

Supplementary Information for “Effect of Chemical Substitution and External Strain on Phase Stability and Ferroelectricity in Two Dimensional M_2CT_2 MXenes”

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I. Optimized structures

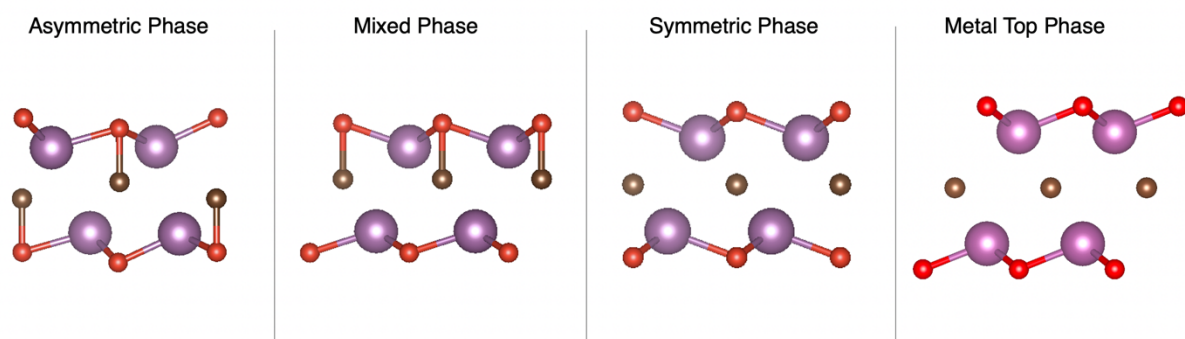


Figure S1. Fully relaxed structures for Sc_2CO_2 .

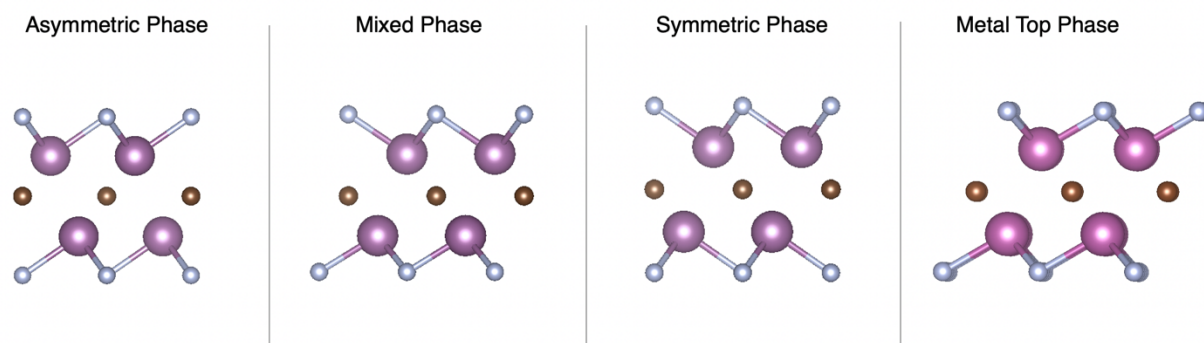


Figure S2. Fully relaxed structures for Sc_2CF_2 .

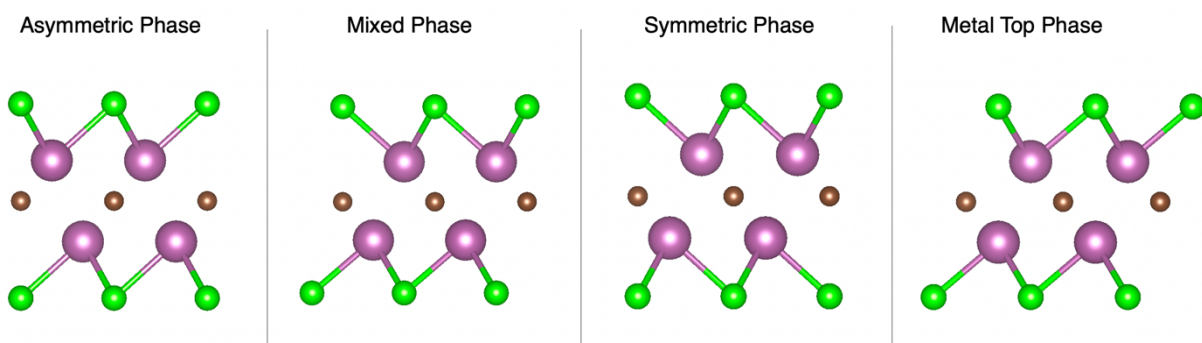


Figure S3. Fully relaxed structures for Sc_2CCl_2 .

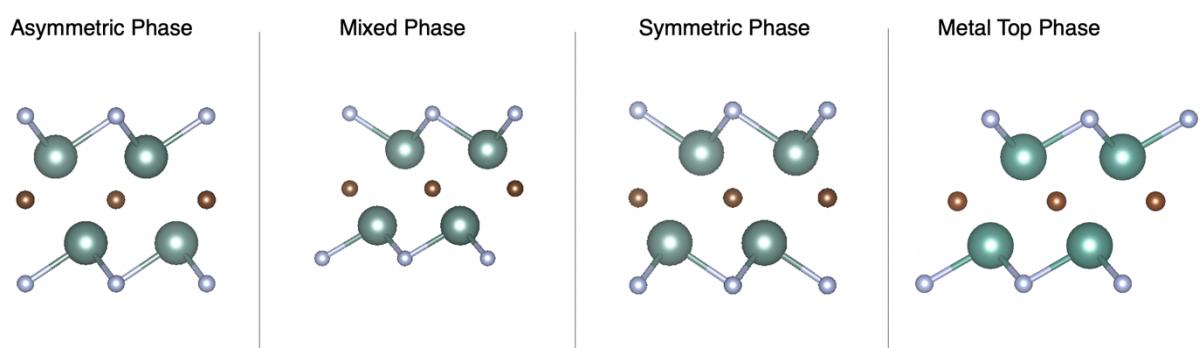


Figure S4. Fully relaxed structures for Y_2CF_2 .

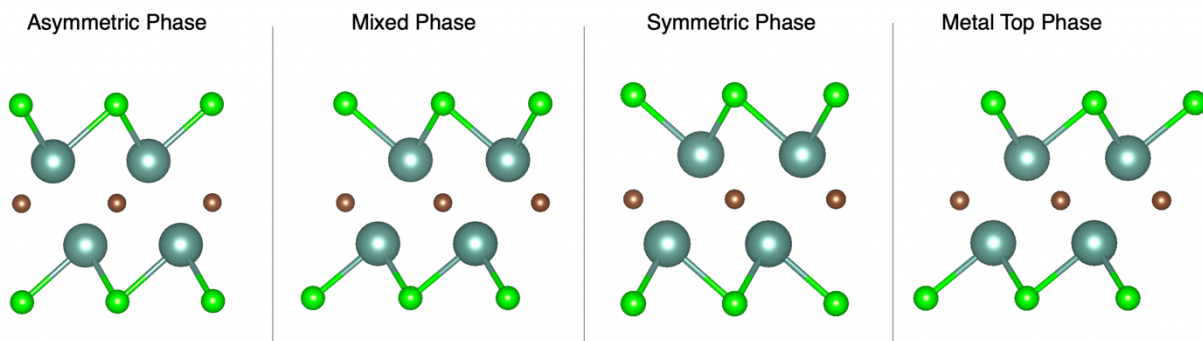


Figure S5. Fully relaxed structures for Y_2CCl_2 .

