Electronic Supplementary Material (ESI) for Nanoscale.

High-throughput computational discovery of ternary-layered MAX phases and the prediction of their exfoliation into 2D MXenes

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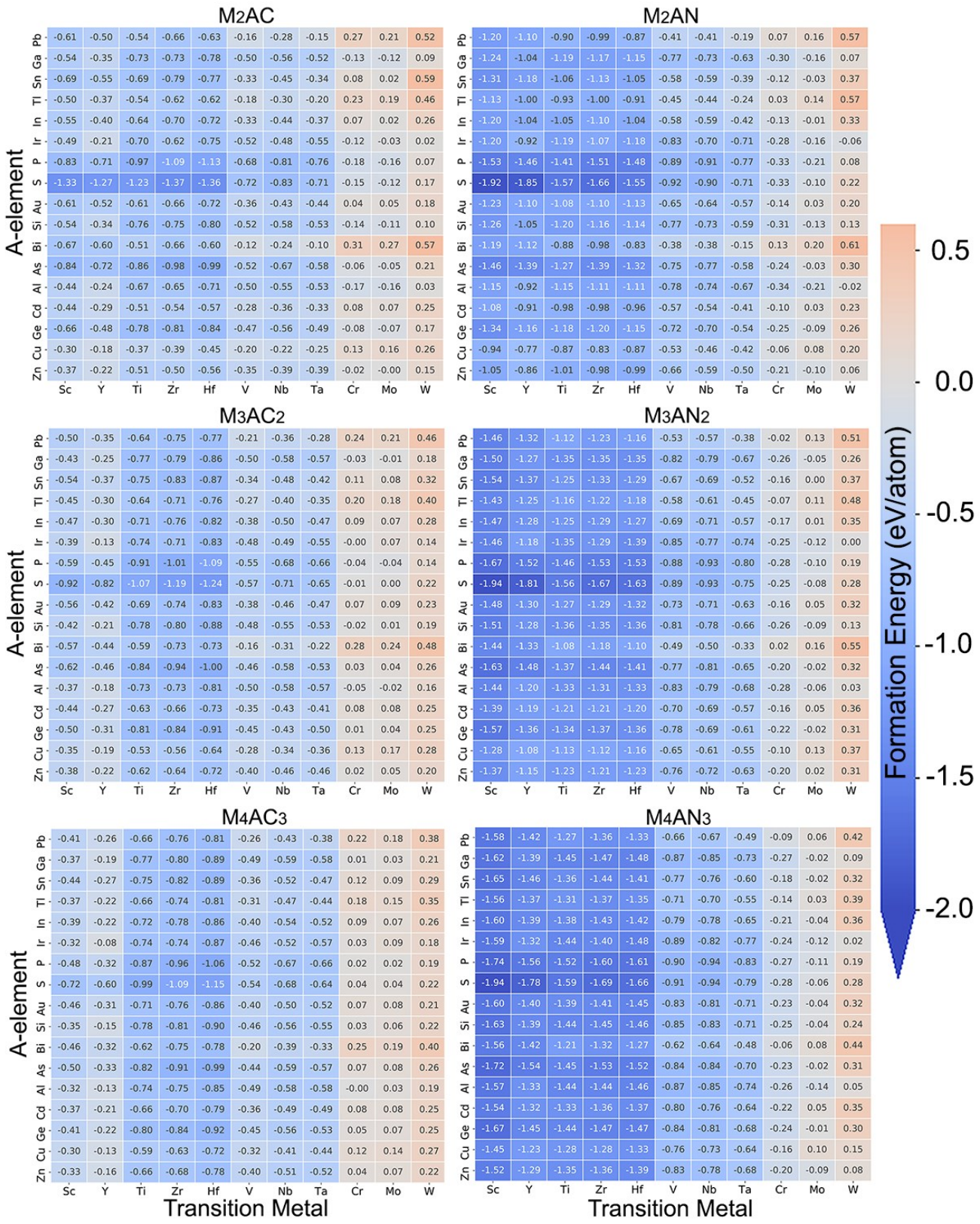

Figure S1. Heatmaps of calculated formation energy for all MAX candidates with respect to the transition metals.

Table S1
The valence electron and atomic radius (Å) values of M-, A-, and X-elements.

