-W-N-Cl-Cl	-1.36946	-2.27873	-1.7443	-1.01847
W-W-C-Cl-Cl	-2.03788	-2.04475	-0.96621	-1.652
W-W-N-Cl-Cl	-2.08605	-2.04898	-0.8726	-1.6853
Y-Cr-C-Cl-Cl	-1.36324	-2.56435	-1.77101	-0.96573
Y-Cr-N-Cl-Cl	-1.36334	-2.39935	-1.72505	-0.76931
Y-Hf-C-Cl-Cl	-1.47727	-2.06538	-1.7428	-0.75425
Y-Hf-N-Cl-Cl	-1.35622	-2.05571	-1.60354	-0.49168
Y-Mo-C-Cl-Cl	-1.33231	-2.13346	-1.79424	-1.36886
Y-Mo-N-Cl-Cl	-1.38024	-2.45871	-1.73181	-1.00782
Y-Nb-C-Cl-Cl	-1.3562	-2.12088	-1.78384	-0.89932
Y-Nb-N-Cl-Cl	-1.37775	-2.13216	-1.72686	-0.72681
Y-Ta-C-Cl-Cl	-1.60929	-2.08556	-1.74999	-0.95292
Y-Ta-N-Cl-Cl	-1.62423	-2.08617	-1.68179	-0.6891
Y-Ti-C-Cl-Cl	-1.33615	-2.21122	-1.76747	-0.95391
Y-Ti-N-Cl-Cl	-1.35144	-2.09478	-1.69265	-0.70374
Y-V-C-Cl-Cl	-1.34132	-2.24279	-1.76155	-0.9731
Y-V-N-Cl-Cl	-1.37049	-2.09783	-1.71817	-0.73206
Y-W-C-Cl-Cl	-1.5698	-2.12309	-1.74312	-1.35371
Y-W-N-Cl-Cl	-1.59969	-2.28999	-1.72415	-1.05042
Y-Y-C-Cl-Cl	-1.57329	-2.14025	-1.76103	-0.57745
Y-Y-N-Cl-Cl	-1.4508	-2.10693	-1.64452	-0.19399
Y-Zr-C-Cl-Cl	-1.46843	-2.09933	-1.75948	-0.74628
Y-Zr-N-Cl-Cl	-1.45357	-2.07707	-1.63165	-0.49119
Zr-Cr-C-Cl-Cl	-1.34428	-2.75791	-1.54373	-0.77493
Zr-Cr-N-Cl-Cl	-1.37307	-2.27564	-1.43026	-0.72504
Zr-Hf-C-Cl-Cl	-1.41109	-1.99763	-1.48882	-0.62464
Zr-Hf-N-Cl-Cl	-1.35796	-1.97832	-1.34548	-0.57411
Zr-Mo-C-Cl-Cl	-1.35661	-2.01951	-1.55068	-0.87434
Zr-Mo-N-Cl-Cl	-1.37602	-2.2789	-1.46967	-0.81625
Zr-Nb-C-Cl-Cl	-1.38531	-2.06961	-1.54513	-0.74379
Zr-Nb-N-Cl-Cl	-1.4084	-2.07223	-1.44211	-0.70903

Zr-Ta-C-Cl-Cl	-1.62854	-2.00289	-1.5197	-0.72863
Zr-Ta-N-Cl-Cl	-1.73556	-2.00968	-1.43617	-0.67935
Zr-V-C-Cl-Cl	-1.34853	-2.24779	-1.54159	-0.76476
Zr-V-N-Cl-Cl	-1.36743	-2.03958	-1.43633	-0.72049
Zr-W-C-Cl-Cl	-1.65611	-1.99093	-1.51855	-0.88869
Zr-W-N-Cl-Cl	-1.68444	-2.13173	-1.48037	-0.85973
Zr-Zr-C-Cl-Cl	-1.45108	-2.0498	-1.50539	-0.63714
Zr-Zr-N-Cl-Cl	-1.45688	-2.00457	-1.37309	-0.56496
Cr-Cr-C-CN-CN	-5.64974	-3.30716	-3.5673	-2.65793
Cr-Cr-N-CN-CN	-5.12736	-3.3025	-3.62041	-2.6089
Cr-Mo-C-CN-CN	-4.73107	-3.00051	-3.20037	-2.68018
Cr-Mo-N-CN-CN	-3.60423	-2.98305	-3.1827	-2.44653
Cr-W-C-CN-CN	-4.3979	-3.02492	-3.12998	-2.6661
Cr-W-N-CN-CN	-3.67053	-2.96846	-3.05227	-2.64212
Hf-Cr-C-CN-CN	-3.21312	-2.85291	-2.71094	-2.44462
Hf-Cr-N-CN-CN	-3.00398	-2.83735	-2.74887	-2.32803
Hf-Hf-C-CN-CN	-2.56921	-3.05775	-2.34137	-2.35225
Hf-Hf-N-CN-CN	-2.54301	-3.12164	-1.92679	-2.35605
Hf-Mo-C-CN-CN	-4.07366	-3.00971	-2.46229	-2.30542
Hf-Mo-N-CN-CN	-3.61748	-3.00652	-2.51562	-2.3217
Hf-Nb-C-CN-CN	-2.50484	-2.9655	-2.48726	-2.30265
Hf-Nb-N-CN-CN	-2.5059	-2.96863	-2.58155	-2.39176
Hf-Ta-C-CN-CN	-2.60458	-3.19839	-2.13949	-2.3508
Hf-Ta-N-CN-CN	-2.50575	-3.32166	-1.58926	-2.40681
Hf-V-C-CN-CN	-2.71818	-3.00015	-2.5605	-2.39721
Hf-V-N-CN-CN	-2.61805	-3.00702	-2.46589	-2.51063
Hf-W-C-CN-CN	-3.61872	-3.09107	-2.1959	-2.23724
Hf-W-N-CN-CN	-3.26753	-3.13415	-2.10698	-2.30088
Mo-Mo-C-CN-CN	-3.51052	-3.21121	-2.96076	-3.34065
Mo-Mo-N-CN-CN	-3.56609	-3.21052	-2.97181	-3.24018
Mo-W-C-CN-CN	-3.33405	-3.17759	-2.93261	-3.31724
Mo-W-N-CN-CN	-3.667	-3.17425	-2.78517	-3.15942
Nb-Cr-C-CN-CN	-2.86611	-3.2464	-3.33416	-3.50153
Nb-Cr-N-CN-CN	-3.08044	-3.30134	-3.36169	-3.64784
Nb-Mo-C-CN-CN	-3.78508	-2.92045	-2.91555	-3.22807
Nb-Mo-N-CN-CN	-3.63105	-2.95889	-2.9537	-3.28823
Nb-Nb-C-CN-CN	-2.58214	-3.07486	-2.93595	-3.21697
Nb-Nb-N-CN-CN	-2.59871	-3.1625	-3.09887	-3.39104
Nb-Ta-C-CN-CN	-2.71395	-3.19049	-2.92801	-3.28493
Nb-Ta-N-CN-CN	-2.6579	-3.25991	-2.50711	-3.31918
Nb-W-C-CN-CN	-3.41016	-2.8514	-2.92819	-3.15847

Nb-W-N-CN-CN	-3.5064	-2.89193	-2.83704	-3.17269
Sc-Cr-C-CN-CN	-3.56656	-2.90249	-3.25952	-0.06353
Sc-Cr-N-CN-CN	-3.06938	-2.90995	-3.36043	-1.62378
Sc-Hf-C-CN-CN	-2.65621	-3.15506	-2.95997	-1.62383
Sc-Hf-N-CN-CN	-2.61815	-3.16877	-2.55112	-2.1334
Sc-Mo-C-CN-CN	-3.79402	-3.14703	-2.94166	-0.93683
Sc-Mo-N-CN-CN	-3.21252	-3.19187	-3.00791	-1.66609
Sc-Nb-C-CN-CN	-2.64031	-3.11485	-2.94937	-1.00848
Sc-Nb-N-CN-CN	-2.58142	-3.08218	-3.17068	-1.67498
Sc-Sc-C-CN-CN	-2.76405	-3.17825	-3.07024	-1.61635
Sc-Sc-N-CN-CN	-2.71722	-3.11693	-2.67204	-2.14536
Sc-Ta-C-CN-CN	-2.68073	-3.26883	-2.95865	-1.86209
Sc-Ta-N-CN-CN	-2.60929	-3.29315	-2.54619	-2.16004
Sc-Ti-C-CN-CN	-2.82603	-3.13502	-3.10689	-1.14963
Sc-Ti-N-CN-CN	-2.66306	-3.17963	-2.8524	-2.24511
Sc-V-C-CN-CN	-2.83146	-3.04097	-3.18633	-1.30779
Sc-V-N-CN-CN	-2.71121	-3.04344	-3.10024	-2.00047
Sc-W-C-CN-CN	-3.46277	-3.13307	-2.95367	-1.10414
Sc-W-N-CN-CN	-3.14083	-3.14926	-2.92136	-1.6417
Sc-Y-C-CN-CN	-2.68468	-3.46016	-2.96935	-1.69298
Sc-Y-N-CN-CN	-2.6541	-3.45114	-2.58433	-2.01322
Sc-Zr-C-CN-CN	-2.67076	-3.15835	-2.96374	-1.6043
Sc-Zr-N-CN-CN	-2.64014	-3.16839	-2.5811	-2.15822
Ta-Cr-C-CN-CN	-2.99493	-4.24982	-2.39741	-5.06252
Ta-Cr-N-CN-CN	-2.73251	-4.28577	-2.41998	-6.05528
Ta-Mo-C-CN-CN	-3.73451	-4.08019	-2.08755	-4.37
Ta-Mo-N-CN-CN	-3.41845	-4.10543	-2.08313	-4.82469
Ta-Ta-C-CN-CN	-2.60659	-4.3431	-1.43055	-4.54188
Ta-Ta-N-CN-CN	-2.54282	-4.63744	-0.55326	-5.18549
Ta-W-C-CN-CN	-3.32845	-4.12927	-1.69558	-4.39614
Ta-W-N-CN-CN	-3.43083	-4.13141	-1.49139	-4.55498
Ti-Cr-C-CN-CN	-4.32804	-2.95512	-3.39892	-2.7815
Ti-Cr-N-CN-CN	-4.26161	-2.94752	-3.558	-2.4436
Ti-Hf-C-CN-CN	-2.51991	-3.18703	-2.94584	-2.46058
Ti-Hf-N-CN-CN	-2.47628	-3.18501	-2.55451	-2.30935
Ti-Mo-C-CN-CN	-3.71448	-3.14893	-3.09079	-2.73352
Ti-Mo-N-CN-CN	-2.93413	-3.10713	-3.19668	-2.25232
Ti-Nb-C-CN-CN	-2.39016	-3.19144	-3.00575	-2.62298
Ti-Nb-N-CN-CN	-2.38705	-3.07214	-3.5507	-2.19917
Ti-Ta-C-CN-CN	-2.55944	-3.35781	-2.97035	-2.608
Ti-Ta-N-CN-CN	-2.53376	-3.3377	-2.7182	-2.44946