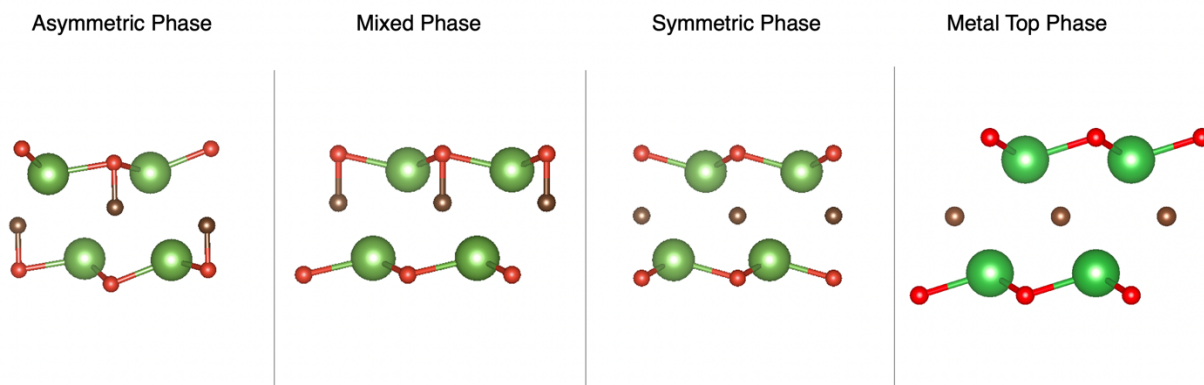


Figure S6. Fully relaxed structures for La_2CO_2 .

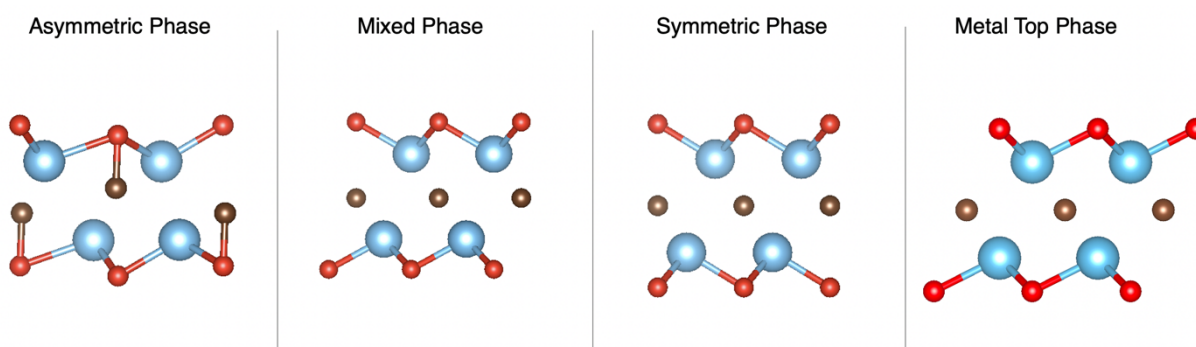


Figure S7. Fully relaxed structures for Ti_2CO_2 .

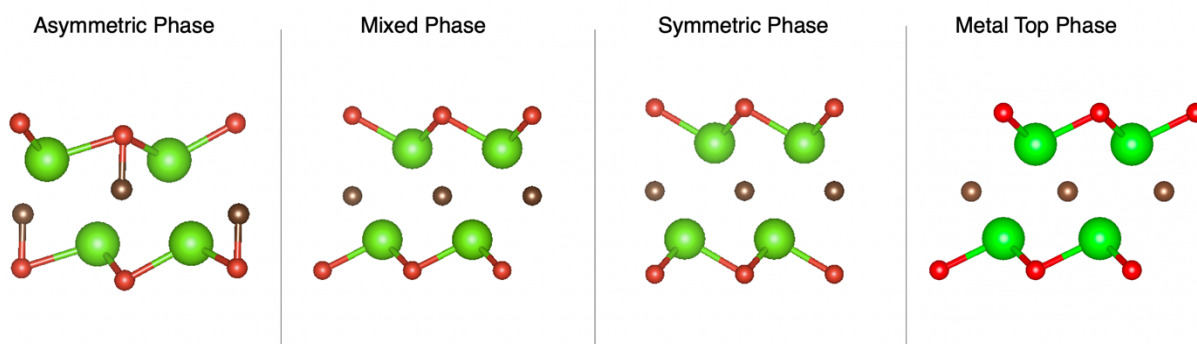


Figure S8. Fully relaxed structures for Zr_2CO_2 .

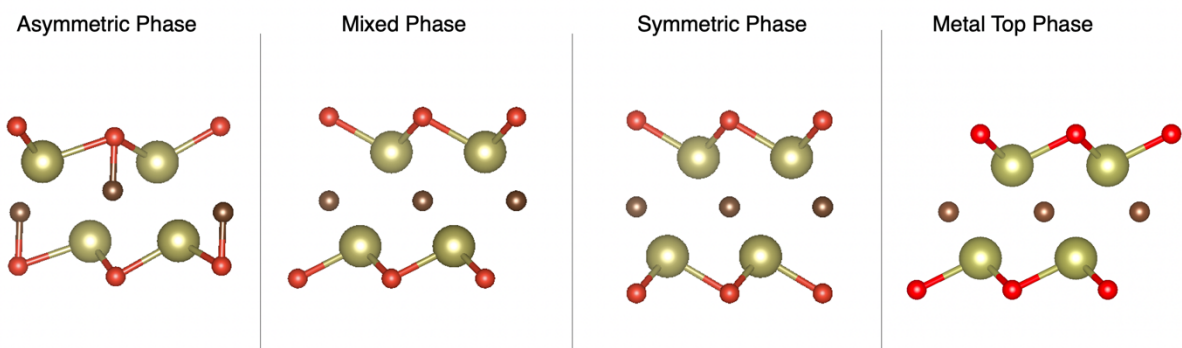


Figure S9. Fully relaxed structures for Hf_2CO_2 .

II. PBE Density of States

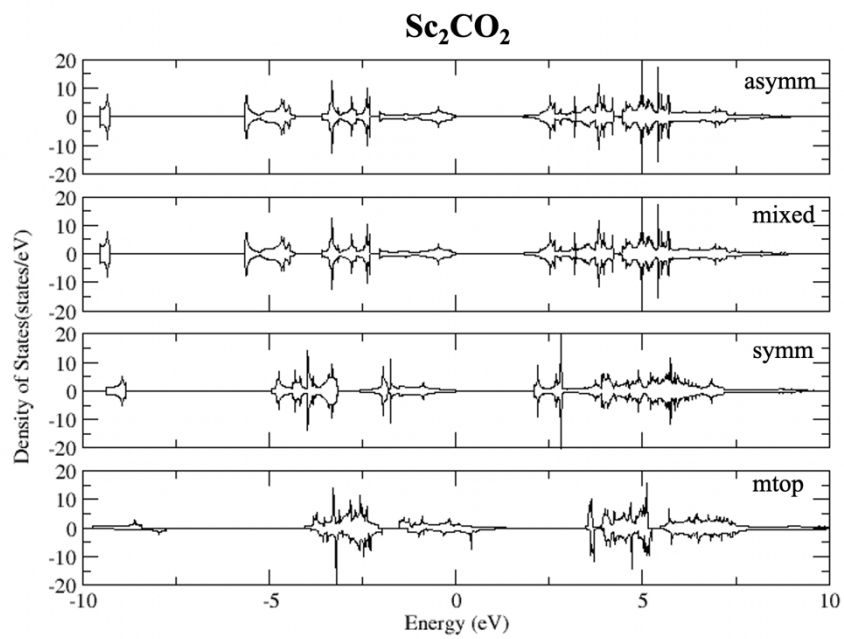


Figure S10. Density of states for Sc_2CO_2 in the four studied phases.

