Supporting Information: Large-scale computational identification of p-type oxide semiconductors by hierarchical screening

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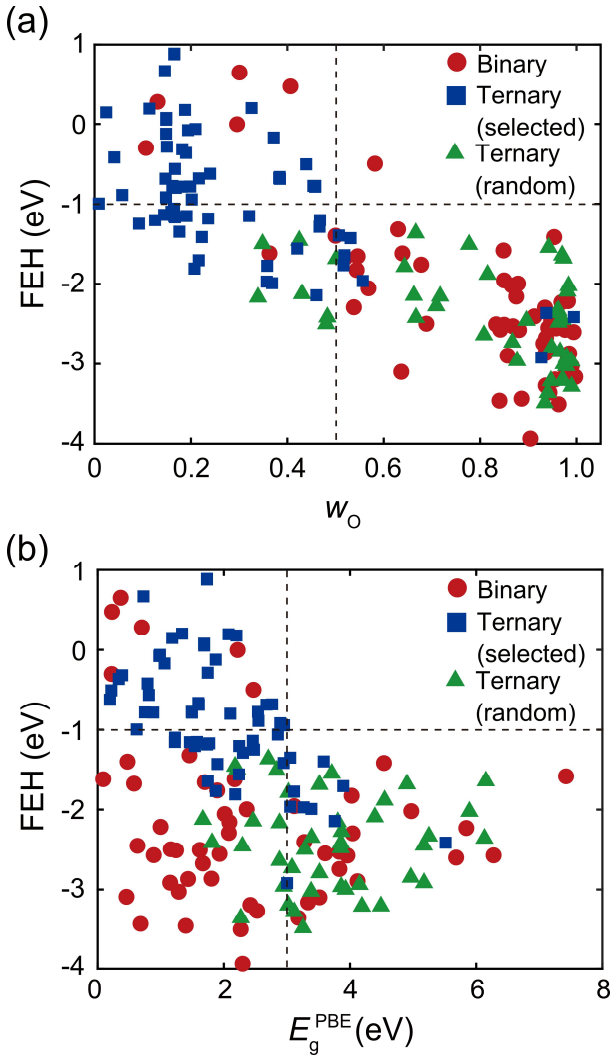

Figure S1. FEH versus (a) oxygen partial weight at the valence band top (w_O) and (b) fundamental band gap with PBE (E_g^{PBE}) for binary, selected ternary and randomly chosen ternary oxides. Vertical and horizontal dashed lines indicate the FEH and simple descriptor criteria for p-type, respectively.

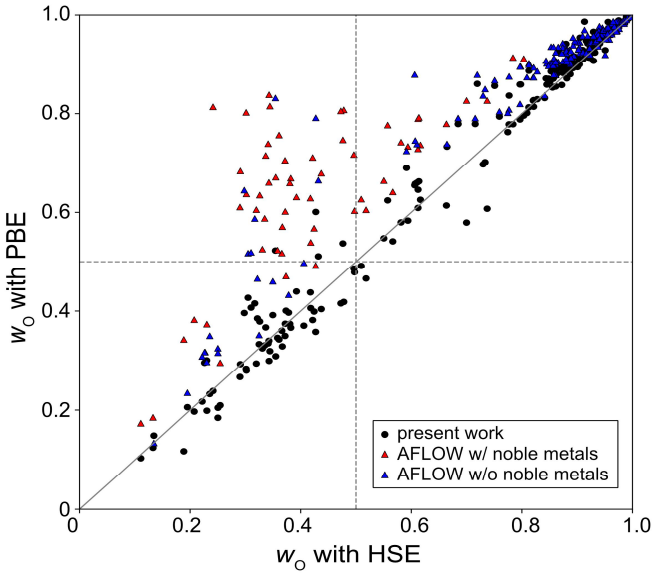

Figure S2. Comparison of oxygen partial weight. Oxygen partial weight by HSE versus oxygen partial weight by PBE in our database (black) and AFLOW (blue or red). In AFLOW database, compounds containing a series of noble metal (Ag, Au, Pd and Pt) have higher w_O compared with w_O by HSE. In our database, there is little difference in root mean square errors (RMSEs) of two groups.

Table S1. RMSEs of w_O in AMP[2] and AFLOW with HSE.

