

Theoretical and experimental exploration of a novel in-plane chemically-ordered
(Cr_{2/3}M_{1/3})₂AlC *i-MAX* phase with M=Sc and Y

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Supporting information

(SUPPLEMENTARY MATERIAL)

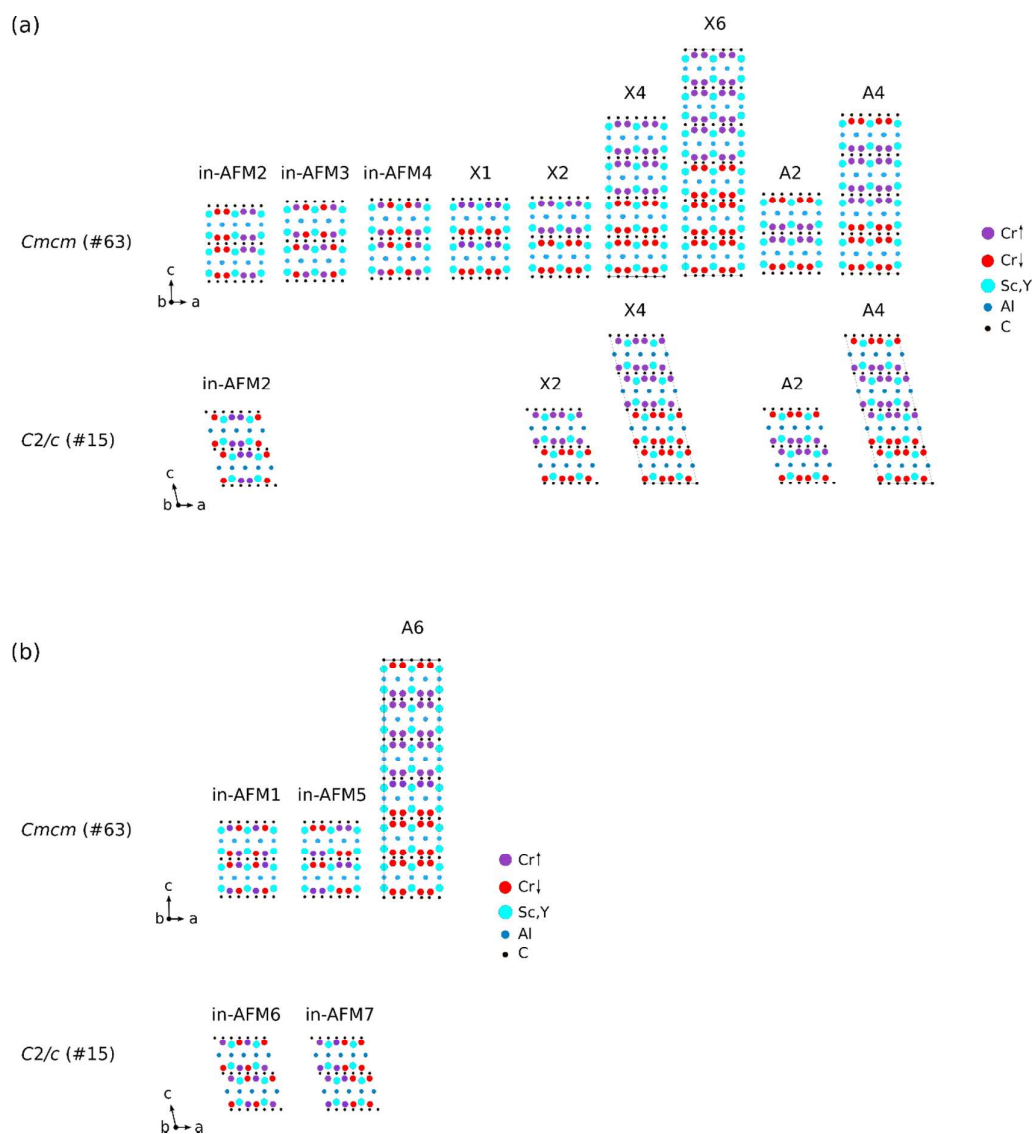


Figure S1. Evaluated antiferromagnetic states for $(\text{Cr}_{2/3}\text{Sc}_{1/3})_2\text{AlC}$ and $(\text{Cr}_{2/3}\text{Y}_{1/3})_2\text{AlC}$. (a) Fully relaxed states. Structural data and energies can be found in Tab. I and II in Supplementary Material. (b) Partially relaxed states. During relaxation, these states either moved towards a ferromagnetic or a nonmagnetic state, or were deemed too high in energy to be of interest.