Ti-Ti-C-CN-CN	-3.16532	-3.12415	-3.17407	-2.77777
Ti-Ti-N-CN-CN	-3.09671	-3.0988	-3.05455	-2.45771
Ti-V-C-CN-CN	-3.69649	-3.0963	-3.25056	-2.7665
Ti-V-N-CN-CN	-3.44051	-3.06783	-3.29712	-2.45882
Ti-W-C-CN-CN	-3.48671	-3.13308	-3.00389	-2.68612
Ti-W-N-CN-CN	-2.9435	-3.11611	-3.02827	-2.31134
Ti-Zr-C-CN-CN	-2.53484	-3.18749	-2.94065	-2.46779
Ti-Zr-N-CN-CN	-2.50364	-3.18419	-2.63422	-2.29677
V-Cr-C-CN-CN	-6.23138	-3.0674	-3.57857	-2.90622
V-Cr-N-CN-CN	-5.12038	-3.01879	-3.61866	-2.79657
V-Mo-C-CN-CN	-4.52673	-3.11061	-3.19722	-2.91049
V-Mo-N-CN-CN	-3.67356	-3.1074	-3.21782	-2.80298
V-Nb-C-CN-CN	-3.02166	-3.14736	-3.29053	-2.97527
V-Nb-N-CN-CN	-2.69316	-3.10358	-3.51801	-2.69089
V-Ta-C-CN-CN	-3.31706	-3.34852	-3.14427	-2.96595
V-Ta-N-CN-CN	-2.80853	-3.39029	-2.75513	-2.69552
V-V-C-CN-CN	-4.63069	-3.21831	-3.38079	-2.90849
V-V-N-CN-CN	-4.17463	-3.09805	-3.34696	-2.80936
V-W-C-CN-CN	-4.25001	-3.11957	-3.11351	-2.8636
V-W-N-CN-CN	-3.59304	-3.12878	-3.05675	-2.76762
W-W-C-CN-CN	-3.32843	-4.15406	-1.89582	-4.55886
W-W-N-CN-CN	-3.27222	-4.18092	-1.66485	-4.42094
Y-Cr-C-CN-CN	-3.21651	-2.97828	-3.21197	-2.27089
Y-Cr-N-CN-CN	-3.10985	-3.33284	-3.23006	-2.13759
Y-Hf-C-CN-CN	-2.68705	-3.15624	-2.89035	-2.43008
Y-Hf-N-CN-CN	-2.63159	-3.12852	-2.48028	-2.35849
Y-Mo-C-CN-CN	-3.48745	-3.13508	-2.78834	-2.43313
Y-Mo-N-CN-CN	-3.41918	-3.15731	-2.86591	-2.2966
Y-Nb-C-CN-CN	-2.68053	-3.14427	-2.84231	-2.37627
Y-Nb-N-CN-CN	-2.63852	-3.11658	-3.01582	-2.26848
Y-Ta-C-CN-CN	-2.70169	-3.20521	-2.8735	-2.43538
Y-Ta-N-CN-CN	-2.61967	-3.21094	-2.46835	-2.35504
Y-Ti-C-CN-CN	-2.75811	-3.15578	-3.04781	-2.42465
Y-Ti-N-CN-CN	-2.76408	-3.16113	-2.76088	-2.31113
Y-V-C-CN-CN	-2.88872	-3.12927	-3.05182	-2.3219
Y-V-N-CN-CN	-2.9319	-3.09556	-2.86758	-2.22078
Y-W-C-CN-CN	-3.28542	-3.10768	-2.83052	-2.34624
Y-W-N-CN-CN	-3.25028	-3.10883	-2.76578	-2.24082
Y-Y-C-CN-CN	-2.75056	-3.50317	-2.90463	-2.40698
Y-Y-N-CN-CN	-2.68377	-3.52383	-2.5294	-2.38407
Y-Zr-C-CN-CN	-2.70595	-3.31692	-2.89355	-2.41034

Y-Zr-N-CN-CN	-2.66029	-3.20911	-2.5166	-2.37322
Zr-Cr-C-CN-CN	-3.5659	-2.88012	-3.22149	-2.25461
Zr-Cr-N-CN-CN	-3.30564	-2.89191	-3.24803	-2.22185
Zr-Hf-C-CN-CN	-2.62075	-3.09885	-2.84307	-2.54508
Zr-Hf-N-CN-CN	-2.59647	-3.12847	-2.49749	-2.41189
Zr-Mo-C-CN-CN	-4.67764	-3.06415	-2.86997	-2.47106
Zr-Mo-N-CN-CN	-3.7455	-3.10338	-2.92521	-2.37483
Zr-Nb-C-CN-CN	-2.63663	-3.07588	-2.89392	-2.44676
Zr-Nb-N-CN-CN	-2.66309	-3.10843	-3.06107	-2.36603
Zr-Ta-C-CN-CN	-2.67533	-3.18671	-2.83648	-2.50847
Zr-Ta-N-CN-CN	-2.73432	-3.23208	-2.49562	-2.40824
Zr-V-C-CN-CN	-2.9467	-3.0284	-2.9915	-2.31443
Zr-V-N-CN-CN	-2.80533	-3.03025	-2.89369	-2.27441
Zr-W-C-CN-CN	-3.95907	-3.02976	-2.82676	-2.39685
Zr-W-N-CN-CN	-3.52584	-3.00765	-2.78703	-2.33171
Zr-Zr-C-CN-CN	-2.63555	-3.16144	-2.82952	-2.52924
Zr-Zr-N-CN-CN	-2.61719	-3.13727	-2.53016	-2.42035
Cr-Cr-C-NCO-NCO	-3.09265	-2.39798	-2.24192	-1.94713
Cr-Cr-N-NCO-NCO	-2.83083	-2.05781	-2.52215	-1.68354
Cr-Mo-C-NCO-NCO	-2.77045	-2.45981	-2.4512	-1.93288
Cr-Mo-N-NCO-NCO	-2.02361	-2.10759	-2.68375	-1.33973
Cr-W-C-NCO-NCO	-3.7935	-2.54199	-2.47045	-2.01456
Cr-W-N-NCO-NCO	-2.32647	-2.24553	-2.66966	-1.33761
Hf-Cr-C-NCO-NCO	-1.31093	-2.67632	-2.09561	-1.09457
Hf-Cr-N-NCO-NCO	-1.2229	-2.13907	-2.21365	-0.76105
Hf-Hf-C-NCO-NCO	-1.23391	-2.53348	-2.11408	-1.04444
Hf-Hf-N-NCO-NCO	-1.20716	-2.04043	-2.10215	-0.7071
Hf-Mo-C-NCO-NCO	-1.30029	-2.75519	-2.22595	-1.08303
Hf-Mo-N-NCO-NCO	-1.23954	-2.16244	-2.39012	-0.7237
Hf-Nb-C-NCO-NCO	-1.29068	-2.57231	-2.24794	-1.06095
Hf-Nb-N-NCO-NCO	-1.2557	-2.04642	-2.31755	-0.76621
Hf-Ta-C-NCO-NCO	-1.26416	-2.67104	-2.12669	-1.03649
Hf-Ta-N-NCO-NCO	-1.22475	-2.12841	-2.11529	-0.7232
Hf-V-C-NCO-NCO	-1.29901	-2.67771	-2.22125	-1.11746
Hf-V-N-NCO-NCO	-1.23779	-2.10073	-2.34175	-0.76506
Hf-W-C-NCO-NCO	-1.37947	-2.96312	-2.1781	-1.05734
Hf-W-N-NCO-NCO	-1.22157	-2.31339	-2.41747	-0.73877
Mo-Mo-C-NCO-NCO	-1.54829	-2.69336	-2.16649	-1.60204
Mo-Mo-N-NCO-NCO	-1.48012	-2.56474	-2.20337	-1.34464
Mo-W-C-NCO-NCO	-1.97146	-2.79437	-2.08067	-1.59999
Mo-W-N-NCO-NCO	-1.77318	-2.52993	-2.16971	-1.3114

Nb-Cr-C-NCO-NCO	-1.41895	-2.68852	-2.01713	-1.35528
Nb-Cr-N-NCO-NCO	-1.30863	-2.51006	-1.9829	-1.04345
Nb-Mo-C-NCO-NCO	-1.3485	-2.7465	-2.08246	-1.26942
Nb-Mo-N-NCO-NCO	-1.18306	-2.63806	-2.15064	-0.95206
Nb-Nb-C-NCO-NCO	-1.40077	-2.74158	-1.98467	-1.28156
Nb-Nb-N-NCO-NCO	-1.18218	-2.74301	-1.89307	-1.01727
Nb-Ta-C-NCO-NCO	-1.50122	-2.85715	-1.96289	-1.2645
Nb-Ta-N-NCO-NCO	-1.17449	-2.72059	-1.80652	-0.9081
Nb-W-C-NCO-NCO	-1.70558	-2.86738	-2.0178	-1.2534
Nb-W-N-NCO-NCO	-1.31475	-2.62163	-2.18333	-0.93226
Sc-Cr-C-NCO-NCO	-1.54469	-2.68027	-2.29133	-1.25832
Sc-Cr-N-NCO-NCO	-1.4535	-2.17711	-2.17703	-1.13456
Sc-Hf-C-NCO-NCO	-1.43207	-2.43354	-2.3034	-1.21048
Sc-Hf-N-NCO-NCO	-1.38481	-2.13922	-2.06599	-1.05127
Sc-Mo-C-NCO-NCO	-1.5385	-2.52371	-2.61888	-1.22637
Sc-Mo-N-NCO-NCO	-1.50682	-2.15592	-2.59984	-1.12366
Sc-Nb-C-NCO-NCO	-1.5124	-2.46586	-2.46977	-1.23629
Sc-Nb-N-NCO-NCO	-1.4416	-2.04692	-2.39588	-1.11584
Sc-Sc-C-NCO-NCO	-1.46949	-2.52674	-2.28384	-1.19479
Sc-Sc-N-NCO-NCO	-1.40399	-2.18902	-2.05614	-1.0697
Sc-Ta-C-NCO-NCO	-1.50666	-2.57054	-2.34942	-1.17619
Sc-Ta-N-NCO-NCO	-1.52588	-2.14956	-2.12793	-1.1002
Sc-Ti-C-NCO-NCO	-1.569	-2.62075	-2.32318	-1.20057
Sc-Ti-N-NCO-NCO	-1.43899	-2.15006	-2.12849	-1.09532
Sc-V-C-NCO-NCO	-1.56939	-2.68273	-2.37941	-1.2912
Sc-V-N-NCO-NCO	-1.50334	-2.08741	-2.23534	-1.16254
Sc-W-C-NCO-NCO	-1.69849	-2.72541	-2.53582	-1.21397
Sc-W-N-NCO-NCO	-1.7499	-2.21118	-2.61117	-1.14146
Sc-Y-C-NCO-NCO	-1.46891	-2.56458	-2.21082	-1.17283
Sc-Y-N-NCO-NCO	-1.36947	-2.15966	-1.9803	-1.0078
Sc-Zr-C-NCO-NCO	-1.46406	-2.46545	-2.30599	-1.19936
Sc-Zr-N-NCO-NCO	-1.37494	-2.19187	-2.05513	-1.0538
Ta-Cr-C-NCO-NCO	-1.22103	-2.68196	-2.02351	-1.16371
Ta-Cr-N-NCO-NCO	-1.02358	-2.10209	-2.21132	-0.63825
Ta-Mo-C-NCO-NCO	-1.16832	-2.7691	-2.07047	-1.11939
Ta-Mo-N-NCO-NCO	-1.0245	-2.13524	-2.11891	-0.59935
Ta-Ta-C-NCO-NCO	-1.28897	-2.68469	-1.98854	-1.10214
Ta-Ta-N-NCO-NCO	-1.06979	-2.1989	-1.89272	-0.6316
Ta-W-C-NCO-NCO	-1.40475	-2.93687	-2.0064	-1.10976
Ta-W-N-NCO-NCO	-1.16	-2.28712	-2.11331	-0.64757
Ti-Cr-C-NCO-NCO	-2.08925	-2.3784	-2.23004	-1.62595

