Supplementary Materials

Unveiling defect physics in gapped metals: a theoretical investigation into defect formation and electronic structure interplay

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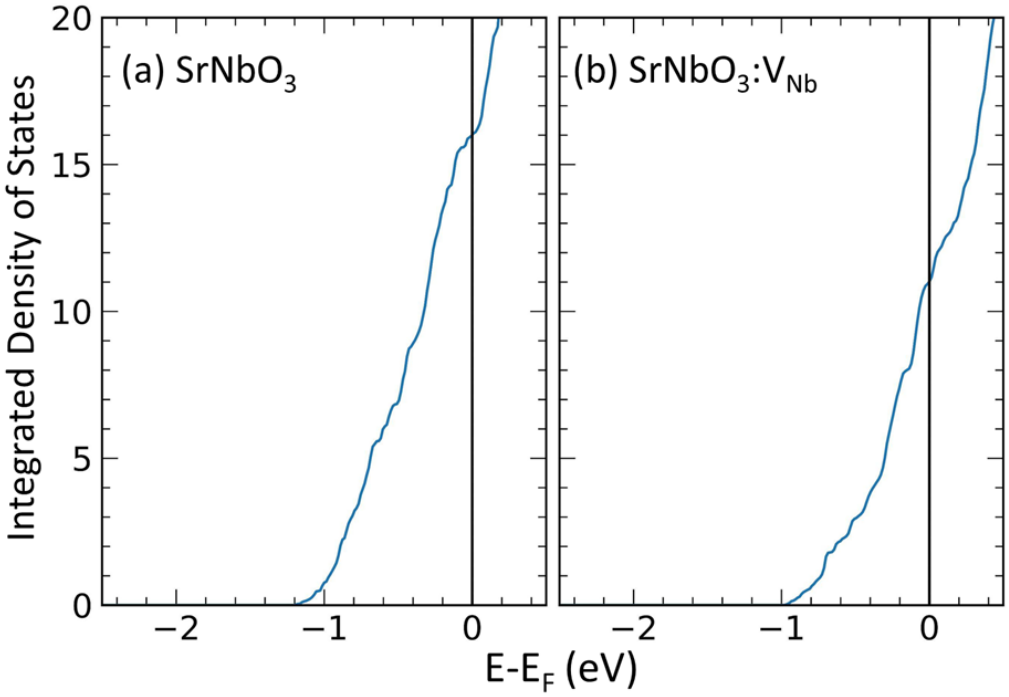
Supplementary Table 1. Supercell sizes used for each material. Supercells are generated from the relaxed primitive structures (given at the end of this file)

Material	Supercell sizes used					
Cu	3×3×3	4×4×4	5×5×5	6×6×6	7×7×7	
Zn	3×3×2	4×4×2	5×5×3	6×6×3	7×7×4	
CaN_2	2×2×2	3×3×3	4×4×4	5×5×5		
$In_{15}SnO_{24}$	1×1×1	1×1×2	1×2×2	2×2×2	2×2×3	2×3×3
$Ca_6Al_7O_{16}$	1×1×1	1×1×2	1×2×2	2×2×2		
$SrNbO_3$	2×2×1	2×2×2	3×2×2	3×3×2		

Supplementary Table 2. Band-filling correction energy (Δ_{BFC}) with electrostatic potentials aligned for the average of 3 most remote atoms of each species and the composition weighed (w) potential alignment are shown. The order of energies (in eV) is shown in the same way as the order of supercell sizes in Supplementary Table 1

