# Supplemental Information: Accessible Chemical Space for Metal Nitride Perovskites

Bastien F. Grosso,<sup>†</sup> Daniel W. Davies,<sup>†</sup> Bonan Zhu,<sup>†</sup> Aron Walsh,<sup>\*,‡</sup> and David O.

 $\mathsf{ScanIon}^{*,\dagger}$ 

†Department of Chemistry, University College London, London, United Kingdom ‡Department of Materials, Imperial College London, London, United Kingdom

E-mail: a.walsh@imperial.ac.uk; d.scanlon@ucl.ac.uk

We present in Fig. S1 to Fig. S8, the effect of the 15 octahedral tilts on the energy of each of the 279 candidates, after one loop of electronic relaxation (dashed lines) and after full relaxation of the ions and lattice (continuous lines).

In Fig. S9 to Fig. S13, we present, for each of the 25 closed-shell candidates, the electronic band structure and density of states for the (A) and (G) structures as well as their respective crystal structures.

Table 1 and 2, contain the convergence parameters for the 25 candidates presented in the main text and for the 86 competing phases used to compute the energy hull, respectively. The corresponding structure can be found in the data repository provided (https://github.com/SMTG-UCL/High\_throughput\_search\_ABN3). Finally, the list of the pseudopotentials used is presented in Table 3.

	Glazer		AIRSS		
	Encut	k-mesh	Encut	k-mesh	
$GaMoN_3$	450	3x5x4	450	5x8x3	
$GaWN_3$	450	6x6x5	450	11x6x4	
$HfNbN_3$	450	4x3x2	450	9x4x2	
$HfSbN_3$	450	5x5x3	450	9x5x3	
$HfTaN_3$	500	4x3x2	500	5x4x3	
HfVN <sub>3</sub>	450	4x5x4	450	9x4x2	
InMoN <sub>3</sub>	550	4x5x6	550	5x2x3	
$InWN_3$	450	4x5x4	450	7x7x7	
$LaMoN_3$	450	5x7x6	450	7x7x6	
$LaWN_3$	450	7x7x7	450	7x7x2	
$ScMoN_3$	450	6x6x4	450	9x4x3	
$ScWN_3$	450	4x5x6	450	9x4x3	
$SnNbN_3$	450	5x6x4	450	11x5x3	
$SnSbN_3$	450	5x5x4	450	7x7x7	
$SnTaN_3$	450	5x5x4	450	5x4x4	
$SnVN_3$	450	5x5x4	450	4x4x3	
$TiVN_3$	450	2x5x5	450	9x5x4	
$TlMoN_3$	550	4x5x6	550	3x5x5	
$TlWN_3$	450	6x6x6	450	9x6x3	
$MON_3$	450	5x6x6	450	5x5x4	
$YWN_3$	450	5x5x6	450	4x4x4	
$ZrNbN_3$	450	4x4x4	450	9x5x4	
$ZrSbN_3$	450	5x5x4	450	5x3x4	
$ZrTaN_3$	450	4x4x3	450	5x4x5	
$ZrVN_3$	450	2x6x6	450	9x4x3	

Table 1: Convergence parameters of the 25 candidates presented in the main text.