Ti-Cr-N-NCO-NCO	-1.8989	-1.34556	-2.84847	-1.31668
Ti-Hf-C-NCO-NCO	-1.61997	-2.14644	-2.31837	-1.25757
Ti-Hf-N-NCO-NCO	-1.46516	-1.16552	-2.46998	-1.02934
Ti-Mo-C-NCO-NCO	-1.83348	-2.50862	-2.59156	-1.52538
Ti-Mo-N-NCO-NCO	-1.43014	-1.35023	-3.07377	-1.09785
Ti-Nb-C-NCO-NCO	-1.60386	-2.18072	-2.72852	-1.32831
Ti-Nb-N-NCO-NCO	-1.44686	-0.37336	-3.41196	-1.08872
Ti-Ta-C-NCO-NCO	-1.81578	-2.34226	-2.41019	-1.3128
Ti-Ta-N-NCO-NCO	-1.64625	-1.0057	-2.82866	-1.06139
Ti-Ti-C-NCO-NCO	-1.98361	-2.32619	-2.27211	-1.56655
Ti-Ti-N-NCO-NCO	-1.81907	-1.18302	-2.72804	-1.29099
Ti-V-C-NCO-NCO	-2.19254	-2.33184	-2.53215	-1.65386
Ti-V-N-NCO-NCO	-1.78926	-1.11383	-3.03476	-1.31469
Ti-W-C-NCO-NCO	-2.25549	-2.65147	-2.53407	-1.5196
Ti-W-N-NCO-NCO	-1.74355	-1.6484	-2.91764	-1.10132
Ti-Zr-C-NCO-NCO	-1.55241	-2.16956	-2.42332	-1.2382
Ti-Zr-N-NCO-NCO	-1.39418	-1.28228	-2.61359	-1.02999
V-Cr-C-NCO-NCO	-2.495	-2.44806	-2.2321	-1.50384
V-Cr-N-NCO-NCO	-2.11647	-1.51172	-2.56961	-1.28181
V-Mo-C-NCO-NCO	-1.53571	-2.5345	-2.43499	-1.24187
V-Mo-N-NCO-NCO	-1.6026	-1.52635	-2.77882	-1.13374
V-Nb-C-NCO-NCO	-1.70661	-2.19227	-2.47926	-1.28309
V-Nb-N-NCO-NCO	-1.54486	-0.9644	-2.82319	-1.10762
V-Ta-C-NCO-NCO	-2.03915	-2.32074	-2.36896	-1.24991
V-Ta-N-NCO-NCO	-1.64576	-1.36013	-2.47148	-1.05239
V-V-C-NCO-NCO	-2.61989	-2.441	-2.3015	-1.63264
V-V-N-NCO-NCO	-2.12708	-1.37484	-2.58828	-1.31318
V-W-C-NCO-NCO	-2.34505	-2.66511	-2.46246	-1.24075
V-W-N-NCO-NCO	-1.73905	-1.87188	-2.72559	-1.08972
W-W-C-NCO-NCO	-2.22474	-2.89723	-2.06449	-1.40615
W-W-N-NCO-NCO	-1.61796	-2.52579	-2.13936	-1.068
Y-Cr-C-NCO-NCO	-1.53105	-2.42957	-2.20045	-1.22081
Y-Cr-N-NCO-NCO	-1.43611	-2.19647	-2.20015	-0.9876
Y-Hf-C-NCO-NCO	-1.4616	-2.47005	-2.20507	-1.17014
Y-Hf-N-NCO-NCO	-1.3558	-2.18274	-2.08085	-0.93895
Y-Mo-C-NCO-NCO	-1.5224	-2.48451	-2.34229	-1.21724
Y-Mo-N-NCO-NCO	-1.42275	-2.2208	-2.44967	-0.9681
Y-Nb-C-NCO-NCO	-1.50779	-2.44453	-2.2233	-1.20519
Y-Nb-N-NCO-NCO	-1.38861	-2.1472	-2.15844	-0.96062
Y-Ta-C-NCO-NCO	-1.46924	-2.56426	-2.24064	-1.18266
Y-Ta-N-NCO-NCO	-1.36265	-2.17341	-2.11652	-0.94884

Y-Ti-C-NCO-NCO	-1.51448	-2.46293	-2.23578	-1.19662
Y-Ti-N-NCO-NCO	-1.41892	-2.20399	-2.14971	-0.93959
Y-V-C-NCO-NCO	-1.55025	-2.48816	-2.2368	-1.21731
Y-V-N-NCO-NCO	-1.39581	-2.19227	-2.18852	-0.96734
Y-W-C-NCO-NCO	-1.4519	-2.75122	-2.3264	-1.19844
Y-W-N-NCO-NCO	-1.4107	-2.22704	-2.51765	-0.98298
Y-Y-C-NCO-NCO	-1.50644	-2.63243	-2.17136	-1.12313
Y-Y-N-NCO-NCO	-1.38918	-2.44607	-2.04	-0.97558
Y-Zr-C-NCO-NCO	-1.50045	-2.49127	-2.20903	-1.1541
Y-Zr-N-NCO-NCO	-1.38782	-2.25859	-2.0847	-0.96584
Zr-Cr-C-NCO-NCO	-1.27326	-2.6972	-2.15551	-0.94001
Zr-Cr-N-NCO-NCO	-1.23341	-2.17338	-2.25291	-0.85403
Zr-Hf-C-NCO-NCO	-1.22105	-2.60995	-2.16259	-0.87521
Zr-Hf-N-NCO-NCO	-1.18724	-2.14311	-2.13835	-0.71459
Zr-Mo-C-NCO-NCO	-1.27261	-2.75571	-2.32907	-0.92066
Zr-Mo-N-NCO-NCO	-1.23196	-2.18796	-2.59541	-0.81253
Zr-Nb-C-NCO-NCO	-1.26754	-2.65614	-2.20513	-0.9225
Zr-Nb-N-NCO-NCO	-1.23791	-2.18035	-2.25935	-0.82106
Zr-Ta-C-NCO-NCO	-1.22089	-2.77363	-2.19048	-0.89416
Zr-Ta-N-NCO-NCO	-1.19657	-2.193	-2.17273	-0.79659
Zr-V-C-NCO-NCO	-1.30071	-2.7003	-2.1728	-0.94202
Zr-V-N-NCO-NCO	-1.24663	-2.19065	-2.24083	-0.85943
Zr-W-C-NCO-NCO	-1.22379	-3.02001	-2.27426	-0.89526
Zr-W-N-NCO-NCO	-1.23576	-2.1976	-2.68895	-0.79182
Zr-Zr-C-NCO-NCO	-1.27778	-2.57658	-2.17897	-0.8689
Zr-Zr-N-NCO-NCO	-1.24455	-2.19759	-2.15066	-0.76657
Cr-Cr-C-NCS-NCS	-1.37464	-3.79994	-1.3505	-1.16082
Cr-Cr-N-NCS-NCS	-1.14434	-1.83511	-1.23982	-1.02476
Cr-Mo-C-NCS-NCS	-1.16473	-2.6985	-1.1817	-1.40629
Cr-Mo-N-NCS-NCS	-1.12781	-2.13007	-1.14942	-1.47545
Cr-W-C-NCS-NCS	-1.4502	-2.59658	-1.15279	-1.47797
Cr-W-N-NCS-NCS	-1.19738	-2.40621	-1.11647	-1.46426
Hf-Cr-C-NCS-NCS	-1.3333	-4.3853	-0.99031	-1.90707
Hf-Cr-N-NCS-NCS	-1.32441	-2.44052	-0.84936	-1.69088
Hf-Hf-C-NCS-NCS	-1.32352	-1.85773	-0.9267	-1.86744
Hf-Hf-N-NCS-NCS	-1.29112	-1.80076	-0.8136	-1.59478
Hf-Mo-C-NCS-NCS	-1.30194	-3.02058	-0.92821	-2.34621
Hf-Mo-N-NCS-NCS	-1.28922	-2.29716	-0.78746	-2.30324
Hf-Nb-C-NCS-NCS	-1.33175	-2.18339	-0.9578	-1.8787
Hf-Nb-N-NCS-NCS	-1.31995	-1.87112	-0.84203	-1.67913
Hf-Ta-C-NCS-NCS	-1.48444	-1.92269	-0.95772	-1.86371

Hf-Ta-N-NCS-NCS	-1.51613	-1.92061	-0.85808	-1.59518
Hf-V-C-NCS-NCS	-1.33813	-2.834	-0.97091	-1.87883
Hf-V-N-NCS-NCS	-1.33058	-1.82089	-0.83425	-1.66678
Hf-W-C-NCS-NCS	-1.46305	-2.86017	-0.91582	-2.29139
Hf-W-N-NCS-NCS	-1.48257	-2.51032	-0.80605	-2.24867
Mo-Mo-C-NCS-NCS	-1.13644	-2.4241	-1.47074	-2.0212
Mo-Mo-N-NCS-NCS	-1.13302	-2.17132	-1.47407	-2.04633
Mo-W-C-NCS-NCS	-1.22616	-2.40763	-1.46657	-2.00068
Mo-W-N-NCS-NCS	-1.23367	-2.39835	-1.63528	-1.95852
Nb-Cr-C-NCS-NCS	-1.13752	-3.7081	-0.9834	-1.07095
Nb-Cr-N-NCS-NCS	-1.09221	-2.03704	-0.96719	-0.83069
Nb-Mo-C-NCS-NCS	-1.11101	-2.47088	-0.83278	-1.47624
Nb-Mo-N-NCS-NCS	-1.07453	-2.30387	-0.87962	-1.358
Nb-Nb-C-NCS-NCS	-1.13634	-2.32411	-0.94107	-1.01954
Nb-Nb-N-NCS-NCS	-1.0867	-1.9713	-0.93208	-0.80698
Nb-Ta-C-NCS-NCS	-1.16425	-2.17695	-0.94216	-1.02071
Nb-Ta-N-NCS-NCS	-1.12978	-1.99335	-0.96084	-0.73668
Nb-W-C-NCS-NCS	-1.18924	-2.47737	-0.77023	-1.44931
Nb-W-N-NCS-NCS	-1.14402	-2.35766	-0.9083	-1.3543
Sc-Cr-C-NCS-NCS	-1.31738	-6.25738	-1.30344	-1.03713
Sc-Cr-N-NCS-NCS	-1.30574	-3.34162	-1.12842	-0.48378
Sc-Hf-C-NCS-NCS	-1.32598	-1.80822	-1.14412	-0.93239
Sc-Hf-N-NCS-NCS	-1.28661	-1.75545	-1.06549	-0.31011
Sc-Mo-C-NCS-NCS	-1.29762	-4.1954	-1.15791	-1.41962
Sc-Mo-N-NCS-NCS	-1.28924	-3.22435	-1.10244	-1.10426
Sc-Nb-C-NCS-NCS	-1.33496	-2.67514	-1.2196	-0.94515
Sc-Nb-N-NCS-NCS	-1.32214	-2.10877	-1.09798	-0.4547
Sc-Sc-C-NCS-NCS	-1.32555	-2.66422	-1.19046	-0.92014
Sc-Sc-N-NCS-NCS	-1.30432	-2.00893	-1.09631	-0.41372
Sc-Ta-C-NCS-NCS	-1.36635	-1.84493	-1.18303	-0.94923
Sc-Ta-N-NCS-NCS	-1.40012	-1.78991	-1.13112	-0.30142
Sc-Ti-C-NCS-NCS	-1.31587	-2.67022	-1.18795	-0.91881
Sc-Ti-N-NCS-NCS	-1.30262	-1.74861	-1.05021	-0.2046
Sc-V-C-NCS-NCS	-1.33067	-3.28145	-1.24049	-0.92538
Sc-V-N-NCS-NCS	-1.31235	-1.76291	-1.07756	-0.47965
Sc-W-C-NCS-NCS	-1.36311	-3.32998	-1.09275	-1.44233
Sc-W-N-NCS-NCS	-1.41758	-2.787	-1.07026	-1.12767
Sc-Y-C-NCS-NCS	-1.32681	-2.27464	-1.20856	-0.89987
Sc-Y-N-NCS-NCS	-1.30293	-1.97899	-1.11938	-0.50322
Sc-Zr-C-NCS-NCS	-1.32792	-1.98393	-1.1584	-0.91746
Sc-Zr-N-NCS-NCS	-1.30207	-1.78917	-1.08393	-0.42475