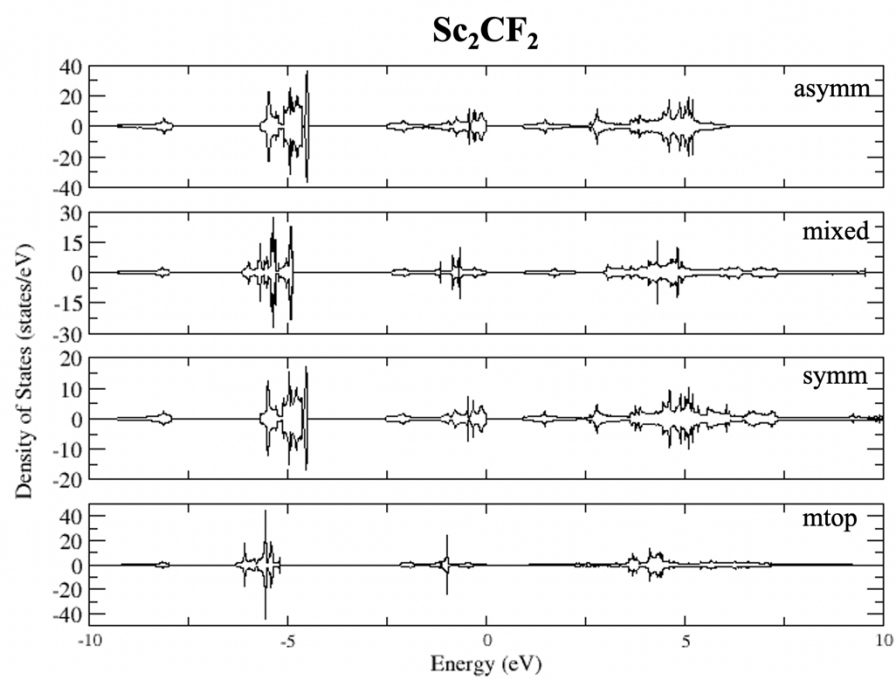


Figure S11. Density of states for Sc₂CF₂ in the four studied phases.

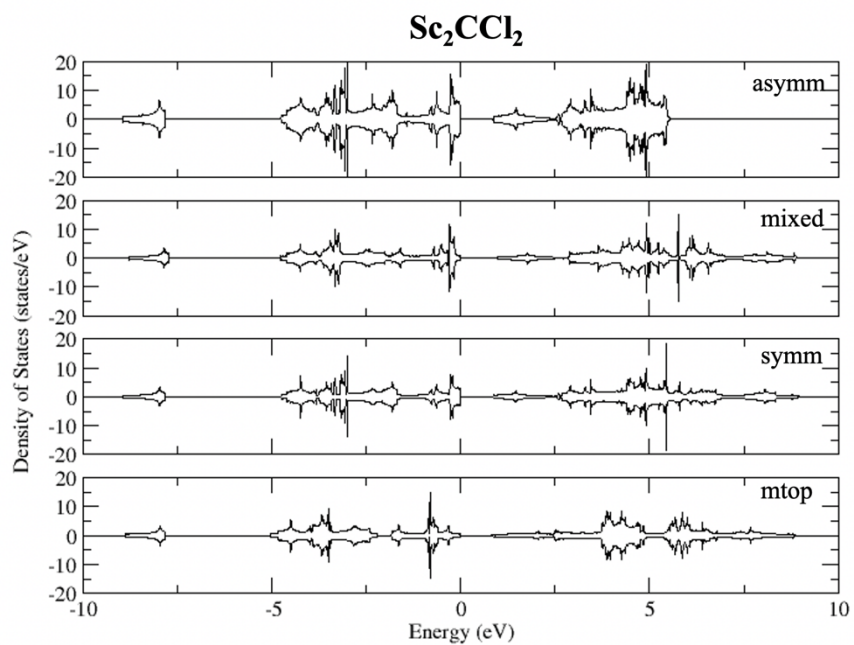


Figure S12. Density of states for Sc₂CCl₂ in the four studied phases.

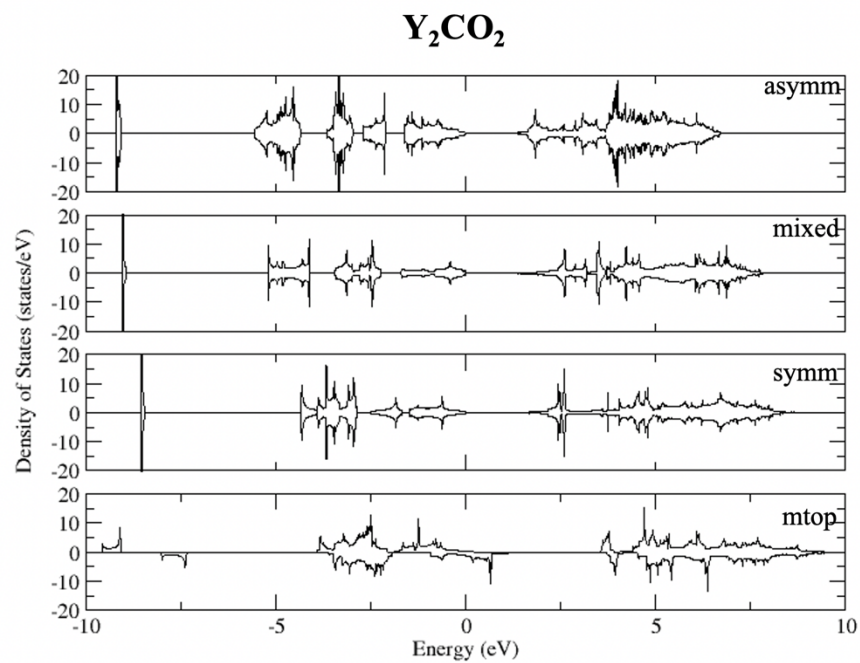


Figure S13. Density of states for Y₂CO₂ in the four studied phases.