Material	Encut	k-mesh	Material	Encut	k-mesh	Material	Encut	k-mesh
Ga <sub>1</sub> N <sub>1</sub>	500	7x7x7	N <sub>4</sub>	750	8x8x6	Tl <sub>3</sub>	400	11x11x11
$Ga_2Mo_6$	400	8x8x8	N <sub>8</sub>	750	9x9x9	$Tl_{29}$	400	бхбхб
$Ga_2N_2$	450	8x8x5	N <sub>8</sub>	750	9x9x9	$V_1$	500	17x17x17
$Ga_4$	400	6x6x6	$Nb_1$	400	17x17x17	$V_1N_1$	500	9x9x9
$Ga_4$	350	12x12x11	$Nb_1N_1$	500	10x10x8	$V_4Sn_8$	400	6x7x6
$Ga_{41}Mo_8$	400	5x5x5	$Nb_4Sn_8$	350	8x8x8	$V_6N_3$	450	5x5x5
$Ga_{62}Mo_{12}$	400	4x4x2	$Nb_6N_3$	450	6x6x5	$V_6Sn_2$	450	9x9x9
$Hf_1N_1$	500	11x11x11	$Nb_6Sn_2$	400	10x10x10	$V_16N_2$	450	4x4x10
$\mathrm{Hf}_2$	450	11x11x6	$Nb_{10}N_{12}$	500	7x7x3	$W_1$	450	16x16x16
$Hf_3N_2$	450	8x8x8	$Nb_{12}Sn_{10}$	400	3x3x5	$W_4N_6$	750	6x6x5
$Hf_4N_2$	500	5x5x11	$Sb_2$	300	11x11x11	$Y_1N_1$	550	8x8x8
$Hf_4Sb_4$	300	11x11x11	$Sc_1N_1$	450	9x9x9	$Y_2$	400	18x18x10
$Hf_6Sb_6$	350	7x7x2	$Sc_2$	450	9x9x5	$Y_3$	400	13x13x13
$\mathrm{Hf}_8\mathrm{Sb}_{16}$	300	12x4x2	$Sn_1Sb_1$	450	15x15x15	$Y_4$	400	9x9x3
$Hf_{10}\text{Sb}_{18}$	350	4x4x4	$Sn_2$	400	11x11x11	$Y_4W_4N_{12}$	450	4x4x4
$Hf_{12}N_{16}$	500	5x5x2	$Ta_1$	450	11x11x11	$Zr_1N_1$	550	16x16x16
$Hf_{12}Sb_4$	350	5x5x4	$Ta_3N_3$	700	7x7x11	$Zr_2$	450	16x16x9
$Hf_{20}\text{Sb}_{12}$	350	3x3x3	$Ta_4Sn_8$	450	10x10x10	$Zr_4N_2$	450	5x5x11
$In_1N_1$	500	8x8x8	$Ta_6N_3$	450	9x9x8	$Zr_4Sb_2$	450	7x7x9
$In_2N_2$	500	8x8x4	$Ta_6N_{10}$	700	7x7x3	$Zr_4Sb_4$	400	10x10x10
In <sub>3</sub>	450	14x14x14	$Ta_6Sn_2$	450	10x10x10	$Zr_6Sb_6$	400	9x9x3
$La_1$	350	16x16x16	$Ta_{30}$	400	4x4x6	$Zr_8Sb_{16}$	400	7x3x2
$La_2N_2$	550	7x7x4	$Ta_{30}$	400	4x4x6	$Zr_{10}Sb_6$	400	4x4x5
$La_2W_2N_6$	450	5x5x5	$Ti_1N_1$	450	16x16x16	$Zr_{12}N_{16}$	550	7x3x3
$La_4$	350	13x13x4	$Ti_2$	400	9x9x5	$Zr_{12}Sb_4$	450	7x7x4
$La_4Mo_4N_{12} \\$	750	2x2x3	Ti <sub>3</sub>	400	7x7x11	$Zr_{20}Sb_{12}$	400	4x3x3
$Mo_1$	400	17x17x17	$Ti_4N_2$	450	7x7x11	$Zr_{22}Sb_{36}$	300	4x4x1
$Mo_4N_2$	450	6x6x8	$Tl_1$	400	24x24x24	$Zr_{28}Sb_{16}$	300	2x3x3
$Mo_8N_8$	550	6x6x6	$Tl_2$	400	16x16x8			

Table 2: List of the competing phases and convergence parameters. The energy cutoff (Encut) and k-mesh grid (k-mesh) are indicated next to each materials.

Table 3: List of pseudopotentials used for each atom.

PAW\_PBE Ga\_d 06Jul2010 PAW PBE Mo pv 04Feb2005 PAW PBE N 08Apr2002 PAW PBE W sv 04Sep2015 PAW PBE Hf pv 06Sep2000 PAW PBE Nb pv 08Apr2002 PAW PBE Sb 06Sep2000 PAW PBE Ta pv 07Sep2000 PAW PBE V pv 07Sep2000 PAW\_PBE In\_d 06Sep2000 PAW PBE La 06Sep2000 PAW PBE Sc sv 07Sep2000 PAW PBE Sn d 06Sep2000 PAW PBE Ti pv 07Sep2000 PAW PBE Tl d 06Sep2000 PAW\_PBE Y\_sv 25May2007 PAW PBE Zr sv 04Jan2005



Figure S1: Energy of tilts for fixed ions (dashed lines) and full relaxation (continuous lines) 5



Figure S2: Energy of tilts for fixed ions (dashed lines) and full relaxation (continuous lines)



Figure S3: Energy of tilts for fixed ions (dashed lines) and full relaxation (continuous lines)