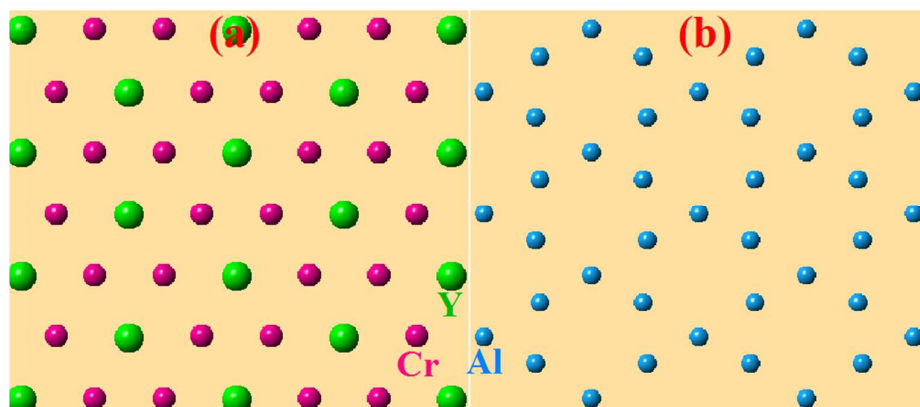


Figure S2: Top view of the *i*-MAX $(\text{Cr}_{2/3}\text{Y}_{1/3})_2\text{AlC}$ (a) *M* layer, where *in-plane* chemical order is given by the $\text{Cr}_{2/3}\text{Y}_{1/3}$ layer composed of Y atoms at the center of hexagon of which the vertices are occupied by Cr atoms, and (b) Al layer, showing a characteristic Kagomé-like structure.

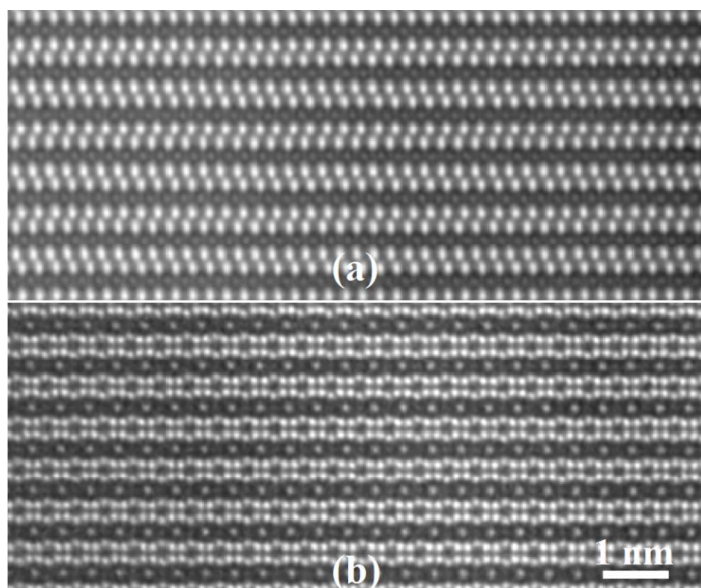


Figure. S3: HRSTEM images of $(\text{Cr}_{2/3}\text{Sc}_{1/3})_2\text{AlC}$ with space group Cmcm (#63), (a) along $[100]$, and (b) along $[010]$ orientation.