$In_{15}SnO_{24}:V_{In}$						
w	4.8707	2.6889	0.6319	0.2290	0.0274	0.0000
In	4.7639	2.4875	0.6038	0.2291	0.0260	0.0000
O	4.6868	2.5417	0.6139	0.2261	0.0272	0.0000
Sn	5.1639	3.0602	0.6781	0.2317	0.0289	0.0000
$SrNbO_3:V_{Nb}$						
w	0.3449	0.1377	0.1253	0.0844		
Nb	0.0041	0.0186	0.0561	0.0664		
O	0.4074	0.1888	0.1520	0.1020		
Sr	1.0253	0.1462	0.1241	0.0558		
$SrNbO_3:V_{Sr}$						
w	0.1739	0.0812	0.0469	0.0095		
Nb	0.0146	0.0402	0.0095	0.0080		
O	0.2621	0.1044	0.0781	0.0156		
Sr	0.1546	0.0733	0.0149	0.0004		
$CaN_2:V_{Ca}$						
w	0.0566	0.3213	0.0031	0.1659		
Ca	0.0018	0.0003	0.0292	0.1890		
N	0.1108	0.7422	0.0001	0.1547		
$Ca_6Al_7O_{16}:V_{Al}$						
w	3.3740	0.0257	0.0000	0.0000		
Al	3.4045	0.0217	0.0006	0.0000		
Ca	3.3730	0.0513	0.0000	0.0001		
O	3.3610	0.0198	0.0000	0.0000		



Supplementary Figure 1. The integrated density of states (IDOS) of the principal conduction band (PCB) of $SrNbO_3$ with (a) and without (b) Nb vacancy in the 2×2×1 supercell. There are 16 electrons in the PCB of $SrNbO_3$, creating an Nb vacancy that leads to the loss of 5 electrons and results in 11 electrons in the PCB. The IDOS on the y-axis is given with respect to the IDOS at the principal conduction band minimum (E_{pcbm}).

Relaxed POSCAR of primitive structure for all materials used.

Crystal structure of Cu (SG: 225)

Cu1

1.00000000000000

2.2260390700239872 0.0000000057329654 1.2852040185709930

0.7420133674538185 2.0987303500495691 1.2852040185709930

0.0000000000930815 0.0000000000658186 2.5704080268195422

Cu

1

Direct

-0.0000000000000000 0.0000000000000000 -0.0000000000000000

Crystal structure of Zn (SG: 194)

Zn2

1.00000000000000

2.6487830749714711 0.0000000149255422 0.0000000000000000

-1.3243905113929617 2.2939132598290133 -0.0000000000000000

0.0000000000000000 0.0000000000000000 5.0319935167634107

Zn

2

Direct

0.3333330000000032 0.6666669999999968 0.2500000000000000

0.6666669999999968 0.3333330000000032 0.7500000000000000

Crystal structure of CaN_2 (SG: 139)

Ca1 N2

1.00000000000000

3.6179146140464997 0.0000000000000001 0.0000000106736897

0.0000000000000001 3.6179146140464997 0.0000000106736897

-1.8089567909851589 -1.8089567909851589 2.9876523243798125

Ca N

1 2

Direct

-0.0000000000000000 -0.0000000000000000 -0.0000000000000000

0.6051671569448525 0.6051671569448525 0.2103323238830390

0.3948328430551475 0.3948328430551475 0.7896676761169611

Crystal structure of $In_{15}SnO_{24}$ (SG: 148)