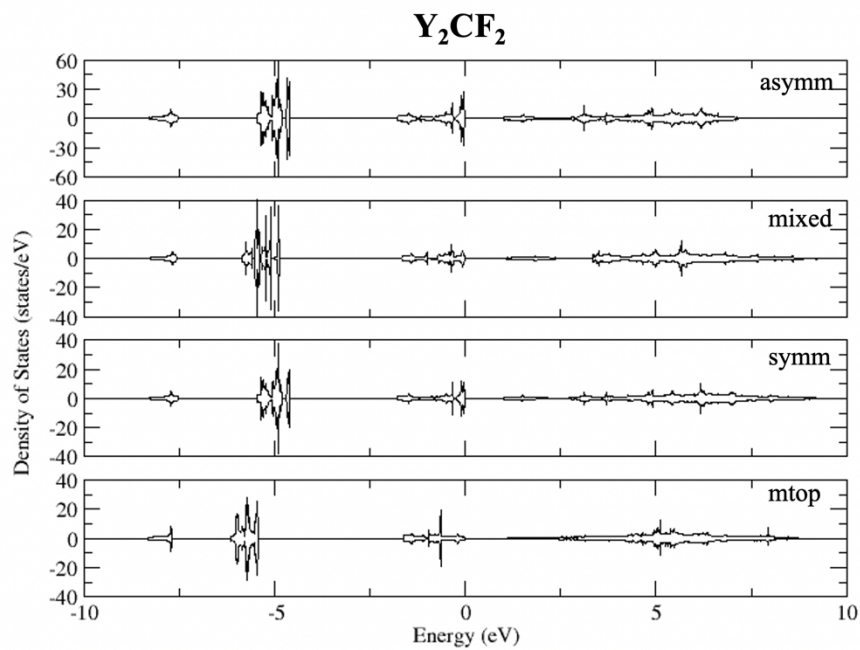


Figure S14. Density of states for Y₂CF₂ in the four studied phases.

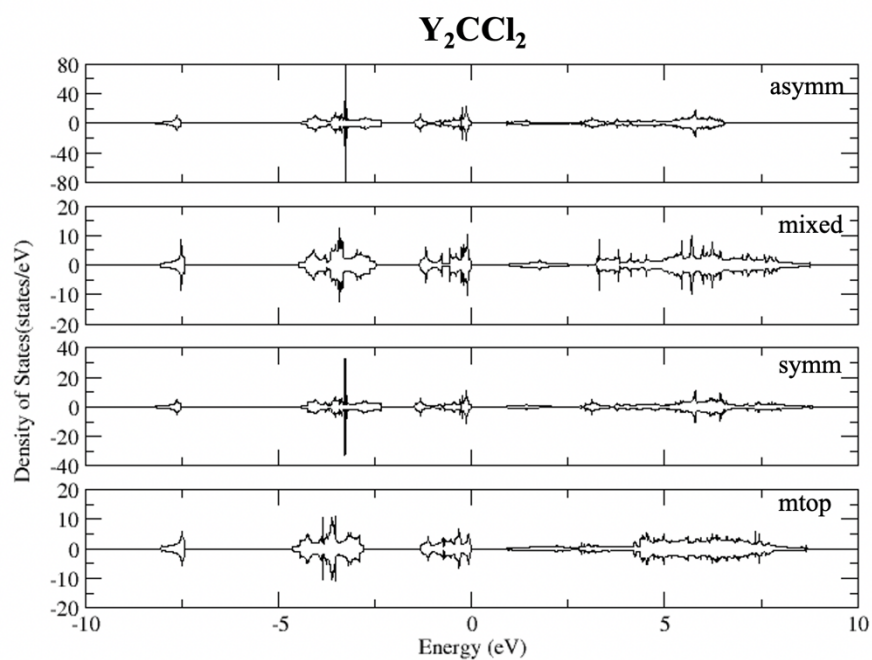


Figure S15. Density of states for Y₂CCl₂ in the four studied phases.

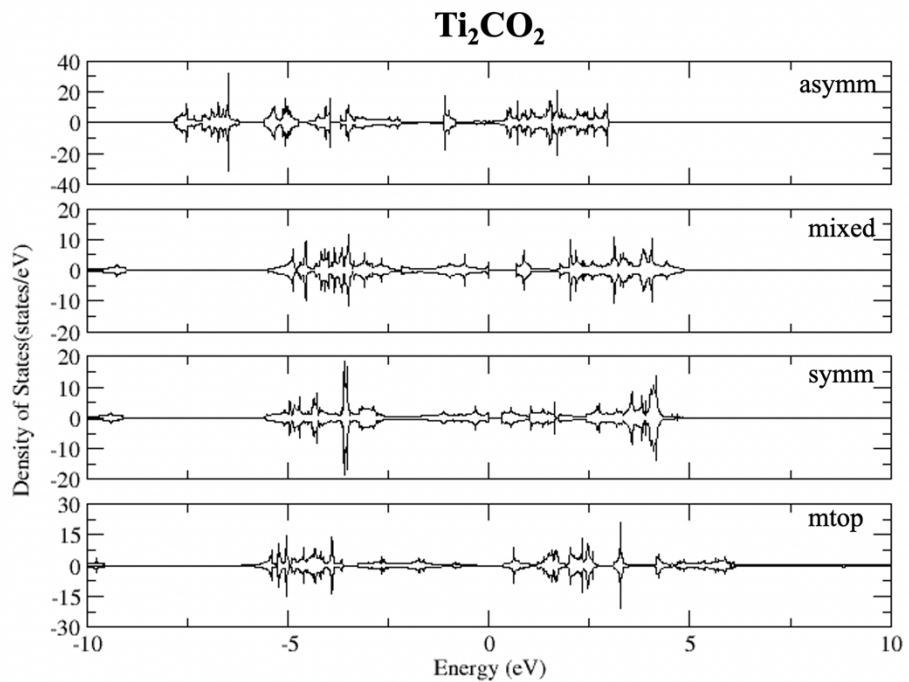


Figure S16. Density of states for Ti₂CO₂ in the four studied phases.

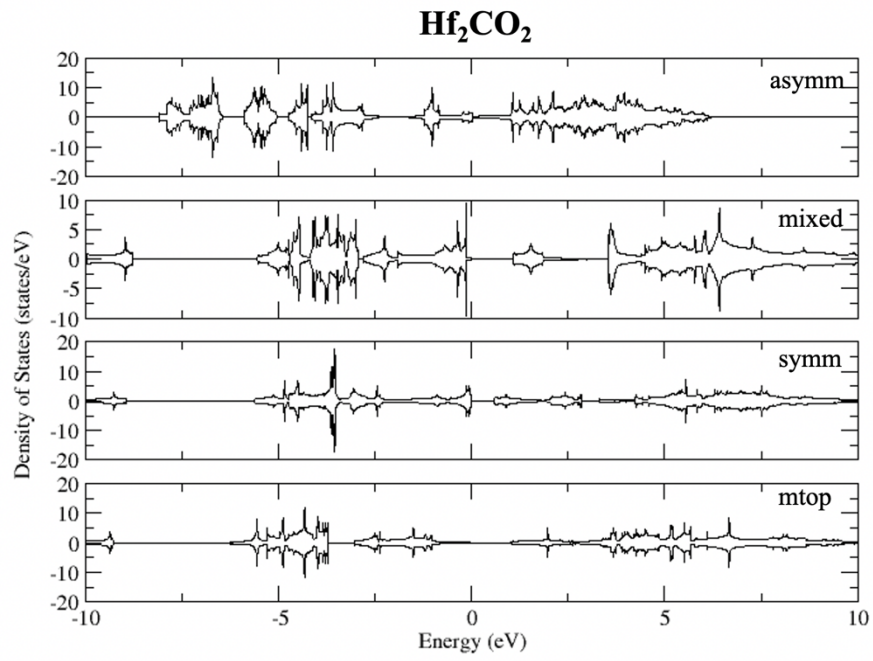


Figure S17. Density of states for Hf₂CO₂ in the four studied phases.