Ta-Cr-C-NCS-NCS	-1.30347	-4.04727	-0.99952	-2.93887
Ta-Cr-N-NCS-NCS	-1.27383	-2.09611	-0.84549	-2.72
Ta-Mo-C-NCS-NCS	-1.24763	-2.67414	-0.93714	-3.42158
Ta-Mo-N-NCS-NCS	-1.26205	-1.79994	-0.71998	-3.45976
Ta-Ta-C-NCS-NCS	-1.7216	-2.11671	-0.96623	-2.85657
Ta-Ta-N-NCS-NCS	-1.73383	-1.95777	-0.83364	-2.64798
Ta-W-C-NCS-NCS	-1.71748	-2.62789	-0.91459	-3.23772
Ta-W-N-NCS-NCS	-1.74116	-2.39811	-0.79436	-3.29489
Ti-Cr-C-NCS-NCS	-1.35566	-4.53963	-1.33624	-1.06175
Ti-Cr-N-NCS-NCS	-1.30888	-2.28754	-1.22683	-0.81365
Ti-Hf-C-NCS-NCS	-1.34464	-1.83949	-1.14336	-0.93243
Ti-Hf-N-NCS-NCS	-1.29177	-1.68204	-1.11068	-0.62983
Ti-Mo-C-NCS-NCS	-1.30663	-3.12015	-1.15449	-1.40869
Ti-Mo-N-NCS-NCS	-1.29616	-2.30549	-1.12772	-1.34923
Ti-Nb-C-NCS-NCS	-1.35849	-2.3712	-1.21473	-0.9522
Ti-Nb-N-NCS-NCS	-1.3307	-1.74089	-1.13718	-0.72559
Ti-Ta-C-NCS-NCS	-1.42207	-2.12733	-1.18823	-0.94338
Ti-Ta-N-NCS-NCS	-1.41176	-1.7578	-1.1899	-0.65476
Ti-Ti-C-NCS-NCS	-1.36656	-2.81762	-1.23188	-0.9774
Ti-Ti-N-NCS-NCS	-1.32349	-1.67741	-1.14669	-0.67528
Ti-V-C-NCS-NCS	-1.3609	-3.02481	-1.25842	-0.99496
Ti-V-N-NCS-NCS	-1.31756	-1.69736	-1.16521	-0.78258
Ti-W-C-NCS-NCS	-1.44454	-2.82482	-1.09105	-1.44059
Ti-W-N-NCS-NCS	-1.39394	-2.39288	-1.09873	-1.37163
Ti-Zr-C-NCS-NCS	-1.3701	-1.98571	-1.15695	-0.92064
Ti-Zr-N-NCS-NCS	-1.32947	-1.73541	-1.11862	-0.6994
V-Cr-C-NCS-NCS	-1.41163	-4.15495	-1.32845	-0.95385
V-Cr-N-NCS-NCS	-1.31251	-1.99242	-1.22347	-0.8909
V-Mo-C-NCS-NCS	-1.31969	-2.86231	-1.13713	-1.29471
V-Mo-N-NCS-NCS	-1.33919	-2.11392	-1.13304	-1.38437
V-Nb-C-NCS-NCS	-1.40578	-2.52696	-1.21989	-0.85409
V-Nb-N-NCS-NCS	-1.32572	-1.70997	-1.14031	-0.78496
V-Ta-C-NCS-NCS	-1.47321	-2.1527	-1.20755	-0.86727
V-Ta-N-NCS-NCS	-1.39667	-1.76061	-1.18018	-0.74105
V-V-C-NCS-NCS	-1.42493	-3.02775	-1.24747	-0.8817
V-V-N-NCS-NCS	-1.32042	-1.77037	-1.15845	-0.85077
V-W-C-NCS-NCS	-1.48456	-2.68497	-1.08433	-1.32159
V-W-N-NCS-NCS	-1.41835	-2.29705	-1.09529	-1.41052
W-W-C-NCS-NCS	-1.80302	-2.69553	-1.17241	-3.07828
W-W-N-NCS-NCS	-1.75418	-2.39985	-1.09604	-3.30582
Y-Cr-C-NCS-NCS	-1.32371	-4.1997	-1.2314	-0.88315

Y-Cr-N-NCS-NCS	-1.31412	-3.01286	-1.08385	-0.50133
Y-Hf-C-NCS-NCS	-1.33285	-1.83749	-1.13296	-0.81367
Y-Hf-N-NCS-NCS	-1.29618	-1.81308	-1.10242	-0.36256
Y-Mo-C-NCS-NCS	-1.31104	-3.14363	-1.10456	-1.32952
Y-Mo-N-NCS-NCS	-1.29978	-2.75805	-1.10848	-1.08089
Y-Nb-C-NCS-NCS	-1.33527	-2.08078	-1.17821	-0.83541
Y-Nb-N-NCS-NCS	-1.31837	-1.77047	-1.0594	-0.45094
Y-Ta-C-NCS-NCS	-1.46909	-1.87534	-1.16987	-0.86744
Y-Ta-N-NCS-NCS	-1.48422	-1.80871	-1.11215	-0.34643
Y-Ti-C-NCS-NCS	-1.32592	-2.27802	-1.15989	-0.82112
Y-Ti-N-NCS-NCS	-1.30887	-1.78398	-1.06431	-0.29745
Y-V-C-NCS-NCS	-1.32477	-2.64243	-1.1879	-0.81666
Y-V-N-NCS-NCS	-1.31503	-1.81044	-1.06681	-0.522
Y-W-C-NCS-NCS	-1.447	-2.92789	-1.06972	-1.3643
Y-W-N-NCS-NCS	-1.47021	-2.61929	-1.0588	-1.12053
Y-Y-C-NCS-NCS	-1.33354	-2.22106	-1.16662	-0.75165
Y-Y-N-NCS-NCS	-1.30714	-2.10558	-1.14954	-0.41189
Y-Zr-C-NCS-NCS	-1.33332	-1.98601	-1.15532	-0.79007
Y-Zr-N-NCS-NCS	-1.30816	-1.87904	-1.11308	-0.46242
Zr-Cr-C-NCS-NCS	-1.33663	-4.55309	-1.14914	-0.50347
Zr-Cr-N-NCS-NCS	-1.32964	-2.5658	-1.06067	-0.53797
Zr-Hf-C-NCS-NCS	-1.32995	-1.7965	-1.0193	-0.43102
Zr-Hf-N-NCS-NCS	-1.29166	-1.7704	-1.02194	-0.3543
Zr-Mo-C-NCS-NCS	-1.3068	-3.12456	-1.01577	-0.91907
Zr-Mo-N-NCS-NCS	-1.29579	-2.5319	-1.01975	-1.08679
Zr-Nb-C-NCS-NCS	-1.33434	-2.17671	-1.09029	-0.43319
Zr-Nb-N-NCS-NCS	-1.31707	-1.82529	-1.03864	-0.51429
Zr-Ta-C-NCS-NCS	-1.48618	-1.87448	-1.07791	-0.44905
Zr-Ta-N-NCS-NCS	-1.50784	-1.83261	-1.06576	-0.37358
Zr-V-C-NCS-NCS	-1.33894	-2.87622	-1.1105	-0.43862
Zr-V-N-NCS-NCS	-1.32973	-1.80793	-1.02597	-0.50481
Zr-W-C-NCS-NCS	-1.46322	-2.88128	-0.96993	-0.94617
Zr-W-N-NCS-NCS	-1.50321	-2.4721	-0.99157	-1.08896
Zr-Zr-C-NCS-NCS	-1.34825	-1.9506	-1.04042	-0.43459
Zr-Zr-N-NCS-NCS	-1.32157	-1.82239	-1.03402	-0.46767
Cr-Cr-C-O-O	-2.66145	-5.27404	-2.59539	-2.36219
Cr-Cr-N-O-O	-4.05933	-4.88072	-2.66109	-2.30629
Cr-Mo-C-O-O	-2.96837	-3.87622	-2.46145	-2.31373
Cr-Mo-N-O-O	-4.18407	-3.70972	-2.62477	-2.34165
Cr-W-C-O-O	-2.97769	-3.63253	-2.45042	-2.32353
Cr-W-N-O-O	-4.3256	-3.55864	-2.39797	-2.24755

Hf-Cr-C-O-O	-2.32872	-2.17634	-2.36612	-2.09361
Hf-Cr-N-O-O	-4.62802	-1.44481	-2.37882	-2.31183
Hf-Hf-C-O-O	-1.75872	-2.95187	-1.52377	-1.85936
Hf-Hf-N-O-O	-2.59291	-2.77235	-0.95685	-2.04252
Hf-Mo-C-O-O	-2.98829	-2.72285	-2.06898	-2.08054
Hf-Mo-N-O-O	-5.37489	-2.64813	-2.0617	-2.23005
Hf-Nb-C-O-O	-1.86608	-2.81406	-2.15452	-1.9951
Hf-Nb-N-O-O	-4.25072	-2.51879	-2.13604	-2.18521
Hf-Ta-C-O-O	-1.96709	-2.83707	-2.09747	-2.01798
Hf-Ta-N-O-O	-3.92346	-2.64533	-1.77389	-2.16947
Hf-V-C-O-O	-2.05698	-2.30941	-2.29761	-2.09339
Hf-V-N-O-O	-4.16622	-1.83986	-2.21189	-2.26068
Hf-W-C-O-O	-3.03229	-2.79436	-2.05722	-2.06616
Hf-W-N-O-O	-5.54567	-2.68568	-2.00163	-2.20226
Mo-Mo-C-O-O	-3.08312	-3.52811	-2.17126	-2.12081
Mo-Mo-N-O-O	-4.91919	-2.84832	-2.14799	-2.09768
Mo-W-C-O-O	-3.09283	-3.19465	-2.19252	-2.13352
Mo-W-N-O-O	-4.85201	-2.8313	-2.09726	-2.11429
Nb-Cr-C-O-O	-2.44195	-6.15769	-2.34946	-2.21955
Nb-Cr-N-O-O	-4.15422	-5.50962	-2.36545	-2.12476
Nb-Mo-C-O-O	-2.94809	-3.60174	-2.13055	-2.18273
Nb-Mo-N-O-O	-4.90022	-3.11759	-2.12092	-2.04979
Nb-Nb-C-O-O	-2.18895	-2.65257	-2.16256	-2.19448
Nb-Nb-N-O-O	-3.9626	-2.88789	-2.17164	-2.15551
Nb-Ta-C-O-O	-2.26931	-2.76314	-2.21741	-2.1964
Nb-Ta-N-O-O	-3.6411	-3.01412	-1.8597	-2.12553
Nb-W-C-O-O	-2.94163	-3.43959	-2.17803	-2.17546
Nb-W-N-O-O	-4.82487	-3.00048	-2.07795	-2.09514
Sc-Cr-C-O-O	-2.36614	-4.69496	-3.37929	-2.70692
Sc-Cr-N-O-O	-4.55597	-4.54262	-3.2115	-2.70569
Sc-Hf-C-O-O	-1.85874	-3.3582	-1.95222	-2.8413
Sc-Hf-N-O-O	-1.95543	-3.47397	-0.99887	-2.9789
Sc-Mo-C-O-O	-2.91703	-3.31297	-2.81547	-2.75465
Sc-Mo-N-O-O	-4.98161	-3.28657	-2.68327	-2.82952
Sc-Nb-C-O-O	-2.14729	-3.07734	-2.81605	-2.76507
Sc-Nb-N-O-O	-4.02562	-2.90954	-2.79307	-2.86135
Sc-Sc-C-O-O	-1.86556	-3.27329	-2.89436	-2.75779
Sc-Sc-N-O-O	-2.34807	-3.45053	-2.08406	-2.91413
Sc-Ta-C-O-O	-2.19497	-3.18859	-2.77357	-2.82806
Sc-Ta-N-O-O	-3.82821	-2.95525	-2.24415	-2.85248
Sc-Ti-C-O-O	-1.94747	-2.82495	-3.43654	-2.82243