RMSE	AMP[2]	AFLOW
w/ noble metals	0.039	0.256
w/o noble metals	0.041	0.086

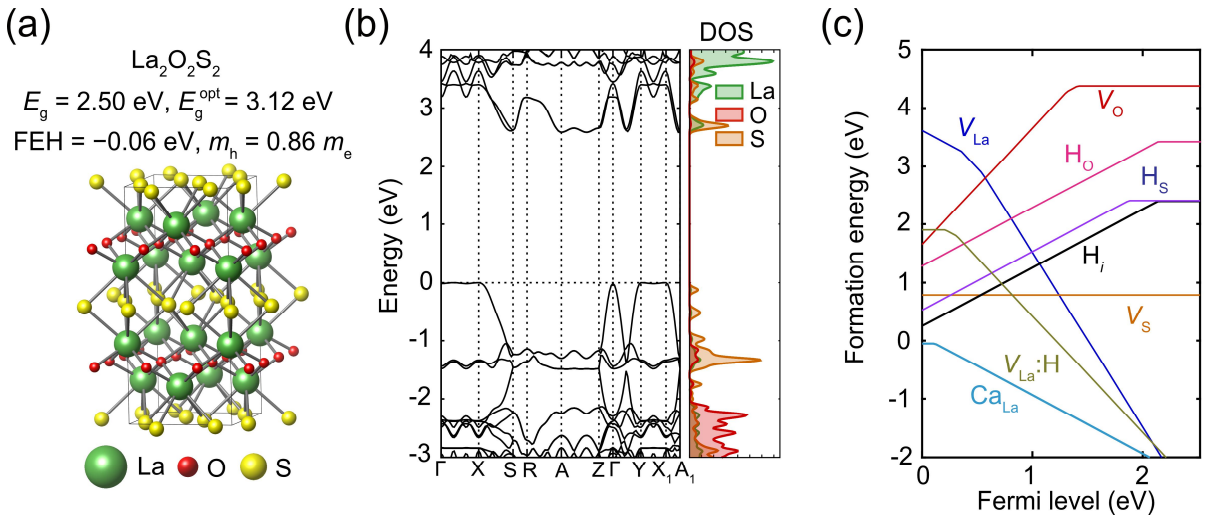

Figure S3. (a) The unit-cell structure of $La_2O_2S_2$ (*Cmce*). (b) Band structure and partial density of states. (The VBM is set to zero.) (c) The formation energies of intrinsic and hydrogen defects at the oxygen-rich condition. For (b), PBE functional is used with scissor-correction with the HSE gap.

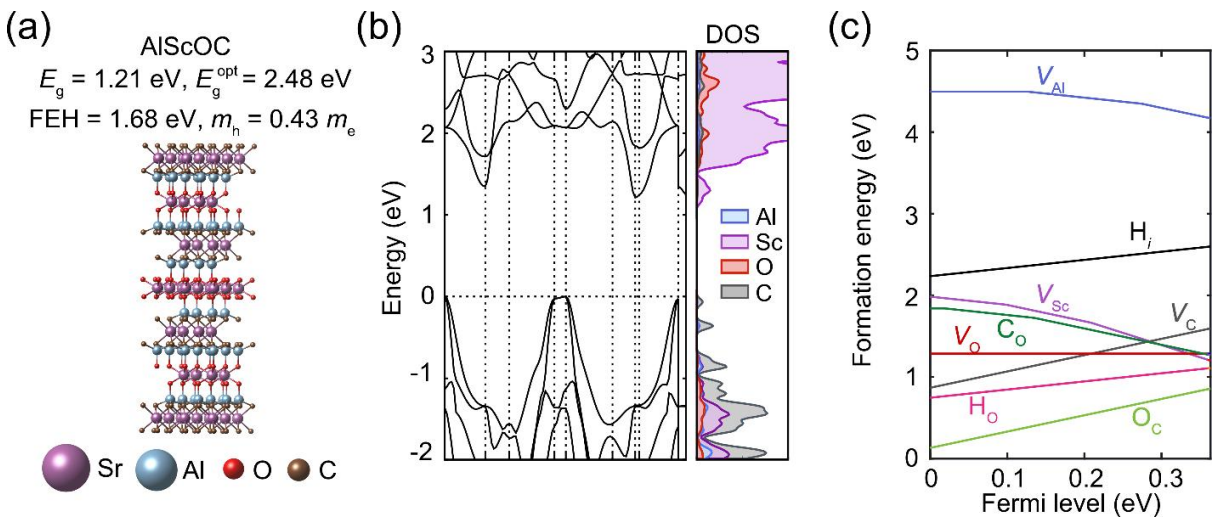

Figure S4. (a) The unit-cell structure of AlScOC. (b) Band structure and partial density of states. (The VBM is set to zero.) (c) The formation energies of intrinsic and hydrogen defects at the oxygen-rich condition with PBE calculation. For (b), PBE functional is used with scissor-correction with the HSE gap.