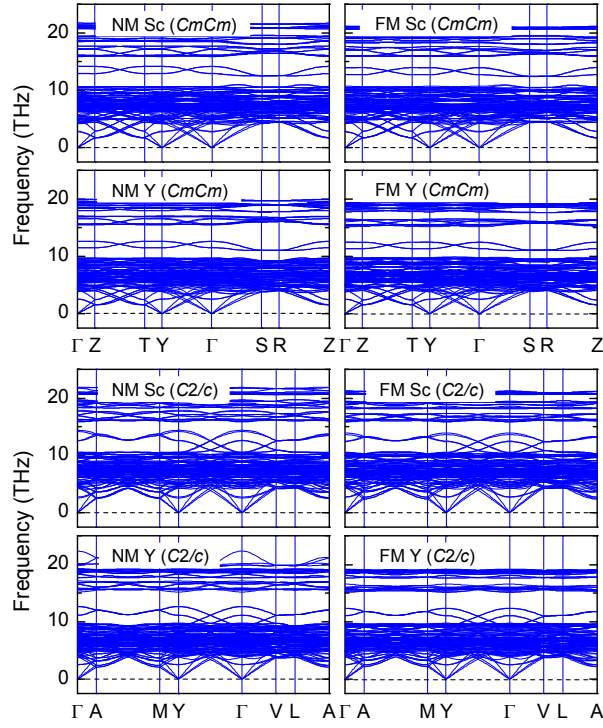


Figure S4. Phonon dispersion in nonmagnetic (NM) and ferromagnetic (FM) $(\text{Cr}_{2/3}\text{Sc}_{1/3})_2\text{AlC}$ and $(\text{Cr}_{2/3}\text{Y}_{1/3})_2\text{AlC}$ for space groups $Cmcm$ and $C2/c$.

Table S1. Structural information for $(\text{Cr}_{2/3}\text{Y}_{1/3})_2\text{AlC}$ from Rietveld refinement.

Space group	$Cmcm$ (#63)
a (Å)	9.33673
b (Å)	5.35495
c (Å)	13.21787
α	90.000
β	90.000
γ	90.000
Cr	16h (0.1652 0.8360 0.4263)
Y	8f (0.0000 0.3353 0.3801) Occupancy of Y = 1.744 and Cr = 0.256
Al	4c (0.0000 0.8249 0.2500) 8g (0.2466 0.0970 0.2500)
C	8e (0.1435 0.5000 0.0000) 4b (0.0000 0.0000 0.0000)

Table S2. Structural information for $(\text{Cr}_{2/3}\text{Sc}_{1/3})_2\text{AlC}$ from Rietveld refinement.

Space group	$C 2/c$ (#15)
a (Å)	9.06908
b (Å)	5.24654
c (Å)	13.21038
α	90.000
β	103.408
γ	90.000
Cr	8f (0.2768 0.4000 0.0792) Occupancy of Cr = 5.435 and Sc = 2.565 8f (0.6077 0.4033 0.0750) Occupancy of Cr = 5.712 and Sc = 2.288
Sc	8f (0.9547 0.40099 0.1090) Occupancy of Sc = 8.00
Al	8f (0.7393 0.1575 0.2496) 4e (0.00000 0.8956 0.25000)
C	8f (0.4401 0.2036 0.00000) 4d (0.25000 0.25000 0.50000)

Table S3. Elastic constants (in GPa) for nonmagnetic (NM), ferromagnetic (FM), and antiferromagnetic (AFM[0001] X_4) $(\text{Cr}_{2/3}\text{Sc}_{1/3})_2\text{AlC}$.

	$(\text{Cr}_{2/3}\text{Sc}_{1/3})_2\text{AlC}$					
	NM		FM		AFM[0001] X_4	
	C_{mcm}	$C_{2/c}$	C_{mcm}	$C_{2/c}$	C_{mcm}	$C_{2/c}$
C_{11}	140	276	144	271	275	268
C_{22}	151	286	154	280	277	273
C_{33}	137	297	136	289	268	278
C_{44}	201	117	197	114	98	116
C_{55}	202	99	198	98	100	98
C_{66}	236	101	231	101	116	101
C_{12}	50	100	60	84	38	85
C_{13}	100	99	91	79	88	81
C_{23}	100	58	81	55	83	49
C_{15}		56		48		43
C_{25}		51		55		41
C_{35}		58		52		47
C_{46}		-1.18		-1.34		-1.53

Table S4. Elastic constants (in GPa) for nonmagnetic (NM), ferromagnetic (FM), and antiferromagnetic (AFM[0001]₄^x) (Cr_{2/3}Y_{1/3})₂AlC.

	(Cr _{2/3} Y _{1/3}) ₂ AlC					
	NM		FM		AFM[0001] ₄ ^x	
	<i>Cmcm</i>	<i>C2/c</i>	<i>Cmcm</i>	<i>C2/c</i>	<i>Cmcm</i>	<i>C2/c</i>
C ₁₁	265	235	271	234	328	234
C ₂₂	290	266	292	280	283	273
C ₃₃	229	282	227	286	226	277
C ₄₄	98	109	95	110	95	110
C ₅₅	96	96	96	95	86	94
C ₆₆	112	98	110	97	109	97
C ₁₂	54	89	63	74	63	76
C ₁₃	89	88	82	74	109	74
C ₂₃	87	57	72	63	72	59
C ₁₅		67		88		71
C ₂₅		75		111		87
C ₃₅		74		92		77
C ₄₆		-1.09		-1.17		-1.84