Sc-Ti-N-O-O	-3.94442	-3.46519	-2.85867	-2.7832
Sc-V-C-O-O	-2.13767	-3.96268	-3.3181	-2.70744
Sc-V-N-O-O	-4.11214	-3.95094	-2.90345	-2.70619
Sc-W-C-O-O	-2.87131	-3.33346	-2.8756	-2.7134
Sc-W-N-O-O	-4.97519	-3.38482	-2.6153	-2.62412
Sc-Y-C-O-O	-1.70641	-3.42451	-2.11012	-2.81372
Sc-Y-N-O-O	-1.88724	-3.5084	-1.30669	-2.95484
Sc-Zr-C-O-O	-1.65798	-3.35408	-1.94673	-2.80608
Sc-Zr-N-O-O	-1.39046	-3.54934	-1.0479	-3.16636
Ta-Cr-C-O-O	-2.77188	-3.20753	-2.16725	-1.87917
Ta-Cr-N-O-O	-5.27843	-3.15084	-2.17316	-1.80398
Ta-Mo-C-O-O	-3.26756	-3.10226	-2.07163	-1.84194
Ta-Mo-N-O-O	-5.8307	-2.60734	-2.03572	-1.63249
Ta-Ta-C-O-O	-2.4761	-2.8153	-2.15488	-1.92446
Ta-Ta-N-O-O	-4.38498	-2.8698	-1.76526	-1.81727
Ta-W-C-O-O	-3.26467	-3.18348	-2.10209	-1.85533
Ta-W-N-O-O	-5.64582	-2.82212	-1.998	-1.73435
Ti-Cr-C-O-O	-2.54001	-4.51528	-2.44856	-2.30981
Ti-Cr-N-O-O	-4.32595	-4.02872	-2.54491	-2.22718
Ti-Hf-C-O-O	-2.13085	-2.88847	-1.79272	-2.31447
Ti-Hf-N-O-O	-2.4846	-3.00264	-1.15378	-2.29638
Ti-Mo-C-O-O	-3.00352	-3.40423	-2.41496	-2.2567
Ti-Mo-N-O-O	-4.86632	-3.41937	-2.47364	-2.16974
Ti-Nb-C-O-O	-2.22256	-2.98103	-2.46675	-2.3162
Ti-Nb-N-O-O	-3.88362	-3.20344	-2.58573	-2.25864
Ti-Ta-C-O-O	-2.31188	-2.93141	-2.476	-2.31471
Ti-Ta-N-O-O	-3.612	-3.15698	-2.12623	-2.27605
Ti-Ti-C-O-O	-2.30603	-2.68473	-2.28105	-2.31186
Ti-Ti-N-O-O	-3.77173	-3.11444	-2.15848	-2.2661
Ti-V-C-O-O	-2.34742	-3.57593	-2.28284	-2.31256
Ti-V-N-O-O	-3.99142	-3.70623	-2.23829	-2.23693
Ti-W-C-O-O	-2.99819	-3.34974	-2.38677	-2.25079
Ti-W-N-O-O	-4.766	-3.39668	-2.35346	-2.16648
Ti-Zr-C-O-O	-1.90931	-3.01014	-1.75336	-2.27006
Ti-Zr-N-O-O	-2.26128	-3.08064	-1.20313	-2.35985
V-Cr-C-O-O	-2.74861	-5.14347	-2.43232	-2.31316
V-Cr-N-O-O	-4.34353	-4.51303	-2.50311	-2.2326
V-Mo-C-O-O	-3.05555	-3.84346	-2.3795	-2.25356
V-Mo-N-O-O	-4.60495	-3.80006	-2.40429	-2.16221
V-Nb-C-O-O	-2.45774	-3.45115	-2.42398	-2.31634
V-Nb-N-O-O	-3.95055	-3.53466	-2.51717	-2.24488

V-Ta-C-O-O	-2.51714	-3.39886	-2.39889	-2.3163
V-Ta-N-O-O	-3.59663	-3.57767	-2.08691	-2.26562
V-V-C-O-O	-2.54084	-4.21661	-2.25016	-2.3136
V-V-N-O-O	-3.82548	-4.04918	-2.21228	-2.23014
V-W-C-O-O	-3.05382	-3.65503	-2.34172	-2.24786
V-W-N-O-O	-4.52717	-3.56435	-2.28987	-2.15156
W-W-C-O-O	-3.26725	-3.21323	-2.1291	-1.83286
W-W-N-O-O	-4.71843	-3.30095	-2.04884	-1.82717
Y-Cr-C-O-O	-3.16581	-4.27145	-3.41785	-1.85438
Y-Cr-N-O-O	-5.29814	-3.93167	-3.55216	-1.84271
Y-Hf-C-O-O	-2.698	-3.3624	-1.94909	-1.85978
Y-Hf-N-O-O	-3.3146	-3.4705	-1.18916	-1.8004
Y-Mo-C-O-O	-3.66476	-3.39986	-2.64917	-1.84477
Y-Mo-N-O-O	-5.43066	-3.63786	-2.61949	-1.86892
Y-Nb-C-O-O	-3.32769	-3.08493	-2.6796	-1.76055
Y-Nb-N-O-O	-5.37586	-3.14677	-2.75128	-1.69809
Y-Ta-C-O-O	-3.23071	-3.12702	-2.593	-1.797
Y-Ta-N-O-O	-4.89692	-3.17613	-2.18943	-1.75823
Y-Ti-C-O-O	-3.08227	-3.17116	-3.24925	-1.79709
Y-Ti-N-O-O	-4.74926	-3.2885	-2.97759	-1.85882
Y-V-C-O-O	-3.01993	-3.60457	-3.2622	-1.86722
Y-V-N-O-O	-5.03356	-3.38604	-3.12441	-1.85919
Y-W-C-O-O	-3.55109	-3.21064	-2.65717	-1.87883
Y-W-N-O-O	-5.47089	-3.25683	-2.52564	-1.85792
Y-Y-C-O-O	-2.57358	-3.44654	-2.05438	-1.86706
Y-Y-N-O-O	-3.09373	-3.5183	-1.46791	-1.89323
Y-Zr-C-O-O	-2.40293	-3.39316	-1.92793	-1.81276
Y-Zr-N-O-O	-3.25059	-3.5111	-1.26078	-1.82272
Zr-Cr-C-O-O	-2.24749	-3.68619	-2.65005	-1.9281
Zr-Cr-N-O-O	-4.61641	-3.42362	-2.57984	-1.9782
Zr-Hf-C-O-O	-1.7366	-3.31281	-1.51573	-1.71035
Zr-Hf-N-O-O	-2.04932	-3.47073	-0.86628	-1.82942
Zr-Mo-C-O-O	-2.97604	-3.01558	-2.14274	-1.91143
Zr-Mo-N-O-O	-5.49781	-3.08738	-2.13076	-1.92336
Zr-Nb-C-O-O	-1.91815	-2.98975	-2.18847	-1.81918
Zr-Nb-N-O-O	-4.23652	-2.98233	-2.18411	-1.89758
Zr-Ta-C-O-O	-1.93441	-3.02986	-2.09422	-1.85705
Zr-Ta-N-O-O	-3.95816	-2.99272	-1.80064	-1.89516
Zr-V-C-O-O	-2.02827	-3.05071	-2.41797	-1.94432
Zr-V-N-O-O	-4.11117	-3.05606	-2.24943	-1.96344
Zr-W-C-O-O	-3.04141	-2.86017	-2.0912	-1.90106

Zr-W-N-O-O	-5.81886	-2.81416	-2.0484	-1.92151
Zr-Zr-C-O-O	-1.29728	-3.31615	-1.47377	-1.59862
Zr-Zr-N-O-O	-1.91291	-3.47229	-0.98429	-1.90252
Cr-Cr-C-OCN-OCN	-4.92354	-3.64185	-3.33365	-2.94719
Cr-Cr-N-OCN-OCN	-4.65355	-3.77352	-3.32214	-2.95032
Cr-Mo-C-OCN-OCN	-3.60057	-4.07429	-3.37919	-3.18282
Cr-Mo-N-OCN-OCN	-3.55595	-4.19537	-3.36016	-3.16597
Cr-W-C-OCN-OCN	-3.60215	-4.03442	-3.41019	-3.13094
Cr-W-N-OCN-OCN	-3.45324	-4.12098	-3.35161	-3.13196
Hf-Cr-C-OCN-OCN	-3.26668	-3.73383	-3.20692	-2.87167
Hf-Cr-N-OCN-OCN	-3.2023	-3.81879	-3.21028	-2.96995
Hf-Hf-C-OCN-OCN	-3.16774	-3.65764	-3.29151	-2.83704
Hf-Hf-N-OCN-OCN	-3.11233	-3.72067	-3.3227	-2.92263
Hf-Mo-C-OCN-OCN	-3.33382	-4.15049	-3.21811	-2.87055
Hf-Mo-N-OCN-OCN	-3.14686	-4.25697	-3.21828	-2.99065
Hf-Nb-C-OCN-OCN	-3.02149	-3.63616	-3.20767	-2.8376
Hf-Nb-N-OCN-OCN	-2.95913	-3.79931	-3.21877	-2.97563
Hf-Ta-C-OCN-OCN	-3.1873	-3.7438	-3.27976	-2.84511
Hf-Ta-N-OCN-OCN	-3.12391	-3.87377	-3.25463	-2.92509
Hf-V-C-OCN-OCN	-3.17654	-3.73711	-3.20362	-2.87653
Hf-V-N-OCN-OCN	-3.16582	-3.76148	-3.21024	-2.96258
Hf-W-C-OCN-OCN	-3.16601	-4.20134	-3.25435	-2.84714
Hf-W-N-OCN-OCN	-3.12228	-4.41375	-3.24838	-2.95722
Mo-Mo-C-OCN-OCN	-3.22976	-4.00519	-3.4553	-3.17484
Mo-Mo-N-OCN-OCN	-3.17804	-4.13267	-3.41011	-3.20128
Mo-W-C-OCN-OCN	-3.1708	-3.96896	-3.46278	-3.13707
Mo-W-N-OCN-OCN	-3.17306	-4.09229	-3.39996	-3.12691
Nb-Cr-C-OCN-OCN	-3.16659	-3.66007	-3.29168	-3.1613
Nb-Cr-N-OCN-OCN	-3.40322	-3.77394	-3.25781	-3.18235
Nb-Mo-C-OCN-OCN	-3.27266	-4.01543	-3.31111	-3.20557
Nb-Mo-N-OCN-OCN	-3.16922	-4.16482	-3.29629	-3.27185
Nb-Nb-C-OCN-OCN	-3.05036	-3.66149	-3.30582	-3.13665
Nb-Nb-N-OCN-OCN	-2.97242	-3.78696	-3.28937	-3.24894
Nb-Ta-C-OCN-OCN	-3.23658	-3.7808	-3.376	-3.16107
Nb-Ta-N-OCN-OCN	-3.15931	-3.77981	-3.29792	-3.17765
Nb-W-C-OCN-OCN	-3.17309	-3.98846	-3.34266	-3.16814
Nb-W-N-OCN-OCN	-3.27857	-4.11056	-3.33011	-3.1931
Sc-Cr-C-OCN-OCN	-3.63622	-3.79273	-3.25328	-3.02256
Sc-Cr-N-OCN-OCN	-3.29547	-3.81217	-3.2471	-2.97636
Sc-Hf-C-OCN-OCN	-3.26718	-3.75123	-3.32249	-2.95992
Sc-Hf-N-OCN-OCN	-3.2388	-3.77378	-3.35159	-3.06433