Figure S4: Energy of tilts for fixed ions (dashed lines) and full relaxation (continuous lines)



Figure S5: Energy of tilts for fixed ions (dashed lines) and full relaxation (continuous lines) 9



Figure S6: Energy of tilts for fixed ions (dashed lines) and full relaxation (continuous lines)



Figure S7: Energy of tilts for fixed ions (dashed lines) and full relaxation (continuous lines)



Figure S8: Energy of tilts for fixed ions (dashed lines) and full relaxation (continuous lines)



Indirect band gap: 2.335 eV Direct band gap: 2.602 eV

**GaWN**<sub>3</sub>



Indirect band gap: 2.439 eV Direct band gap: 2.798 eV



Direct band gap: 1.064 eV



Indirect band gap: 1.876 eV Direct band gap: 2.080 eV



Indirect band gap: 0.550 eV Direct band gap: 1.146 eV



HfSbN<sub>3</sub>





Figure S9: Electronic structure, DOS and relative crystal structures.

13



Glazer

Total DOS

Ga (s)



Indirect band gap: 2.605 eV Direct band gap: 2.801 eV



Direct band gap: 2.348 eV



Indirect band gap: 3.443 eV Direct band gap: 3.532 eV











**AIRSS** 





Glazer





Figure S10: Electronic structure, DOS and relative crystal structures.



Indirect band gap: 2.076 eV Direct band gap: 2.102 eV

ScWN<sub>3</sub>



Indirect band gap: 2.194 eV Direct band gap: 2.238 eV





Direct band gap: 1.170 eV



Indirect band gap: 1.896 eV Direct band gap: 2.083 eV



Indirect band gap: 1.896 eV Direct band gap: 2.083 eV





Indirect band gap: 2.026 eV Direct band gap: 2.269 eV

- N (p) - Sc (d) - W (s) (v) W (p) Energy W (d)

Indirect band gap: 2.563 eV Direct band gap: 2.648 eV



Indirect band gap: 2.502 eV Direct band gap: 2.674 eV

# SnSbN<sub>3</sub>

SnTaN<sub>3</sub>

(eV)

ergy



Indirect band gap: 1.697 eV Direct band gap: 1.829 eV









Total DOS







Figure S11: Electronic structure, DOS and relative crystal structures.

Glazer

AIRSS

# **SnVN**<sub>3</sub>

(eV)

Energy

(eV)

ergy



Indirect band gap: 2.028 eV Direct band gap: 2.736 eV





Indirect band gap: 0.938 eV Direct band gap: 1.179 eV



Glazer

## TIMoN<sub>3</sub>



Indirect band gap: 1.506 eV Direct band gap: 2.020 eV

## **TIWN3**

Energy (eV)



Metallic





Indirect band gap: 2.184 eV Direct band gap: 2.271 eV



Indirect band gap: 1.406 eV

Indirect band gap: 2.221 eV Direct band gap: 2.305 eV



Total DOS

N (s)

N (p)

Sn (p)

Total DOS

N (p) Ti (d)

V (d)

— Sn (s)

- Sn (d) — V (d)





Glazer





-0





Figure S12: Electronic structure, DOS and relative crystal structures.

Total DOS

N (p) TI (s)

W (d)

— W (p)



Indirect band gap: 2.250 eV Direct band gap: 2.533 eV

ZrNbN<sub>3</sub>



Indirect band gap: 0.744 eV Direct band gap: 1.278 eV



ZrTaN<sub>3</sub>

**ZrVN**<sub>3</sub>



Indirect band gap: 1.725 eV Direct band gap: 1.898 eV



Indirect band gap: 0.457 eV Direct band gap: 1.067 eV



Indirect band gap: 1.416 eV Direct band gap: 1.662 eV





Total DOS

Indirect band gap: 2.252 eV Direct band gap: 2.533 eV



Direct band gap: 2.220 eV



Indirect band gap: 3.251 eV Direct band gap: 3.312 eV



Direct band gap: 2.135 eV

6 4 () 2		<ul> <li>Total DOS</li> <li>N (p)</li> <li>V (s)</li> <li>V (p)</li> </ul>
0 0 -2 Euergy -4 -6	ZT Y S RUX TY	— V (d) — Zr (d)

Indirect band gap: 2.251 eV Direct band gap: 2.359 eV









AIRSS



Glazer





Figure S13: Electronic structure, DOS and relative crystal structures.