

Supporting Information for Continued Challenges in High-Throughput Materials Predictions: MatterGen predicts compounds from the training dataset.

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Table S1: Refined parameters for the Rietveld refinement in Figure 2A.

$\text{Ta}_{0.43}\text{Cr}_{0.57}\text{O}_2$ $P4_2/mnm$
 $a = b = 4.6520(15) \text{ \AA}$ $c = 3.03050(12) \text{ \AA}$

Atom	x	y	z	Occ	B_{iso}
Cr	0	0	0	0.57 (2)	0.88 (7)
Ta	0	0	0	0.43 (2)	0.88 (7)
O1	0.302 (11)	0.302 (11)	0	1	0.8 (4)
Zero error	0.0513 (1)				
U	V	W	Y	X	Z
-0.045 (15)	0.090 (15)	-0.285 (3)	0	0.180 (17)	0
Simple axial model	13 (1)				

Cr_2O_3 $R-3c$ (Hexagonal setting)
 $a = b = 4.9625 (15) \text{ \AA}$ $c = 13.5960 (12) \text{ \AA}$

Atom	x	y	z	Occ	B_{iso}
Cr	0	0	0.346 (11)	1	0.88 (7)
O1	0.303	0	0.25	1	0.8 (4)
Zero error	0.0513 (1)				
U	V	W	Y	X	Z
-0.045 (15)	0.090 (15)	-0.285 (3)	0	0.180 (17)	0
Simple axial model	13 (1)				

Table S2: Table of fixed Atomic Displacement Parameters used for quantifying the robustness of the refinement.

Fixed ADP value	Refined occupancies	R_{Bragg} (%) for $\text{Ta}_{1-x}\text{Cr}_x\text{O}_2$
0.1	Ta 0.41 Cr 0.59	4.95
0.3	Ta 0.41 Cr 0.59	4.09
0.5	Ta 0.42 Cr 0.58	3.28
0.7	Ta 0.42 Cr 0.58	2.52
0.9	Ta 0.43 Cr 0.57	1.81
1.1	Ta 0.44 Cr 0.56	1.78
1.3	Ta 0.44 Cr 0.56	2.46
1.5	Ta 0.44 Cr 0.56	3.25