M-elements	Valence Electrons	Atomic Radius	A-elements	Valence Electrons	Atomic Radius	X-elements	Valence Electrons	Atomic Radius
Sc	3	1.59	Ir	2	1.32	C	4	0.75
Y	3	1.62	Cu	1	1.22	N	5	0.71
Ti	4	1.48	Au	1	1.30			
Zr	4	1.64	Zn	2	1.20			
Hf	4	1.64	Cd	2	1.40			
V	5	1.44	Al	3	1.24			
Nb	5	1.56	Ga	3	1.23			
Ta	5	1.58	In	3	1.42			
Cr	6	1.30	Tl	3	1.44			
Mo	6	1.46	Si	4	1.14			
W	6	1.30	Ge	4	1.20			
			Sn	4	1.40			
			Pb	4	1.45			
			P	5	1.09			
			As	5	1.20			
			Bi	5	1.44			
			S	6	1.04			

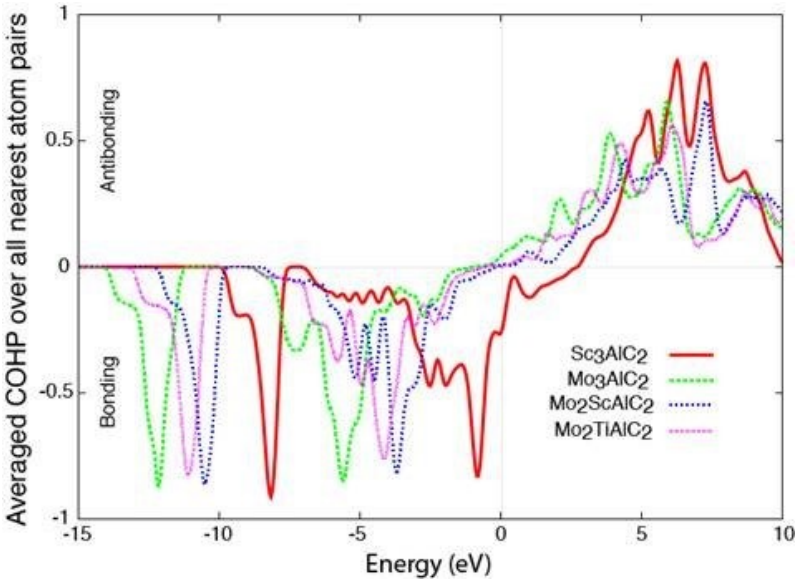

Figure S2. Averaged COHP over all nearest atom pairs. COHP stands for chemical orbital Hamilton population