Sc-Mo-C-OCN-OCN	-3.6172	-4.25309	-3.26727	-3.09511
Sc-Mo-N-OCN-OCN	-3.32254	-4.18896	-3.27393	-3.0765
Sc-Nb-C-OCN-OCN	-3.17517	-3.75685	-3.27008	-2.91342
Sc-Nb-N-OCN-OCN	-2.98478	-3.74695	-3.26762	-2.99709
Sc-Sc-C-OCN-OCN	-3.34003	-3.81601	-3.25596	-2.94442
Sc-Sc-N-OCN-OCN	-3.30102	-3.83873	-3.25576	-3.07403
Sc-Ta-C-OCN-OCN	-3.34931	-3.83446	-3.32523	-2.9677
Sc-Ta-N-OCN-OCN	-3.26825	-3.82858	-3.31795	-3.04665
Sc-Ti-C-OCN-OCN	-3.41285	-3.82316	-3.25227	-2.99268
Sc-Ti-N-OCN-OCN	-3.18997	-3.76387	-3.2509	-2.98192
Sc-V-C-OCN-OCN	-3.28537	-3.83195	-3.25625	-3.00456
Sc-V-N-OCN-OCN	-3.14812	-3.76233	-3.24963	-2.97425
Sc-W-C-OCN-OCN	-3.43878	-4.21909	-3.29951	-3.09315
Sc-W-N-OCN-OCN	-3.36373	-4.22749	-3.28528	-3.06466
Sc-Y-C-OCN-OCN	-3.18664	-4.22228	-3.24177	-2.92882
Sc-Y-N-OCN-OCN	-3.20411	-4.28009	-3.2504	-3.04465
Sc-Zr-C-OCN-OCN	-3.26787	-3.76535	-3.2509	-2.92879
Sc-Zr-N-OCN-OCN	-3.25038	-3.7893	-3.24811	-3.05776
Ta-Cr-C-OCN-OCN	-3.16336	-3.73328	-3.13129	-2.90679
Ta-Cr-N-OCN-OCN	-3.26545	-3.77597	-3.11486	-3.43783
Ta-Mo-C-OCN-OCN	-3.23437	-4.11737	-3.15412	-2.87029
Ta-Mo-N-OCN-OCN	-3.08198	-4.12876	-3.12011	-3.39151
Ta-Ta-C-OCN-OCN	-3.20348	-3.7595	-3.12516	-2.88838
Ta-Ta-N-OCN-OCN	-3.11728	-3.83253	-2.93482	-3.26866
Ta-W-C-OCN-OCN	-3.13816	-4.12748	-3.13662	-2.84495
Ta-W-N-OCN-OCN	-3.1058	-4.29133	-3.05765	-3.28006
Ti-Cr-C-OCN-OCN	-3.88688	-3.80305	-3.2916	-3.1308
Ti-Cr-N-OCN-OCN	-3.65476	-3.7564	-3.33372	-3.04503
Ti-Hf-C-OCN-OCN	-3.24848	-3.70466	-3.35412	-3.08358
Ti-Hf-N-OCN-OCN	-3.19727	-3.70767	-3.35824	-3.03681
Ti-Mo-C-OCN-OCN	-3.55681	-4.33978	-3.34498	-3.2168
Ti-Mo-N-OCN-OCN	-3.3136	-4.31175	-3.31505	-3.11732
Ti-Nb-C-OCN-OCN	-3.03264	-3.80703	-3.31459	-3.12763
Ti-Nb-N-OCN-OCN	-3.10567	-3.72133	-3.34612	-3.04156
Ti-Ta-C-OCN-OCN	-3.30615	-3.87731	-3.35261	-3.11141
Ti-Ta-N-OCN-OCN	-3.25457	-3.82778	-3.34046	-3.0587
Ti-Ti-C-OCN-OCN	-3.5183	-3.83687	-3.30633	-3.16004
Ti-Ti-N-OCN-OCN	-3.3772	-3.72428	-3.32807	-3.04638
Ti-V-C-OCN-OCN	-4.21534	-3.78929	-3.28922	-3.06069
Ti-V-N-OCN-OCN	-3.46185	-3.70671	-3.33443	-3.0186
Ti-W-C-OCN-OCN	-3.62003	-4.29238	-3.35258	-3.17205

Ti-W-N-OCN-OCN	-3.21245	-4.2812	-3.31914	-3.09185
Ti-Zr-C-OCN-OCN	-3.24164	-3.71598	-3.28596	-3.06328
Ti-Zr-N-OCN-OCN	-3.22668	-3.75637	-3.2663	-3.05388
V-Cr-C-OCN-OCN	-4.93222	-3.76543	-3.33388	-3.0237
V-Cr-N-OCN-OCN	-4.16531	-3.71986	-3.33986	-3.06731
V-Mo-C-OCN-OCN	-3.55043	-4.2967	-3.37468	-3.20773
V-Mo-N-OCN-OCN	-3.54935	-4.31729	-3.36242	-3.18508
V-Nb-C-OCN-OCN	-3.24844	-3.79498	-3.38367	-3.12128
V-Nb-N-OCN-OCN	-3.30817	-3.7085	-3.37052	-3.15573
V-Ta-C-OCN-OCN	-3.49469	-3.92305	-3.42953	-3.13694
V-Ta-N-OCN-OCN	-3.44081	-3.78362	-3.37369	-3.11735
V-V-C-OCN-OCN	-4.44728	-3.7462	-3.3251	-2.97603
V-V-N-OCN-OCN	-3.84627	-3.67124	-3.33834	-3.04186
V-W-C-OCN-OCN	-3.51725	-4.29843	-3.40298	-3.21137
V-W-N-OCN-OCN	-3.38884	-4.30541	-3.37301	-3.17288
W-W-C-OCN-OCN	-3.17318	-4.11171	-3.57452	-2.87769
W-W-N-OCN-OCN	-3.14525	-4.20278	-3.45201	-3.09155
Y-Cr-C-OCN-OCN	-3.37148	-3.74705	-3.22776	-3.11398
Y-Cr-N-OCN-OCN	-3.38742	-3.81579	-3.22409	-3.04882
Y-Hf-C-OCN-OCN	-3.26009	-3.74388	-3.30113	-3.08471
Y-Hf-N-OCN-OCN	-3.22104	-3.76709	-3.33336	-3.0467
Y-Mo-C-OCN-OCN	-3.48482	-4.13115	-3.24441	-3.19292
Y-Mo-N-OCN-OCN	-3.36398	-4.20498	-3.24459	-3.10804
Y-Nb-C-OCN-OCN	-3.10248	-3.72151	-3.24146	-3.11313
Y-Nb-N-OCN-OCN	-3.04309	-3.78849	-3.23894	-3.04968
Y-Ta-C-OCN-OCN	-3.31017	-3.8362	-3.3032	-3.1061
Y-Ta-N-OCN-OCN	-3.2337	-3.80388	-3.28648	-3.06365
Y-Ti-C-OCN-OCN	-3.28034	-3.7383	-3.23084	-3.11665
Y-Ti-N-OCN-OCN	-3.27811	-3.77869	-3.22857	-3.04521
Y-V-C-OCN-OCN	-3.3641	-3.75847	-3.22817	-3.11386
Y-V-N-OCN-OCN	-3.25219	-3.76699	-3.22261	-3.04769
Y-W-C-OCN-OCN	-3.31062	-4.15521	-3.28198	-3.14463
Y-W-N-OCN-OCN	-3.24843	-4.20324	-3.27544	-3.09375
Y-Y-C-OCN-OCN	-3.20371	-4.23191	-3.2666	-3.06752
Y-Y-N-OCN-OCN	-3.17375	-4.26309	-3.28915	-3.02162
Y-Zr-C-OCN-OCN	-3.24581	-3.79399	-3.22794	-3.05425
Y-Zr-N-OCN-OCN	-3.21958	-3.79038	-3.21518	-3.02149
Zr-Cr-C-OCN-OCN	-3.40788	-3.775	-3.22598	-3.09577
Zr-Cr-N-OCN-OCN	-3.35694	-3.78066	-3.225	-3.07092
Zr-Hf-C-OCN-OCN	-3.19756	-3.68772	-3.30441	-3.10871
Zr-Hf-N-OCN-OCN	-3.15034	-3.70845	-3.3306	-3.03558

Zr-Mo-C-OCN-OCN	-3.47515	-4.1485	-3.24438	-3.22596
Zr-Mo-N-OCN-OCN	-3.36282	-4.2468	-3.252	-3.17954
Zr-Nb-C-OCN-OCN	-3.04823	-3.6789	-3.2386	-3.12564
Zr-Nb-N-OCN-OCN	-3.00252	-3.76358	-3.23738	-3.09147
Zr-Ta-C-OCN-OCN	-3.24325	-3.76334	-3.30504	-3.11376
Zr-Ta-N-OCN-OCN	-3.21048	-3.76684	-3.28021	-3.06405
Zr-V-C-OCN-OCN	-3.24905	-3.7536	-3.22638	-3.12441
Zr-V-N-OCN-OCN	-3.21686	-3.73211	-3.22041	-3.05715
Zr-W-C-OCN-OCN	-3.27901	-4.14846	-3.28193	-3.16637
Zr-W-N-OCN-OCN	-3.21856	-4.16792	-3.28102	-3.1192
Zr-Zr-C-OCN-OCN	-3.18851	-3.71267	-3.22632	-3.07892
Zr-Zr-N-OCN-OCN	-3.16566	-3.74516	-3.20279	-3.05751
Cr-Cr-C-PO-PO	-3.78863	-4.3964	-4.01216	-3.96996
Cr-Cr-N-PO-PO	-4.07715	-4.34215	-4.06194	-3.97772
Cr-Mo-C-PO-PO	-3.82183	-4.39502	-4.04329	-3.97468
Cr-Mo-N-PO-PO	-4.17521	-4.36037	-4.04678	-3.98178
Cr-W-C-PO-PO	-3.83438	-4.42178	-4.0455	-3.89124
Cr-W-N-PO-PO	-4.1541	-4.39609	-4.02174	-3.89046
Hf-Cr-C-PO-PO	-4.33259	-4.2025	-4.02273	-3.75463
Hf-Cr-N-PO-PO	-5.17486	-4.22784	-3.88197	-3.92648
Hf-Hf-C-PO-PO	-5.0015	-4.24718	-4.2037	-2.96271
Hf-Hf-N-PO-PO	-4.8441	-4.5082	-3.93581	-3.29662
Hf-Mo-C-PO-PO	-4.5401	-4.24566	-4.04313	-3.38112
Hf-Mo-N-PO-PO	-5.27295	-4.34541	-3.85856	-3.53969
Hf-Nb-C-PO-PO	-4.72003	-4.21422	-4.16896	-3.29413
Hf-Nb-N-PO-PO	-5.38124	-4.39333	-3.89082	-3.48662
Hf-Ta-C-PO-PO	-4.65674	-4.3294	-4.16477	-3.28572
Hf-Ta-N-PO-PO	-5.23188	-4.61265	-3.84225	-3.49393
Hf-V-C-PO-PO	-4.30162	-4.22853	-4.04613	-3.69403
Hf-V-N-PO-PO	-5.25801	-4.28811	-3.84969	-3.88819
Hf-W-C-PO-PO	-4.5012	-4.29196	-4.06075	-3.27095
Hf-W-N-PO-PO	-5.24249	-4.41428	-3.86258	-3.40823
Mo-Mo-C-PO-PO	-3.71391	-4.34844	-4.05427	-3.90845
Mo-Mo-N-PO-PO	-4.17347	-4.33347	-4.03421	-3.95325
Mo-W-C-PO-PO	-3.70149	-4.35136	-4.07482	-3.75471
Mo-W-N-PO-PO	-4.18238	-4.31728	-4.02719	-3.8384
Nb-Cr-C-PO-PO	-3.72096	-4.33298	-4.0142	-4.01436
Nb-Cr-N-PO-PO	-3.91839	-4.32332	-3.95743	-4.00772
Nb-Mo-C-PO-PO	-3.71406	-4.32993	-4.05652	-3.79247
Nb-Mo-N-PO-PO	-4.22479	-4.36009	-3.96514	-3.67931
Nb-Nb-C-PO-PO	-3.8571	-4.32966	-4.16891	-3.61376