III. Phonon Stability

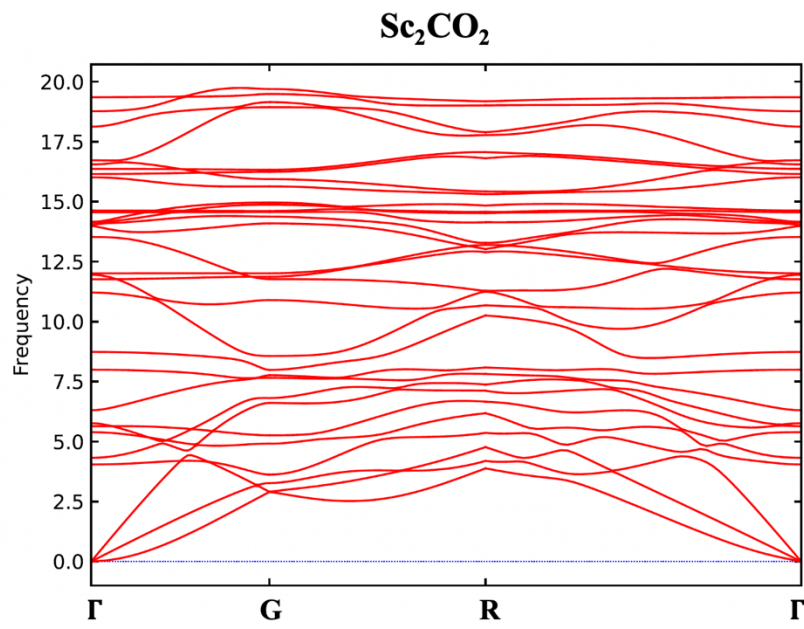


Figure S18. Phonon frequencies for Sc₂CO₂ in the mixed phase.

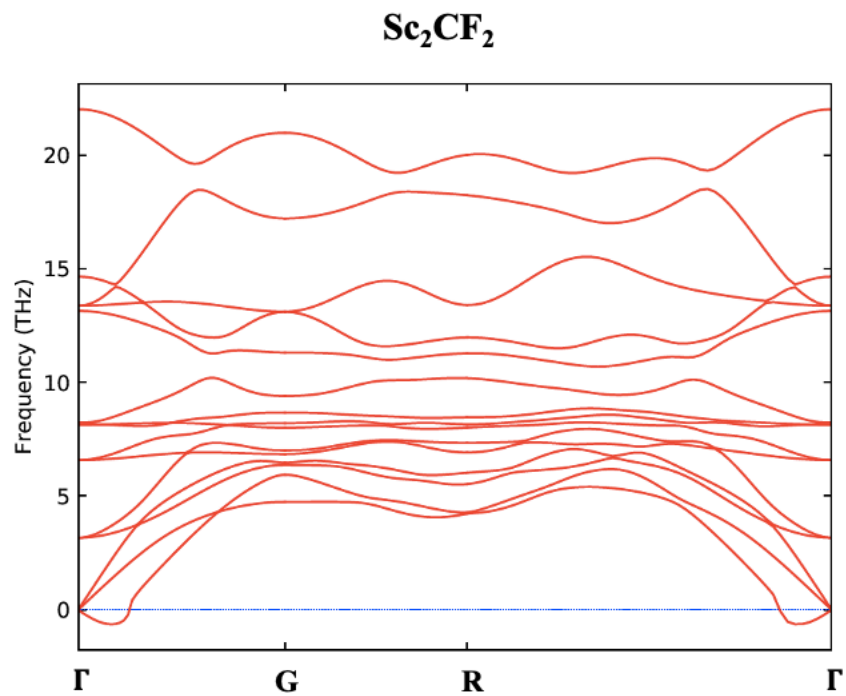


Figure S19. Phonon frequencies for Sc₂CF₂ in the mixed phase.

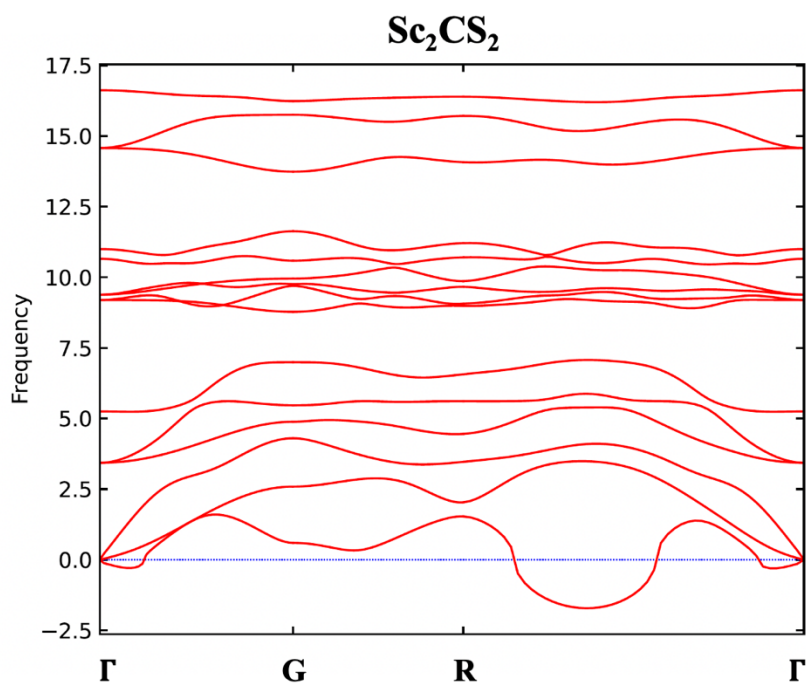


Figure S20. Phonon frequencies for Sc₂CS₂ in the mixed phase.

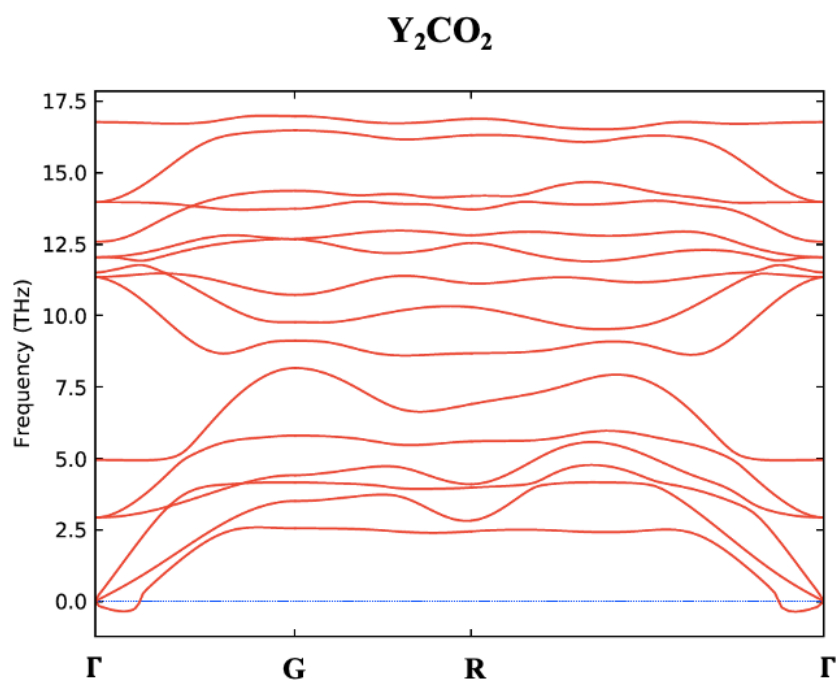


Figure S21. Phonon frequencies for Y₂CO₂ in the mixed phase.