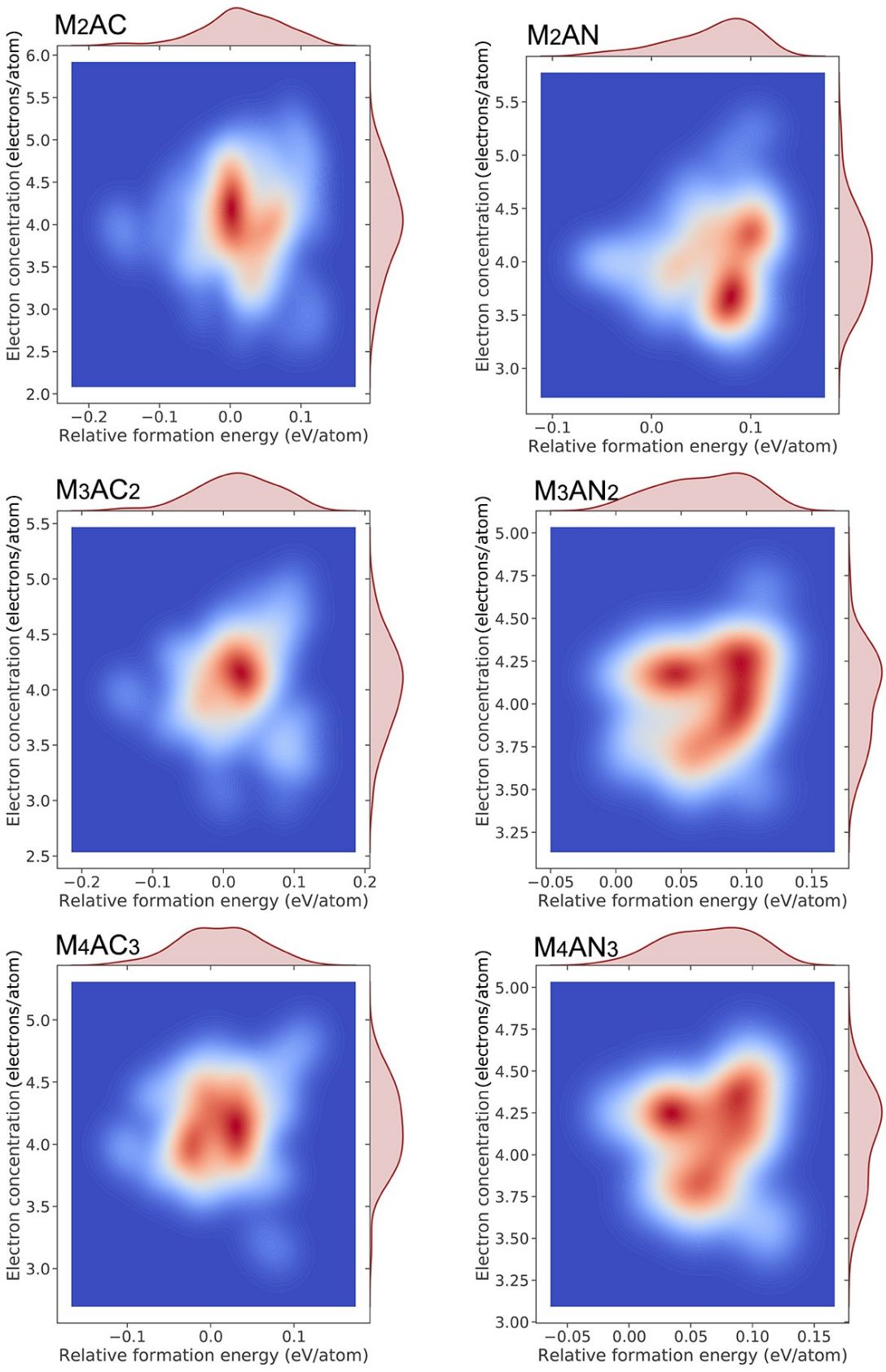

Figure S3. Calculated electron concentration (electron/atom) of the predicted MAX phases for all MAX candidates with reference to their relative formation energy.