Nb-Nb-N-PO-PO	-4.2404	-4.40488	-3.99304	-3.6042
Nb-Ta-C-PO-PO	-3.86052	-4.36891	-4.15774	-3.62661
Nb-Ta-N-PO-PO	-4.10564	-4.51477	-3.9583	-3.56325
Nb-W-C-PO-PO	-3.77209	-4.32389	-4.06351	-3.57491
Nb-W-N-PO-PO	-4.22676	-4.37146	-3.95552	-3.55243
Sc-Cr-C-PO-PO	-4.56823	-4.45523	-3.97661	-3.76188
Sc-Cr-N-PO-PO	-5.20235	-4.42209	-3.84184	-3.79403
Sc-Hf-C-PO-PO	-5.16979	-4.57681	-4.34517	-3.42415
Sc-Hf-N-PO-PO	-5.29347	-4.79339	-3.94662	-3.66504
Sc-Mo-C-PO-PO	-4.62616	-4.49297	-4.02832	-3.71276
Sc-Mo-N-PO-PO	-5.28408	-4.53633	-3.82206	-3.77014
Sc-Nb-C-PO-PO	-4.89222	-4.45615	-4.17399	-3.58071
Sc-Nb-N-PO-PO	-5.3556	-4.57565	-3.85031	-3.77046
Sc-Sc-C-PO-PO	-5.0977	-4.49503	-4.18976	-3.47471
Sc-Sc-N-PO-PO	-5.49496	-4.63914	-3.82509	-3.65064
Sc-Ta-C-PO-PO	-4.88132	-4.58388	-4.17082	-3.55638
Sc-Ta-N-PO-PO	-5.23764	-4.81288	-3.79897	-3.75281
Sc-Ti-C-PO-PO	-4.87963	-4.41147	-3.98949	-3.56185
Sc-Ti-N-PO-PO	-5.29012	-4.40228	-3.5865	-3.76177
Sc-V-C-PO-PO	-4.58351	-4.44796	-4.00133	-3.73962
Sc-V-N-PO-PO	-5.20476	-4.44365	-3.80722	-3.78811
Sc-W-C-PO-PO	-4.64706	-4.53797	-4.03869	-3.5956
Sc-W-N-PO-PO	-5.16331	-4.60183	-3.80946	-3.68475
Sc-Y-C-PO-PO	-5.03123	-4.57365	-4.18589	-3.38093
Sc-Y-N-PO-PO	-5.00101	-4.72245	-3.8426	-3.4818
Sc-Zr-C-PO-PO	-5.05366	-4.55216	-4.40352	-3.44772
Sc-Zr-N-PO-PO	-5.84623	-4.79179	-4.01927	-3.69117
Ta-Cr-C-PO-PO	-3.87215	-4.16031	-4.07378	-3.80844
Ta-Cr-N-PO-PO	-4.71177	-4.14422	-3.93974	-4.00856
Ta-Mo-C-PO-PO	-3.71248	-4.1967	-4.09384	-3.74707
Ta-Mo-N-PO-PO	-4.64899	-4.24187	-3.90555	-4.02503
Ta-Ta-C-PO-PO	-3.88909	-4.26202	-4.14567	-3.68449
Ta-Ta-N-PO-PO	-4.54248	-4.41015	-3.89401	-3.64717
Ta-W-C-PO-PO	-3.77919	-4.2152	-4.10562	-3.58394
Ta-W-N-PO-PO	-4.72026	-4.2665	-3.93635	-3.64292
Ti-Cr-C-PO-PO	-3.82191	-4.42126	-4.00328	-4.01287
Ti-Cr-N-PO-PO	-4.35133	-4.40158	-3.94731	-4.00107
Ti-Hf-C-PO-PO	-4.08521	-4.62261	-4.16683	-3.83938
Ti-Hf-N-PO-PO	-3.74885	-4.75502	-3.91312	-3.97344
Ti-Mo-C-PO-PO	-3.81295	-4.49194	-4.0279	-4.01376
Ti-Mo-N-PO-PO	-4.42867	-4.49501	-3.94406	-4.00984

Ti-Nb-C-PO-PO	-3.87178	-4.48984	-4.14751	-3.98078
Ti-Nb-N-PO-PO	-4.31091	-4.56282	-3.94291	-3.96659
Ti-Ta-C-PO-PO	-3.86385	-4.59502	-4.14624	-3.9714
Ti-Ta-N-PO-PO	-4.18528	-4.75709	-3.9001	-3.98384
Ti-Ti-C-PO-PO	-3.80477	-4.45336	-3.97921	-4.01668
Ti-Ti-N-PO-PO	-4.34539	-4.51386	-3.76989	-4.00778
Ti-V-C-PO-PO	-3.77435	-4.47345	-4.01995	-4.014
Ti-V-N-PO-PO	-4.23624	-4.48421	-3.91379	-3.99882
Ti-W-C-PO-PO	-3.8285	-4.54218	-4.03202	-3.91409
Ti-W-N-PO-PO	-4.40505	-4.54659	-3.929	-3.91183
Ti-Zr-C-PO-PO	-4.15024	-4.61944	-4.19425	-3.74667
Ti-Zr-N-PO-PO	-3.77191	-4.84382	-3.94091	-3.95149
V-Cr-C-PO-PO	-3.86598	-4.19314	-4.04472	-4.02264
V-Cr-N-PO-PO	-4.21943	-4.16126	-4.1003	-4.0372
V-Mo-C-PO-PO	-3.85928	-4.25616	-4.06992	-4.0213
V-Mo-N-PO-PO	-4.28533	-4.23045	-4.07444	-4.03005
V-Nb-C-PO-PO	-3.92671	-4.22107	-4.18924	-4.01421
V-Nb-N-PO-PO	-4.17791	-4.256	-4.08506	-4.02759
V-Ta-C-PO-PO	-3.92918	-4.32647	-4.18173	-3.99348
V-Ta-N-PO-PO	-4.02153	-4.42201	-4.03809	-4.01906
V-V-C-PO-PO	-3.82434	-4.20021	-4.06218	-4.01756
V-V-N-PO-PO	-4.14451	-4.19135	-4.06564	-4.03585
V-W-C-PO-PO	-3.86961	-4.30395	-4.07171	-3.9301
V-W-N-PO-PO	-4.22706	-4.26569	-4.04923	-3.9304
W-W-C-PO-PO	-3.78537	-4.2566	-4.10879	-3.79102
W-W-N-PO-PO	-4.31826	-4.22739	-4.06657	-3.77856
Y-Cr-C-PO-PO	-5.39307	-4.66206	-3.98952	-3.52452
Y-Cr-N-PO-PO	-6.29139	-4.60347	-3.85658	-3.60136
Y-Hf-C-PO-PO	-5.37176	-4.88183	-4.22694	-3.28734
Y-Hf-N-PO-PO	-5.66771	-5.12123	-3.90637	-3.39097
Y-Mo-C-PO-PO	-5.44586	-4.81157	-4.02838	-3.43075
Y-Mo-N-PO-PO	-6.17241	-4.82827	-3.81763	-3.52544
Y-Nb-C-PO-PO	-5.58151	-4.78211	-4.16647	-3.39435
Y-Nb-N-PO-PO	-6.10111	-4.90432	-3.83683	-3.49772
Y-Ta-C-PO-PO	-5.51167	-5.07038	-4.16401	-3.38101
Y-Ta-N-PO-PO	-6.16781	-5.49719	-3.78303	-3.53152
Y-Ti-C-PO-PO	-5.67969	-4.5976	-4.06657	-3.3547
Y-Ti-N-PO-PO	-6.82212	-4.5233	-3.72417	-3.53749
Y-V-C-PO-PO	-5.5548	-4.70433	-4.01236	-3.50565
Y-V-N-PO-PO	-6.49607	-4.66403	-3.82988	-3.55899
Y-W-C-PO-PO	-5.38805	-4.97359	-4.0273	-3.32691

Y-W-N-PO-PO	-6.10212	-5.04592	-3.80373	-3.41477
Y-Y-C-PO-PO	-5.40096	-4.7707	-4.10277	-3.27805
Y-Y-N-PO-PO	-5.49655	-4.94671	-3.83947	-3.32694
Y-Zr-C-PO-PO	-5.53243	-4.7945	-4.24891	-3.30001
Y-Zr-N-PO-PO	-5.614	-5.00423	-3.96168	-3.38447
Zr-Cr-C-PO-PO	-4.63755	-4.17437	-4.02804	-3.53698
Zr-Cr-N-PO-PO	-5.3983	-4.22297	-3.8822	-3.58472
Zr-Hf-C-PO-PO	-5.19325	-4.20643	-4.24058	-2.84193
Zr-Hf-N-PO-PO	-5.15939	-4.46395	-3.95278	-3.03555
Zr-Mo-C-PO-PO	-4.78001	-4.19676	-4.0739	-3.13046
Zr-Mo-N-PO-PO	-5.60639	-4.29181	-3.85502	-3.30776
Zr-Nb-C-PO-PO	-4.98168	-4.15702	-4.20774	-3.05576
Zr-Nb-N-PO-PO	-5.6457	-4.33146	-3.89738	-3.17916
Zr-Ta-C-PO-PO	-4.96288	-4.25157	-4.18897	-3.05588
Zr-Ta-N-PO-PO	-5.53006	-4.51825	-3.8545	-3.11037
Zr-V-C-PO-PO	-4.66587	-4.18797	-4.05702	-3.50237
Zr-V-N-PO-PO	-5.44311	-4.24423	-3.86445	-3.57532
Zr-W-C-PO-PO	-4.77174	-4.25103	-4.08134	-3.04179
Zr-W-N-PO-PO	-5.52794	-4.3573	-3.85504	-3.15538
Zr-Zr-C-PO-PO	-5.29487	-4.11589	-4.31397	-2.79435
Zr-Zr-N-PO-PO	-5.0998	-4.42528	-3.97978	-3.02503
Cr-Cr-C-SCN-SCN	-3.59428	-3.53057	-3.28302	-2.8059
Cr-Cr-N-SCN-SCN	-3.50495	-3.67249	-3.23701	-2.95186
Cr-Mo-C-SCN-SCN	-3.12841	-3.34145	-3.24551	-2.56657
Cr-Mo-N-SCN-SCN	-3.24307	-3.54503	-3.26915	-2.75928
Cr-W-C-SCN-SCN	-3.09218	-3.34661	-3.29125	-2.54847
Cr-W-N-SCN-SCN	-3.15499	-3.40246	-3.327	-2.72182
Hf-Cr-C-SCN-SCN	-3.12922	-3.49468	-3.22016	-2.78392
Hf-Cr-N-SCN-SCN	-3.04553	-4.02537	-3.20137	-3.04065
Hf-Hf-C-SCN-SCN	-3.13425	-3.65318	-3.37799	-2.80226
Hf-Hf-N-SCN-SCN	-3.05402	-3.58218	-3.51855	-3.1008
Hf-Mo-C-SCN-SCN	-3.19431	-3.37674	-3.20959	-2.57427
Hf-Mo-N-SCN-SCN	-3.06667	-3.84261	-3.28822	-2.78682
Hf-Nb-C-SCN-SCN	-2.90212	-3.66861	-3.24329	-2.77278
Hf-Nb-N-SCN-SCN	-2.73917	-5.28331	-3.21524	-3.05578
Hf-Ta-C-SCN-SCN	-3.12902	-3.38081	-3.27859	-2.70277
Hf-Ta-N-SCN-SCN	-3.04365	-4.02297	-3.28356	-3.01532
Hf-V-C-SCN-SCN	-3.14007	-3.5211	-3.21795	-2.78133
Hf-V-N-SCN-SCN	-3.0659	-3.90888	-3.22731	-3.04977
Hf-W-C-SCN-SCN	-3.06071	-3.32722	-3.20583	-2.49614
Hf-W-N-SCN-SCN	-3.00953	-3.61832	-3.27586	-2.72904