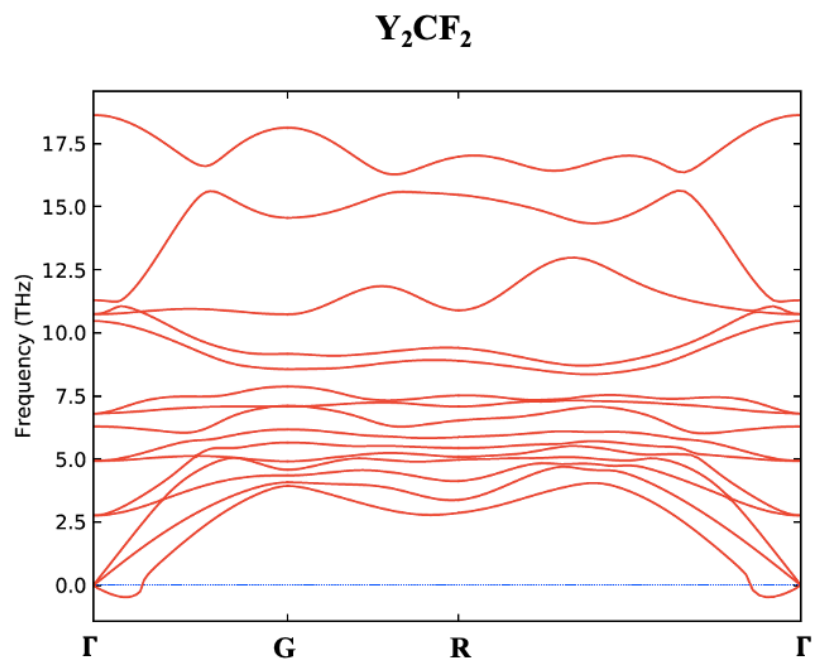


Figure S22. Phonon frequencies for Y₂CF₂ in the mixed phase.

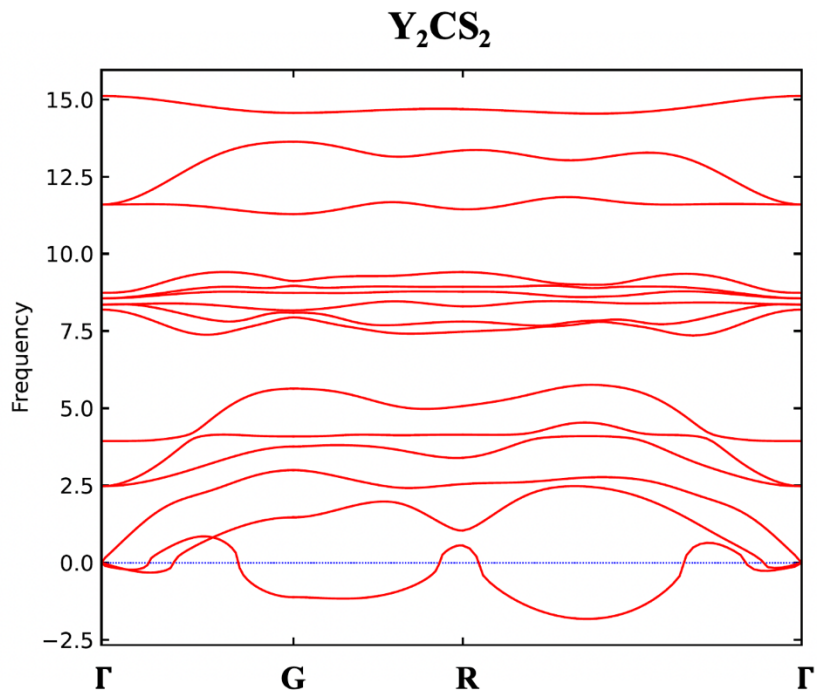


Figure S23. Phonon frequencies for Y₂CS₂ in the mixed phase.

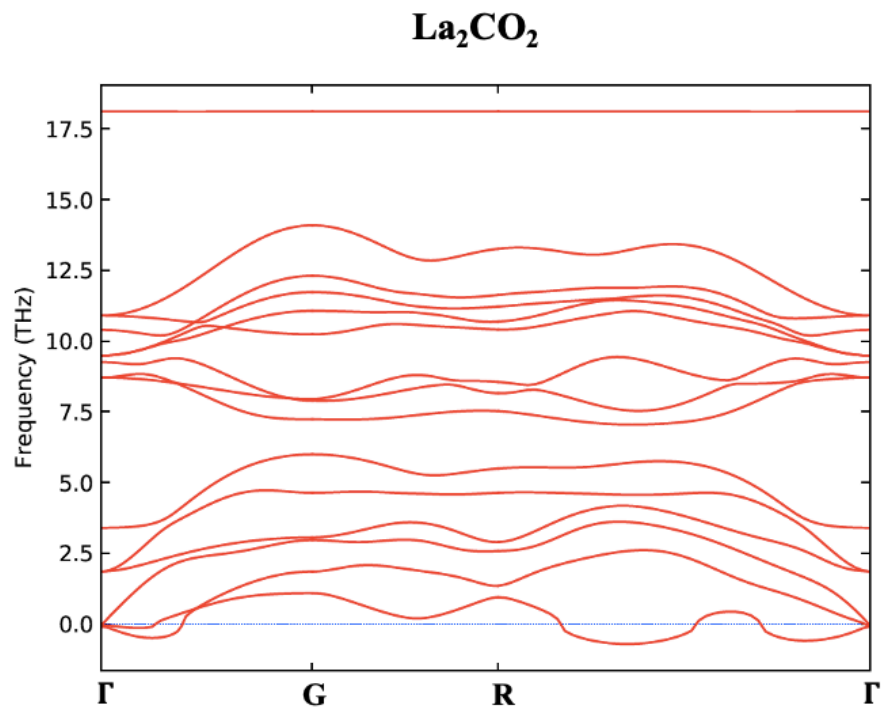


Figure S24. Phonon frequencies for La₂CO₂ in the mixed phase.

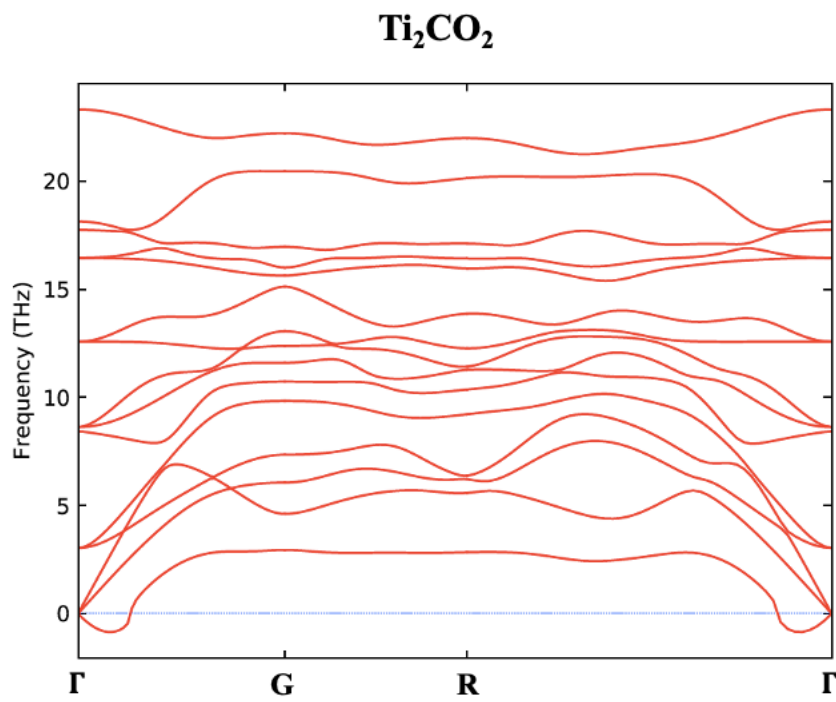


Figure S25. Phonon frequencies for Ti₂CO₂ in the mixed phase.