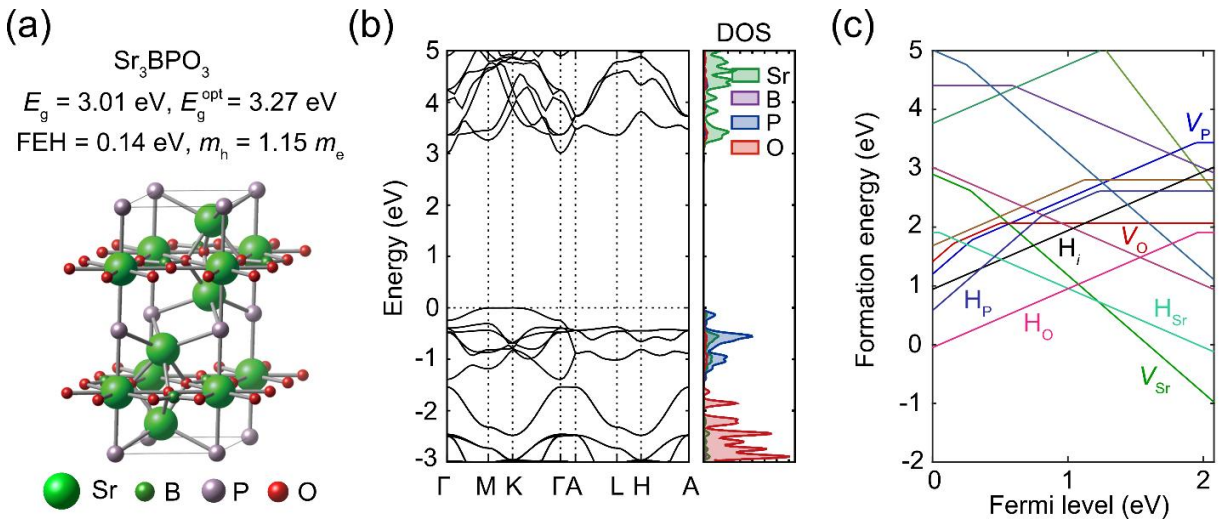

Figure S5. (a) The unit-cell structure of Sr_3BPO_3. (b) Band structure and partial density of states. (The VBM is set to zero.) (c) The formation energies of intrinsic and hydrogen defects at the oxygen-rich condition with PBE calculation. For (b), PBE functional is used with scissor-correction with the HSE gap.

Table S2. Names, ICSD numbers, space groups, fundamental and optical band gaps and hole effective masses of Group I: unpaired electrons in Figure 5b.