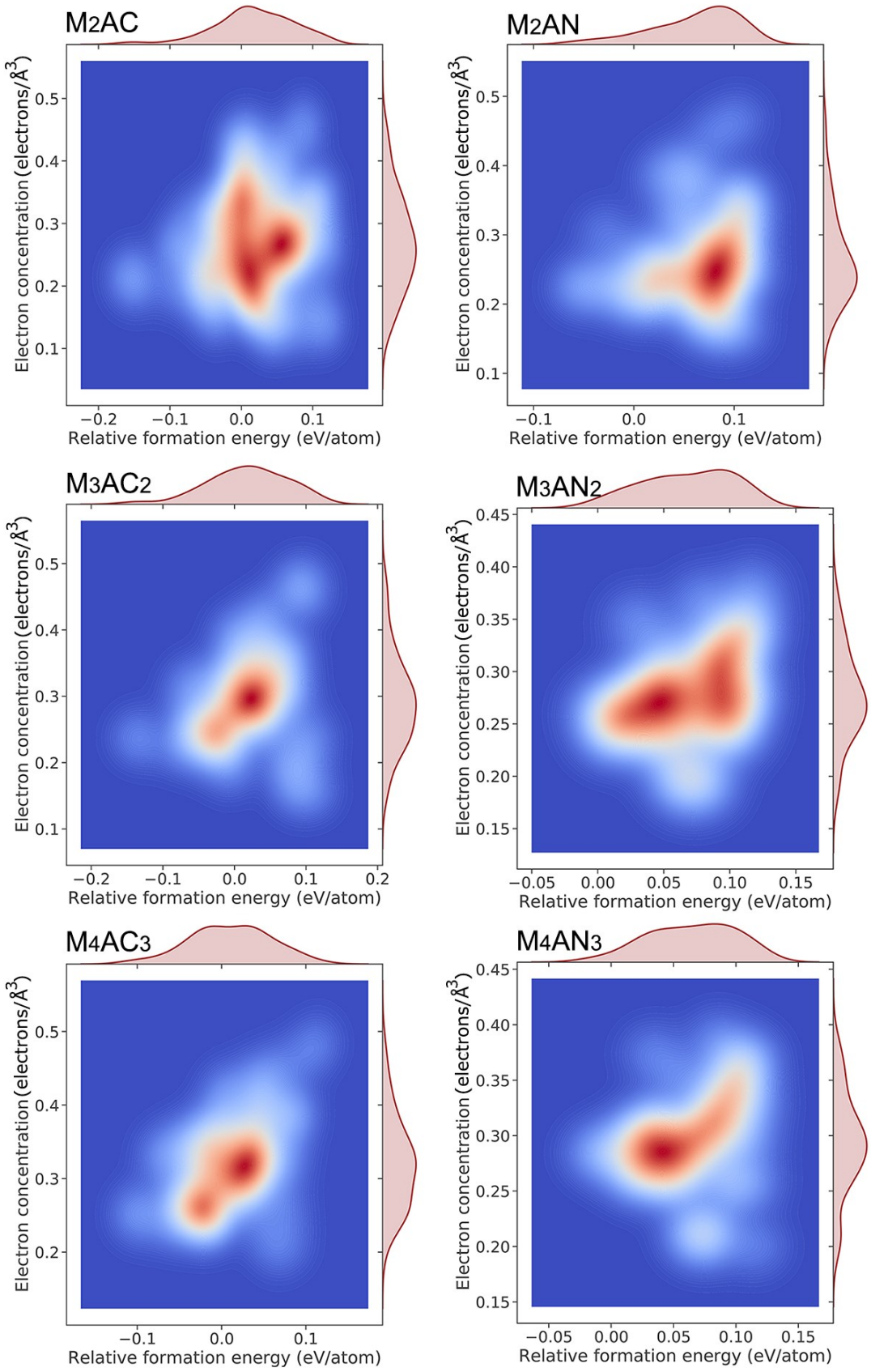

Figure S4. Calculated electron concentration (electron/Å^3) of the predicted MAX phases for all MAX candidates with reference to their relative formation energy.