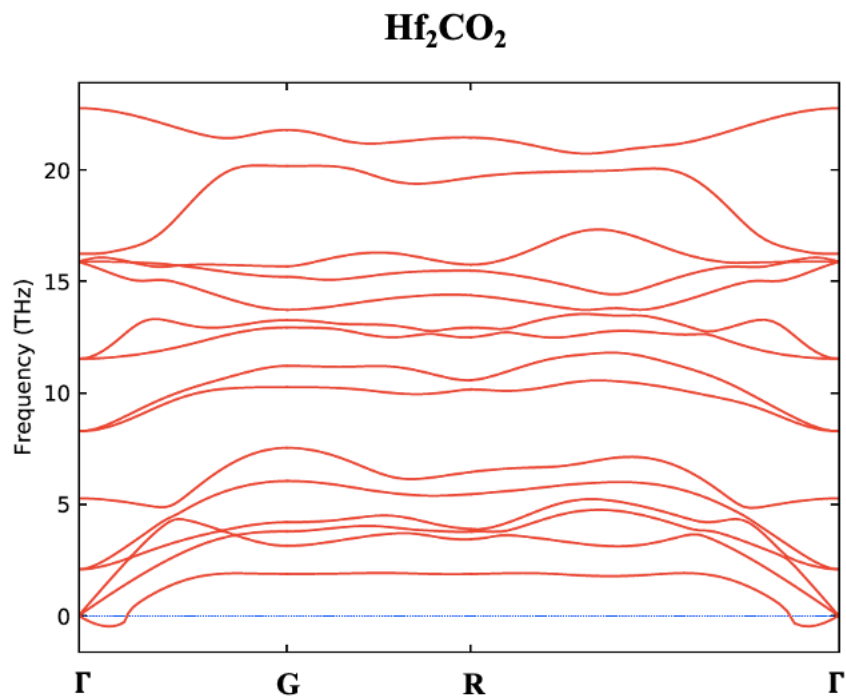


Figure S26. Phonon frequencies for Hf₂CO₂ in the mixed phase.

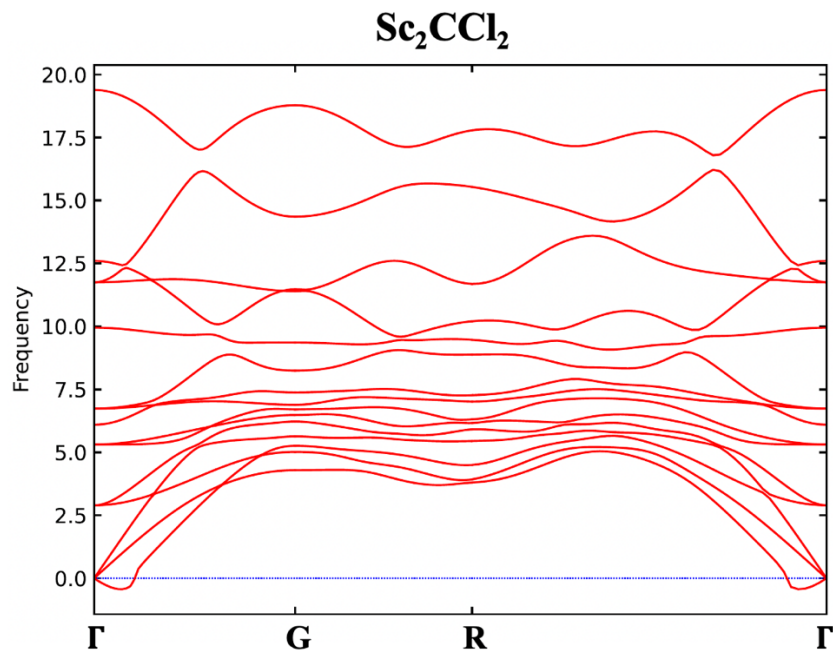


Figure S27. Phonon frequencies for Sc₂CCl₂ in the mixed phase.

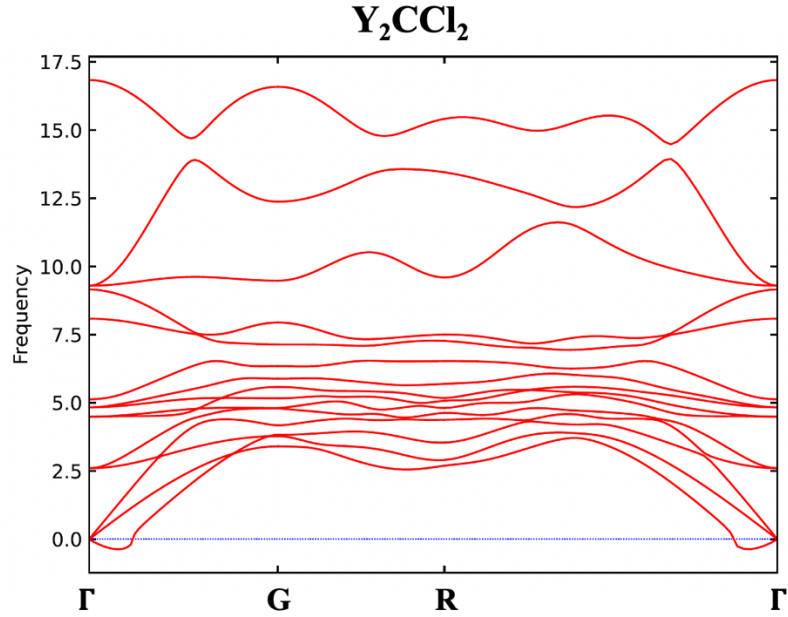


Figure S28. Phonon frequencies for Y₂CCl₂ in the mixed phase.

Table S1. Born effective charges for mixed phase compounds not reported in the main text.