In15 Sn1 O24

1.00000000000000

5.1590089023797496 -7.2846976031268449 0.0006514768827309

5.1590088982768227 7.2846975986892755 0.0006514825135962

-5.1281573945802279 -0.0000000057901851 7.3064496335646183

In Sn O

15 1 24

Direct

0.9657959360519921 0.7501121957111972 0.2175828890160473

0.7153420146844205 0.4666047645038204 0.7493439837749650

0.7824171109838477 0.0342040639479410 0.2498878042884651

0.2498878042887749 0.7824171109838914 0.0342040639479345

0.2506560162250128 0.2846579853155622 0.5333952354961042

0.5000000000000000 0.5000000000000000 0.0000000000000000

0.5333952354961660 0.2506560162250176 0.2846579853155458

0.0000000000000000 0.5000000000000000 0.5000000000000000

0.4666047645038339 0.7493439837749826 0.7153420146844542

0.5000000000000000 0.0000000000000000 0.5000000000000000

0.7493439837749870 0.7153420146844378 0.4666047645038956

0.7501121957112251 0.2175828890161086 0.9657959360520653

0.2846579853155794 0.5333952354961797 0.2506560162250350

0.2175828890161521 0.9657959360520590 0.7501121957115349

0.0342040639480079 0.2498878042888026 0.7824171109839527

0.0000000000000000 0.0000000000000000 0.0000000000000000

0.0457899839542068 0.0395587250837473 0.2635708601416736

0.4560337425480880 0.2277904922141403 0.4939040660260973

0.7299611288071328 0.7744903728309496 0.2361959134254589

0.0395587250835838 0.2635708601404517 0.0457899839543311

0.5336883016362527 0.9925329668193521 0.2616477760650023

0.2277904922141442 0.4939040660263447 0.4560337425479027

0.7638040865748550 0.2700388711928888 0.2255096271689243
0.7383522239349708 0.4663116983638305 0.0074670331811654
0.5060959339736261 0.5439662574518710 0.7722095077858969
0.2635708601403235 0.0457899839538992 0.0395587250831274
0.2255096271692161 0.7638040865749993 0.2700388711934438
0.9925329668193943 0.2616477760651619 0.5336883016363797
0.0074670331806058 0.7383522239348382 0.4663116983636202
0.4939040660263740 0.4560337425481290 0.2277904922141030
0.7744903728307838 0.2361959134250006 0.7299611288065562
0.7364291398596765 0.9542100160461007 0.9604412749168727
0.2361959134251450 0.7299611288071112 0.7744903728310756
0.2616477760650293 0.5336883016361695 0.9925329668188348
0.4663116983637473 0.0074670331806480 0.7383522239349974
0.7722095077858558 0.5060959339736550 0.5439662574520975
0.2700388711928671 0.2255096271690503 0.7638040865745410
0.9604412749164162 0.7364291398595483 0.9542100160456686
0.5439662574519120 0.7722095077858597 0.5060959339739026
0.9542100160457935 0.9604412749162526 0.7364291398583264

Crystal structure of $SrNbO_3$ (SG: 62)

Sr4 Nb4 O12

1.00000000000000

5.7317703281525354 -0.0000000000000000 0.0000000000000000

0.0000000000000000 5.7279045419366890 0.0000000000000000

0.0000000000000000 0.0000000000000000 8.1206281687158341

Sr Nb O

4 4 12

Direct

0.0005159495616428 0.9892406187262446 0.7500000000000000

0.4994840504383573 0.4892406187262448 0.7500000000000000

0.5005159495616428 0.5107593812737554 0.2500000000000000

0.9994840504383572 0.0107593812737552 0.2500000000000000

0.5000000000000000 -0.0000000000000000 0.5000000000000000

-0.0000000000000000 0.5000000000000000 0.0000000000000000

-0.0000000000000000 0.5000000000000000 0.5000000000000000

0.5000000000000000 -0.0000000000000000 0.0000000000000000

0.7274359500609601 0.2725145844408953 0.4850776051952833

0.7725640499390399 0.7725145844408958 0.0149223948047166

0.2274359500609602 0.2274854155591044 0.5149223948047165

0.2725640499390399 0.7274854155591042 0.9850776051952835

0.2725640499390399 0.7274854155591042 0.5149223948047165

0.2274359500609602 0.2274854155591044 0.9850776051952835

0.7725640499390399 0.7725145844408958 0.4850776051952833

0.7274359500609601 0.2725145844408953 0.0149223948047166

0.0293259341224857 0.4967768401769211 0.2500000000000000

0.4706740658775143 0.9967768401769211 0.2500000000000000

0.5293259341224855 0.0032231598230789 0.7500000000000000

0.9706740658775145 0.5032231598230789 0.7500000000000000

Crystal structure of $Ca_6Al_7O_{16}$ (SG: 220)