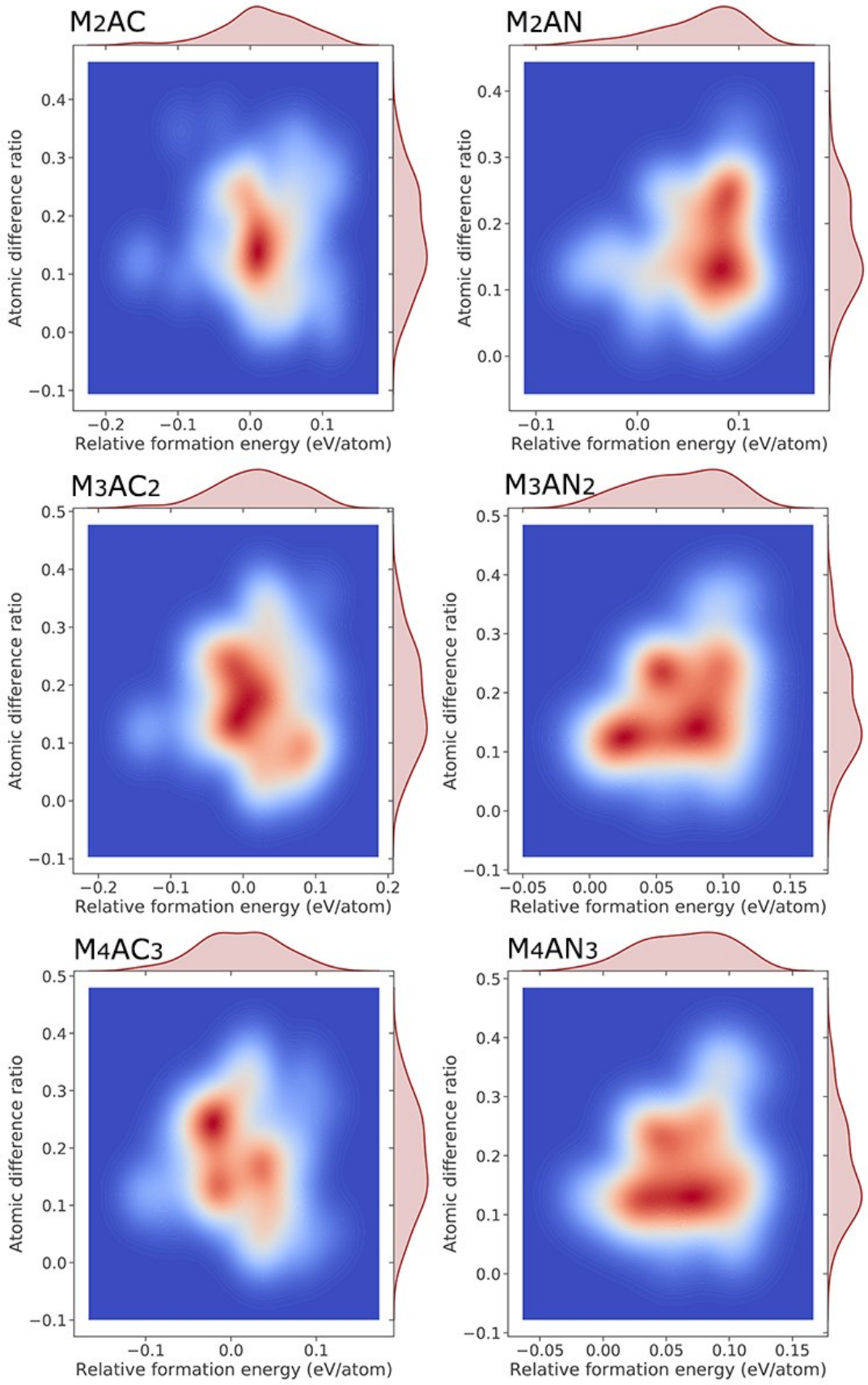

Figure S5. Calculated size factor (electron/Å^3) of the predicted MAX phases for all MAX candidates with reference to their relative formation energy.

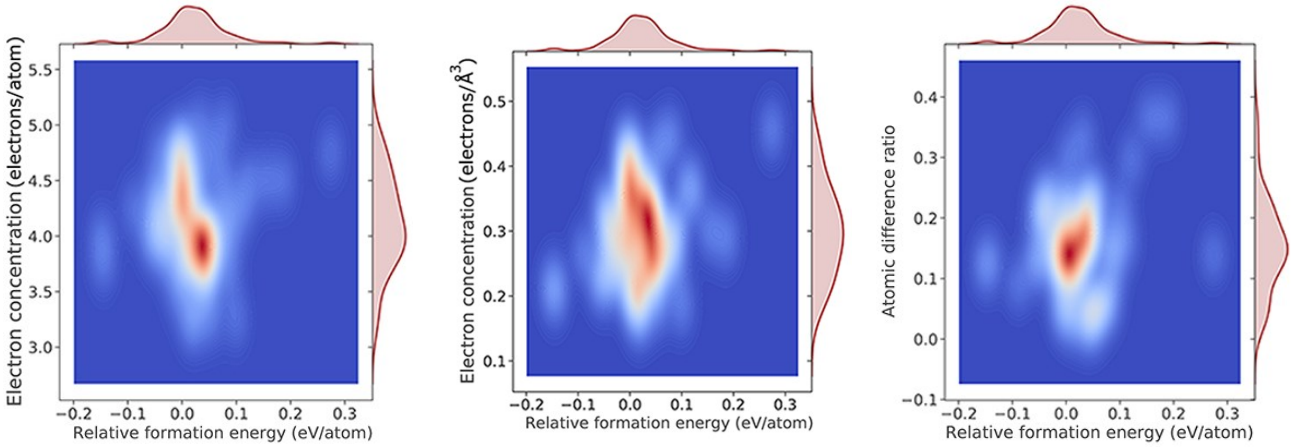

Figure S6. Calculated electron concentration and size factors of the synthesized MAX phases with reference to their relative formation energy.