		Born effective charges		
	Element	Z11	Z22	Z33
Sc ₂ CF ₂	C	-5.33	-5.31	-0.44
	F1	-1.05	-1.11	-0.52
	F2	-1.77	-1.76	-0.50
	Sc1	4.36	4.36	0.73
	Sc2	3.78	3.82	0.72
SC ₂ CCl ₂	C	-5.51	-5.51	-0.46
	Cl1	-1.08	-1.08	-0.29
	Cl2	-1.57	-1.57	-0.27
	Sc1	4.35	4.35	0.52
	Sc2	3.82	3.82	0.50
Y ₂ CF ₂	C	-5.38	-5.38	-0.47
	F1	-0.99	-0.99	-0.58
	F2	-1.81	-1.81	-0.55
	Y1	4.42	4.42	0.80
	Y2	3.76	3.76	0.80

Y2CCl2	C	-5.62	-5.62	-0.52
	Cl1	-1.06	-1.06	-0.37
	Cl2	-1.60	-1.60	-0.35
	Y1	4.42	4.42	0.63
	Y2	3.86	3.86	0.62
Ti2CO2	C	-4.36	-4.36	-0.21
	O1	-2.32	-2.33	-0.38
	O2	-4.26	-4.25	-0.38
	Ti1	6.95	6.95	0.53
	Ti2	3.99	3.99	0.43
Hf2CO2	C	-4.44	-4.44	-0.37
	O1	-2.21	-2.21	-0.51
	O2	-3.53	-3.53	-0.52
	Hf1	5.90	5.90	0.75
	Hf2	4.28	4.28	0.66

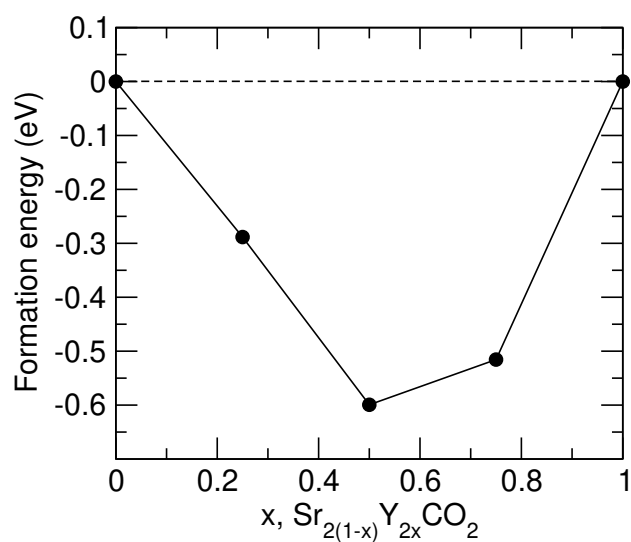
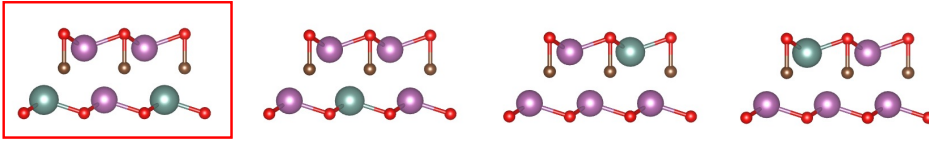
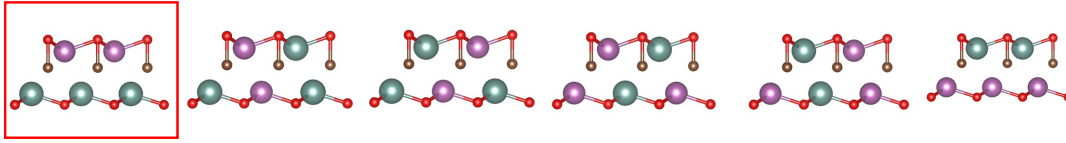


Figure S29. Formation energy of Sr_{2(1-x)}Y_{2x}CO₂ alloys as a function of concentration.

$\text{Sr}_{0.75}\text{Y}_{0.25}\text{CO}_2$



$\text{Sr}_{0.5}\text{Y}_{0.5}\text{CO}_2$



$\text{Sr}_{0.25}\text{Y}_{0.75}\text{CO}_2$

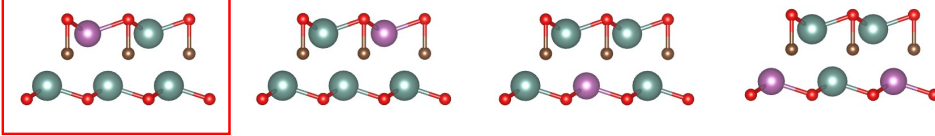
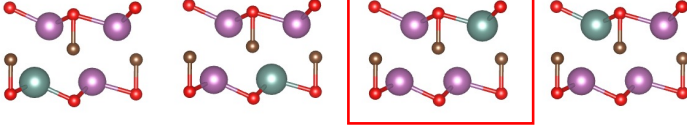
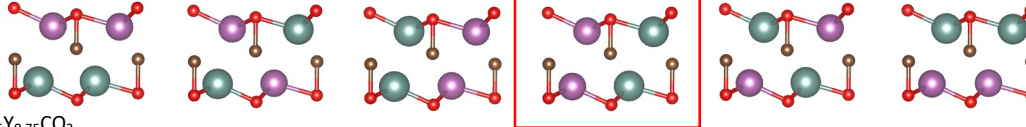


Figure S30. Relaxed structures of all $\text{Sr}_{2(1-x)}\text{Y}_{2x}\text{CO}_2$ alloy structures tested in the mixed phase. The lowest energy structure is circled in red.

$\text{Sr}_{0.75}\text{Y}_{0.25}\text{CO}_2$



$\text{Sr}_{0.5}\text{Y}_{0.5}\text{CO}_2$



$\text{Sr}_{0.25}\text{Y}_{0.75}\text{CO}_2$

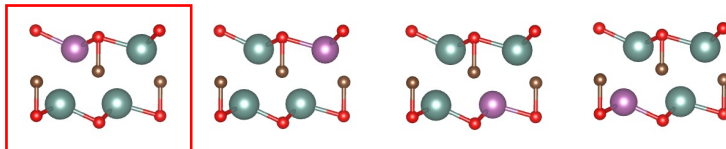


Figure S31. Relaxed structures of all $\text{Sr}_{2(1-x)}\text{Y}_{2x}\text{CO}_2$ alloy structures tested in the asymmetric phase. The lowest energy structure is circled in red.

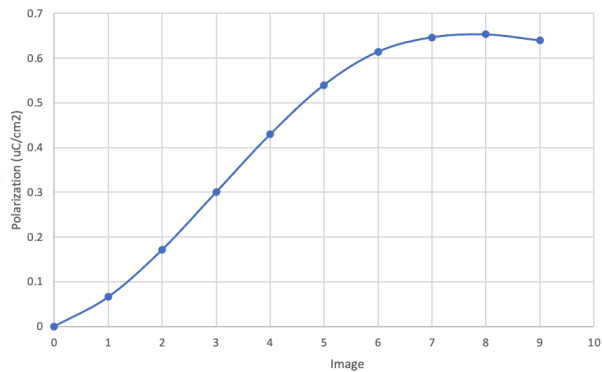


Figure S32. Polarization quantum for Sc_2CO_2 .

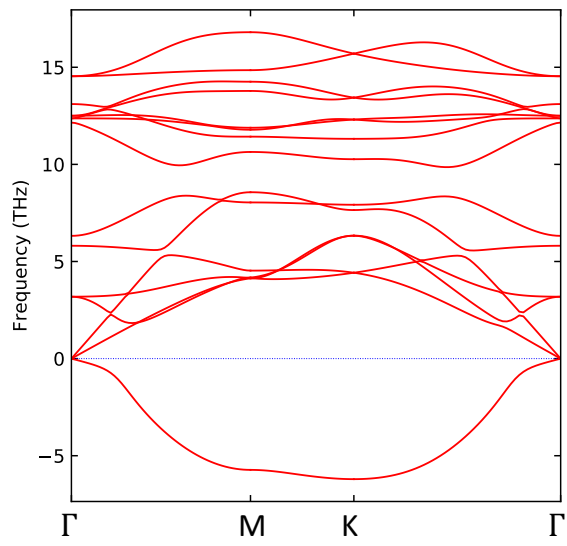


Figure S33. Phonon band structure of the Y_2CO_2 symmetric phase.