Mo-Mo-C-SCN-SCN	-3.08438	-3.34849	-3.32513	-2.58656
Mo-Mo-N-SCN-SCN	-3.05046	-3.53281	-3.34028	-2.77893
Mo-W-C-SCN-SCN	-3.11316	-3.28007	-3.36861	-2.5538
Mo-W-N-SCN-SCN	-3.11128	-3.36885	-3.38123	-2.74716
Nb-Cr-C-SCN-SCN	-3.15526	-3.46478	-3.25703	-2.76209
Nb-Cr-N-SCN-SCN	-3.05744	-3.81594	-3.24423	-3.10866
Nb-Mo-C-SCN-SCN	-3.13883	-3.26449	-3.32103	-2.57208
Nb-Mo-N-SCN-SCN	-3.02169	-4.38137	-3.32046	-2.95611
Nb-Nb-C-SCN-SCN	-2.91355	-3.50378	-3.28835	-2.73004
Nb-Nb-N-SCN-SCN	-2.83453	-3.906	-3.38663	-3.09788
Nb-Ta-C-SCN-SCN	-3.13211	-3.38915	-3.31455	-2.68361
Nb-Ta-N-SCN-SCN	-3.06848	-3.50113	-3.41734	-3.02395
Nb-W-C-SCN-SCN	-3.04769	-3.20659	-3.3356	-2.57509
Nb-W-N-SCN-SCN	-3.11139	-3.32367	-3.33006	-2.9051
Sc-Cr-C-SCN-SCN	-3.30532	-3.65403	-3.26512	-3.04523
Sc-Cr-N-SCN-SCN	-3.24998	-3.81955	-3.21758	-3.09668
Sc-Hf-C-SCN-SCN	-3.24889	-3.71123	-3.35458	-3.12091
Sc-Hf-N-SCN-SCN	-3.18739	-3.67227	-3.40804	-3.12923
Sc-Mo-C-SCN-SCN	-3.30575	-3.52781	-3.2527	-2.6679
Sc-Mo-N-SCN-SCN	-3.21596	-3.76332	-3.25024	-2.8091
Sc-Nb-C-SCN-SCN	-2.99698	-3.68669	-3.27992	-3.06921
Sc-Nb-N-SCN-SCN	-2.92017	-4.36569	-3.24887	-3.06066
Sc-Sc-C-SCN-SCN	-3.22878	-4.33922	-3.32346	-3.06179
Sc-Sc-N-SCN-SCN	-3.20164	-3.91169	-3.29976	-3.10479
Sc-Ta-C-SCN-SCN	-3.23523	-3.53189	-3.29051	-3.05662
Sc-Ta-N-SCN-SCN	-3.16568	-3.79416	-3.27873	-3.06845
Sc-Ti-C-SCN-SCN	-3.27767	-3.68895	-3.26913	-3.08816
Sc-Ti-N-SCN-SCN	-3.21745	-3.76696	-3.23841	-3.0676
Sc-V-C-SCN-SCN	-3.30635	-3.73047	-3.26884	-3.05184
Sc-V-N-SCN-SCN	-3.22542	-3.78987	-3.22468	-3.05916
Sc-W-C-SCN-SCN	-3.15473	-3.50027	-3.28409	-2.59034
Sc-W-N-SCN-SCN	-3.08845	-3.71075	-3.25566	-2.76311
Sc-Y-C-SCN-SCN	-3.22255	-4.40188	-3.30027	-3.09634
Sc-Y-N-SCN-SCN	-3.19284	-4.49561	-3.34975	-3.12901
Sc-Zr-C-SCN-SCN	-3.23473	-4.02827	-3.31787	-3.05825
Sc-Zr-N-SCN-SCN	-3.18606	-4.21571	-3.3076	-3.1185
Ta-Cr-C-SCN-SCN	-3.07531	-3.53567	-2.99045	-2.65362
Ta-Cr-N-SCN-SCN	-3.01081	-3.8264	-3.00641	-3.32753
Ta-Mo-C-SCN-SCN	-3.12495	-3.51557	-2.99791	-2.64946
Ta-Mo-N-SCN-SCN	-2.99729	-4.48865	-3.02962	-3.29258
Ta-Ta-C-SCN-SCN	-3.1203	-3.26874	-3.02016	-2.48835

Ta-Ta-N-SCN-SCN	-3.04615	-3.48354	-3.11197	-3.11592
Ta-W-C-SCN-SCN	-3.04618	-3.50019	-2.94777	-2.64799
Ta-W-N-SCN-SCN	-2.99892	-3.62377	-2.95121	-3.22535
Ti-Cr-C-SCN-SCN	-3.11875	-3.57597	-3.27172	-2.79206
Ti-Cr-N-SCN-SCN	-3.06899	-3.63185	-3.23243	-2.89696
Ti-Hf-C-SCN-SCN	-3.15981	-3.55569	-3.32694	-2.8188
Ti-Hf-N-SCN-SCN	-3.10116	-3.53579	-3.38939	-2.99444
Ti-Mo-C-SCN-SCN	-3.14143	-3.42469	-3.24928	-2.59215
Ti-Mo-N-SCN-SCN	-3.04661	-3.57106	-3.25579	-2.76748
Ti-Nb-C-SCN-SCN	-2.93052	-3.58921	-3.26644	-2.79767
Ti-Nb-N-SCN-SCN	-2.83345	-3.98075	-3.25578	-2.91239
Ti-Ta-C-SCN-SCN	-3.15378	-3.43222	-3.27326	-2.75735
Ti-Ta-N-SCN-SCN	-3.06602	-3.48323	-3.29699	-2.96754
Ti-Ti-C-SCN-SCN	-3.16719	-3.57907	-3.25319	-2.80414
Ti-Ti-N-SCN-SCN	-3.09237	-3.64313	-3.22683	-2.91516
Ti-V-C-SCN-SCN	-3.17464	-3.61461	-3.26566	-2.8044
Ti-V-N-SCN-SCN	-3.11689	-3.65141	-3.2243	-2.90718
Ti-W-C-SCN-SCN	-3.05091	-3.37084	-3.2811	-2.56556
Ti-W-N-SCN-SCN	-3.01512	-3.38129	-3.31569	-2.72011
Ti-Zr-C-SCN-SCN	-3.15167	-3.74666	-3.25954	-2.77788
Ti-Zr-N-SCN-SCN	-3.10534	-3.66175	-3.27699	-2.96011
V-Cr-C-SCN-SCN	-3.55536	-3.63306	-3.27303	-2.81805
V-Cr-N-SCN-SCN	-3.44474	-3.63051	-3.23721	-2.96723
V-Mo-C-SCN-SCN	-3.0788	-3.37311	-3.24739	-2.58468
V-Mo-N-SCN-SCN	-3.08031	-3.5121	-3.24779	-2.81469
V-Nb-C-SCN-SCN	-2.97762	-3.56672	-3.27603	-2.80825
V-Nb-N-SCN-SCN	-2.90119	-3.76005	-3.28208	-3.04354
V-Ta-C-SCN-SCN	-3.20001	-3.44594	-3.28895	-2.77124
V-Ta-N-SCN-SCN	-3.12988	-3.50479	-3.30811	-2.98578
V-V-C-SCN-SCN	-3.43453	-3.66455	-3.26677	-2.8313
V-V-N-SCN-SCN	-3.3783	-3.65801	-3.22509	-2.97686
V-W-C-SCN-SCN	-3.04832	-3.36758	-3.28254	-2.56576
V-W-N-SCN-SCN	-3.12743	-3.43263	-3.31621	-2.76436
W-W-C-SCN-SCN	-3.01431	-3.49363	-3.20513	-2.65221
W-W-N-SCN-SCN	-3.02116	-3.60911	-3.14901	-3.00794
Y-Cr-C-SCN-SCN	-3.37814	-3.76964	-3.33175	-2.98964
Y-Cr-N-SCN-SCN	-3.3033	-4.07708	-3.35784	-2.97882
Y-Hf-C-SCN-SCN	-3.26943	-3.97023	-3.37053	-3.20473
Y-Hf-N-SCN-SCN	-3.21613	-3.824	-3.49021	-3.13045
Y-Mo-C-SCN-SCN	-3.38151	-3.46551	-3.30571	-2.69133
Y-Mo-N-SCN-SCN	-3.29462	-4.15822	-3.34872	-2.71082

Y-Nb-C-SCN-SCN	-3.0316	-3.71703	-3.35617	-3.0678
Y-Nb-N-SCN-SCN	-2.93654	-4.56198	-3.40806	-3.00902
Y-Ta-C-SCN-SCN	-3.27082	-3.55209	-3.34763	-3.06589
Y-Ta-N-SCN-SCN	-3.18663	-3.90768	-3.41741	-3.02406
Y-Ti-C-SCN-SCN	-3.29165	-3.69892	-3.33353	-3.08684
Y-Ti-N-SCN-SCN	-3.23023	-3.96578	-3.37699	-3.02113
Y-V-C-SCN-SCN	-3.30185	-3.70303	-3.28223	-3.03011
Y-V-N-SCN-SCN	-3.25013	-4.09155	-3.36417	-2.99794
Y-W-C-SCN-SCN	-3.21701	-3.42351	-3.32014	-2.62475
Y-W-N-SCN-SCN	-3.1821	-3.65611	-3.36287	-2.69944
Y-Y-C-SCN-SCN	-3.30226	-4.40065	-3.31513	-3.16631
Y-Y-N-SCN-SCN	-3.23371	-4.60374	-3.40012	-3.14263
Y-Zr-C-SCN-SCN	-3.25663	-4.38781	-3.33654	-3.13004
Y-Zr-N-SCN-SCN	-3.21071	-4.54646	-3.40225	-3.07183
Zr-Cr-C-SCN-SCN	-3.26226	-3.56963	-3.32372	-2.90154
Zr-Cr-N-SCN-SCN	-3.1691	-3.93514	-3.34476	-3.01765
Zr-Hf-C-SCN-SCN	-3.16273	-3.68809	-3.43987	-2.99225
Zr-Hf-N-SCN-SCN	-3.10628	-3.59354	-3.52504	-3.08243
Zr-Mo-C-SCN-SCN	-3.26777	-3.36563	-3.37835	-2.57148
Zr-Mo-N-SCN-SCN	-3.17174	-3.74475	-3.43869	-2.75608
Zr-Nb-C-SCN-SCN	-2.91481	-3.64711	-3.35943	-2.9267
Zr-Nb-N-SCN-SCN	-2.80516	-4.23991	-3.50651	-3.04353
Zr-Ta-C-SCN-SCN	-3.14958	-3.43629	-3.37252	-2.87086
Zr-Ta-N-SCN-SCN	-3.06661	-3.66757	-3.48144	-3.02451
Zr-V-C-SCN-SCN	-3.19258	-3.61292	-3.32521	-2.91752
Zr-V-N-SCN-SCN	-3.12031	-3.93667	-3.38851	-3.03127
Zr-W-C-SCN-SCN	-3.0918	-3.30024	-3.38895	-2.47568
Zr-W-N-SCN-SCN	-3.05452	-3.47516	-3.43431	-2.70147
Zr-Zr-C-SCN-SCN	-3.14068	-4.18806	-3.40206	-2.93999
Zr-Zr-N-SCN-SCN	-3.10917	-4.13989	-3.46674	-3.05554

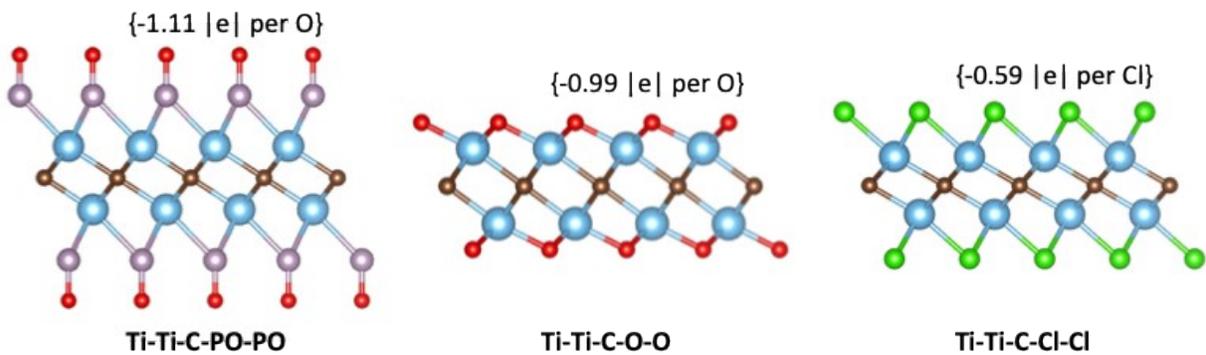


Fig. S11. Bader charges on terminal atom for representative PO-, O-, and Cl- terminating MXenes.

Table S10. Calculated ΔE_{diff} in gas phase and dimethyl sulfoxide solvent medium.

MXenes	ΔE_{diff} (Gas phase) (eV)	ΔE_{diff} (Solvent medium) (eV)
Ti-Ti-C-O-O	0.37	0.37
Cr-Cr-N-PO-PO	0.67	0.75
Cr-Mo-N-PO-PO	0.64	0.72