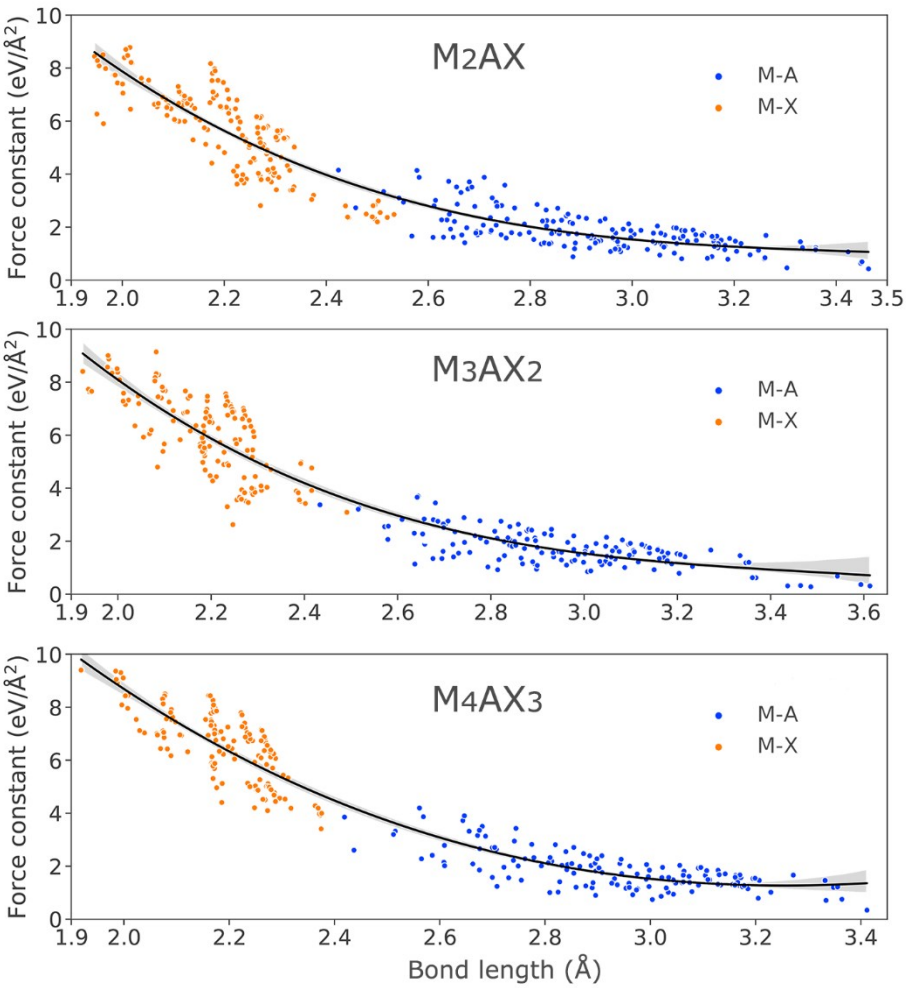

Figure S7. Calculated force constants for M-A and M-X bonds with reference to the bond length for each predicted MAX phases separately. The solid line is a third order of a polynomial regression