Ca12 Al14 O32

1.00000000000000

-6.0544659836645680 6.0547986214486489 6.0548573392406357

6.0544886839032355 -6.0548289554224057 6.0549103921286909

6.0544942561415782 6.0548572402993859 -6.0548876919144874

Ca Al O

12 14 32

Direct

0.6377231320045896 0.2498660797087929 0.8879173413094695

0.8621785375245056 0.7501960233058260 0.6120467883450406

0.3880114428894950 0.7500220019030177 0.1379909970433312

0.1120895563140992 0.2499742108845632 0.3621031436452991

0.8879330341482209 0.6379601389019782 0.2499997004088316

0.6120957921331326 0.8620623970805590 0.7500191261318471

0.1380754743554058 0.3878879337857014 0.7501150174402492

0.3618807600776764 0.1120325920348487 0.2497940017776718

0.2500180857569513 0.8884896958975531 0.6385006280810714

0.7500069224667705 0.6121742619332976 0.8621921447132578

0.7499897005268713 0.1378179878607877 0.3878158171312695

0.2500035171762980 0.3615243810440393 0.1115059984442062

0.3749714389666730 0.2499938358622765 0.6250410571173507

0.1250297310351704 0.7500644079799784 0.8750182926196337

0.6249551690389320 0.3749508666888935 0.2499236251491830

0.8750584321197358 0.1249944010064954 0.7500248570814753

0.2499819817159631 0.6249866094304545 0.3749966440369990

0.7500067083213825 0.8750123815930357 0.1249935276703027

0.4999697269688632 0.0000655077872513 0.0340203784325834

0.0340293766355443 0.5000441184603797 0.0000126072015656

0.0000554468229879 0.0340805847778697 0.5000913111890900

0.4659376820145008 0.4659598324813500 0.4660168159382175

0.5339694787822107 0.4998937459325742 -0.0000722470098493
0.5000440303424888 -0.0000040528345813 0.5340466102116864
-0.0000329075185752 0.5339743838600400 0.4999372152646606
0.9660295660164453 0.9659857847152490 0.9659517580158560
0.5003483008713554 -0.0000966511188376 0.8678685333850407
0.8677348970110096 0.4999843770124809 -0.0000825027671305
0.9997295512449523 0.8675846380649350 0.4995686127280879
0.6322094812500463 0.6321246649343931 0.6322845310596112
0.3679723176323060 0.5004003046235072 0.0000719360462198
0.5001075807008557 0.0001198127492164 0.3678785914744381
0.9998903654573980 0.3677086512575912 0.4999430731313201
0.1319963310356414 0.1321653988684299 0.1324702572804898
0.4089072139968656 0.0942694195499029 0.6148120860149477
0.5206684389469178 0.4058335436126793 0.8145720051639368
0.0911357484792625 0.7059146842406953 0.6853489569772586
0.9793003530295898 0.7938892200109674 0.8851758246268385
0.1147084290020074 0.5941429006366230 0.9087176943750370
0.3147044926754503 0.9055961651294197 0.0208179170110486
0.1853113204546253 0.2061003693746624 0.5908570344019446
0.3852739306108204 0.2940159060122790 0.4794601355341558
0.6152196738064273 0.4091249920072932 0.0944221687183022
0.8145712795656751 0.5205694889993332 0.4058435667002249
0.6854341652133916 0.0912621185189694 0.7059728947469364
0.8847603947358006 0.9791824674742426 0.7938847572848122
0.9087630753254153 0.1148711604167646 0.5941768546150897
0.0205487097433533 0.3146434247761419 0.9057911628186633
0.5913064250260286 0.1854172138508177 0.2060982257104263
0.4794314621372727 0.3851731587063664 0.2940834585022866
0.0941000104307351 0.6147170909421871 0.4087097500404714
0.4058332430680505 0.8146095825834905 0.5206202167902979
0.7059621704586529 0.6853547921303178 0.0910214304307309

0.7940503134812088 0.8851447705339719 0.9794073048677928
0.5942927250532504 0.9089371805367252 0.1149023659021659
0.9056927244797573 0.0205838327307355 0.3146401982434414
0.2060216630656954 0.5912507344265180 0.1853923052283974
0.2940003953738468 0.4793965143249376 0.3852664855664197