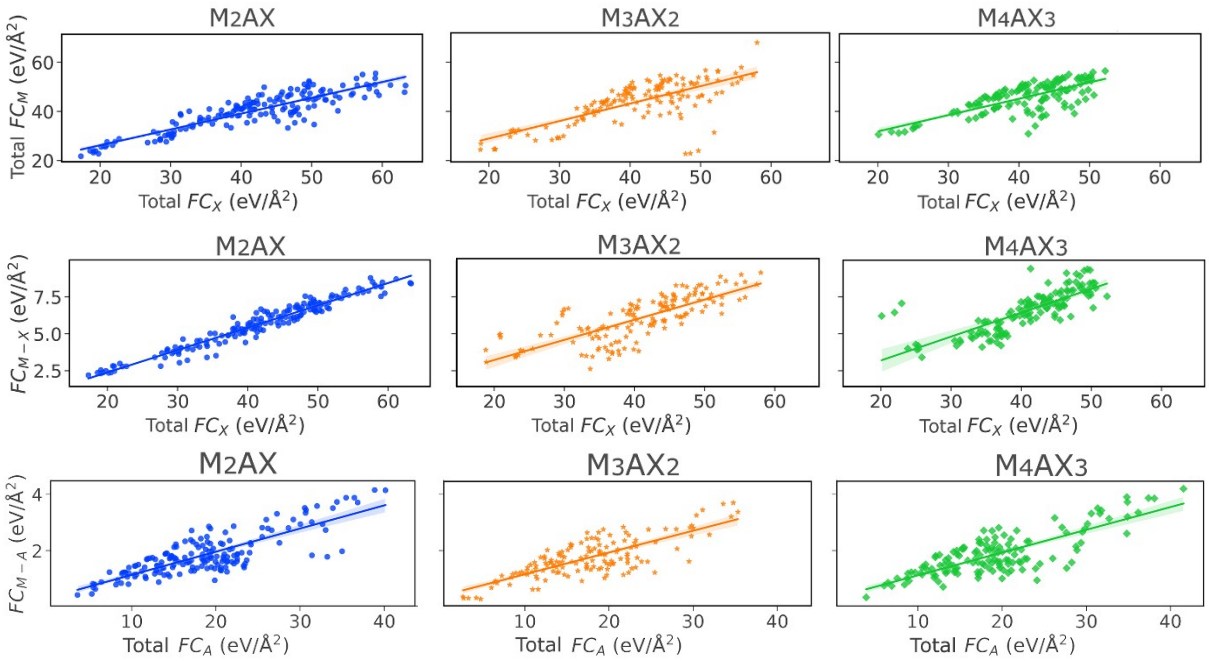

Figure S8. Calculated total force constants on M-element with reference to the calculated total force constants on X-element atoms, the force constants between M- and X-element atoms with reference to the calculated total force constants on X-element atoms, and the force constants between M- and A-element atoms with reference to the calculated total force constants on A-element atoms for each MAX phase separately. The solid line is the linear regression.

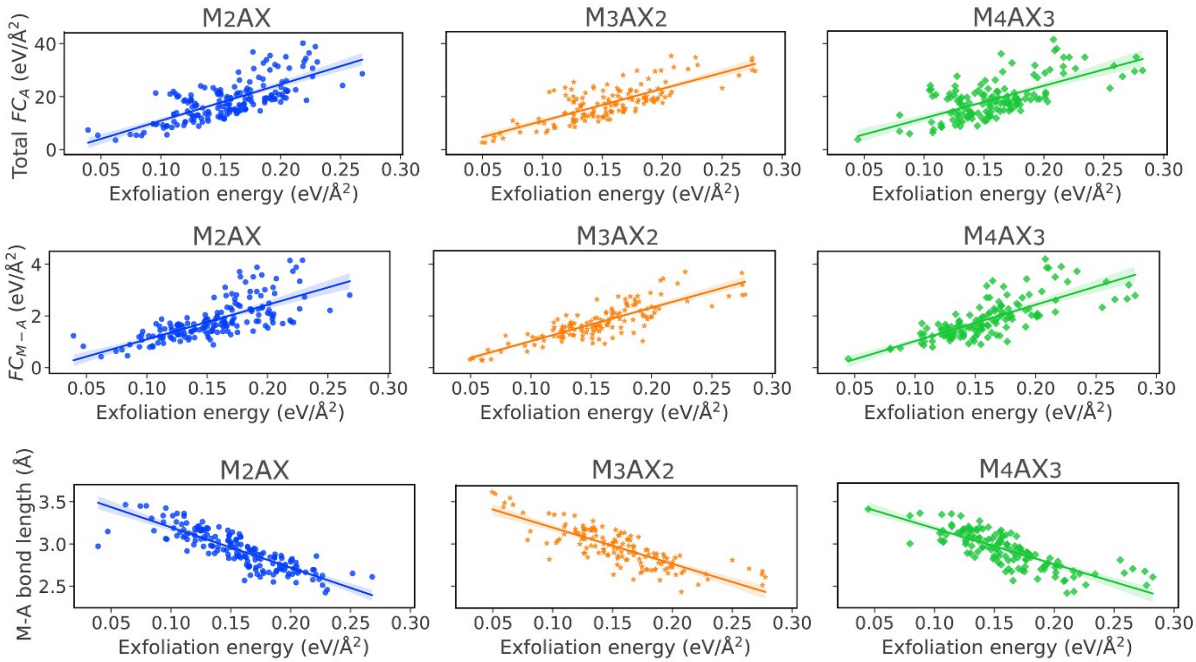

Figure S9. Calculated total force constants on A-element, the force constants between M- and A-element atoms, and M-A bond length for each MAX phase separately with reference to exfoliation energy. The solid line is the linear regression.