Name	ICSD	Space group	E_g (eV)	E_g^{opt} (eV)	FEH (eV)	m_h^* (m_e)
$NaNbO_2$	29282	$P6_3/mmc$	2.25	2.40	2.14	0.74
$LiNbO_2$	451	$P6_3/mmc$	2.40	2.40	1.21	0.74
$CaNb_2O_4$	88779	$Pbcm$	2.05	2.24	1.14	0.75
$Mg_3Nb_6O_{11}$	62662	$P\bar{3}m1$	1.21	1.67	0.47	2.07
Cr_2O_3	25781	$R\bar{3}c$	3.88	4.00	0.00	3.92
$CaFeSi_2O_6$	10226	$C2/c$	3.57	3.57	-0.05	3.59
$Ba_2FeGe_2O_7$	22358	$P\bar{4}2_1m$	2.18	2.18	-0.06	4.54
$NaVO_2$	420138	$C2/m$	2.44	2.46	-0.09	1.36
Ta_2VO_6	23600	$P4_2/mnm$	1.51	1.59	-0.12	3.18
$CaFeO_2$	246244	$I4_1/amd$	1.83	1.83	-0.14	1.46
Li_2FeSiO_4	161649	$Pmn2_1$	3.59	3.59	-0.19	4.14
Fe_2GeO_4	93973	$Fd\bar{3}m$	1.69	1.75	-0.20	21.90
$NaTiSi_2O_6$	281615	$P\bar{1}$	2.73	2.78	-0.30	2.99
NbO_2	35181	$I4_1$	1.30	1.75	-0.30	2.88
Fe_2SiO_4	41003	$P6_3/mmc$	2.44	2.55	-0.33	22.67
Cr_2SiO_4	75639	$P6_3/mmc$	3.01	3.17	-0.34	3.19
$LiFeAsO_4$	245182	$Pnma$	2.71	2.77	-0.35	1.83
$NaTiSi_2O_6$	39194	$C2/c$	2.73	2.75	-0.35	3.29
Li_2FeSiO_4	246132	$P2_1$	3.62	3.69	-0.38	7.44
Cr_2MnO_4	167400	$Fd\bar{3}m$	3.69	3.81	-0.43	5.17
$LiTiSi_2O_6$	96292	$C2/c$	2.74	2.75	-0.45	3.51
$FeGeO_3$	89788	$I4/mmm$	1.54	1.54	-0.50	17.40
Ba_2VO_4	40708	$Fd\bar{3}m$	2.46	2.49	-0.55	29.86
$FeTe_6O_{13}$	417293	$P4_2/ncm$	2.46	2.74	-0.63	93.05
FeB_2O_4	420403	$C2/c$	3.15	3.15	-0.63	5.43
$FeTiO_3$	9805	$R\bar{3}$	2.13	2.13	-0.64	5.15
WO_2	74774	$Pnma$	1.52	1.59	-0.64	1.62
Mn_2TiO_4	22313	$R\bar{3}$	2.19	2.19	-0.65	1.82
Mn_5VO_8	262807	$P\bar{1}$	1.88	1.90	-0.66	2.14
$KCrO_2$	425293	$P6_3/mmc$	4.22	4.31	-0.67	2.98
$AgCoO_2$	246157	$P6_3/mmc$	2.70	3.46	-0.68	3.99
$CrWO_4$	8269	$C2/m$	1.53	1.63	-0.69	1.14
$LaCrO_3$	91271	$R\bar{3}c$	3.38	3.40	-0.71	2.67

Name	ICSD	Space group	E_g (eV)	E_g^{opt} (eV)	FEH (eV)	m_h^* (m_e)
$KCrO_2$	40267	$R\bar{3}m$	4.22	4.36	-0.72	2.83
K_3FeO_2	73215	$P4_12_12$	2.17	2.30	-0.73	11.06
$FeTi_2O_5$	37231	$Cmcm$	1.68	1.82	-0.76	13.30
$MgCr_2O_4$	290588	$I4_1/amd$	4.20	4.20	-0.76	3.60
$MgCr_2O_4$	290589	$C2/c$	4.19	4.19	-0.79	3.40
$MgCr_2O_4$	52386	$Fd\bar{3}m$	4.19	4.19	-0.79	3.39
$CaFeTi_2O_6$	79353	$P4_2/nmc$	1.47	1.47	-0.80	12.58
$Rb_5Co_2O_4$	73190	$P\bar{1}$	2.20	2.41	-0.85	108.98
BVO_3	45060	$P2_1/c$	2.61	2.71	-0.90	6.95
Li_6CoO_4	62688	$P2_1/c$	3.87	3.87	-0.91	3.01
Rb_3CoO_2	94437	$Pnma$	2.22	2.30	-0.94	62.96
$PbVO_3$	152276	$P4mm$	2.23	2.23	-0.98	3.29
$ZnCr_2O_4$	50047	$Fd\bar{3}m$	4.02	4.02	-0.99	4.16

Table S3. Names, ICSD numbers, space groups, fundamental and optical band gaps and hole effective masses of Group I: quasi-closed shell d^6 (Rh^{3+}) or d^8 (Pd^{2+} and Pt^{2+}) in Figure 5c.

Name	ICSD	Space group	E_g (eV)	E_g^{opt} (eV)	FEH (eV)	m_h^* (m_e)
$Na_2Pd_3O_4$	6157	*Immm*	2.00	2.01	0.74	0.88
$MgPt_3O_6$	35340	*Cmmm*	1.28	1.28	0.25	0.90
Na_2PtO_2	25018	*Immm*	3.15	3.32	0.21	2.64
$CoRh_2O_4$	109301	$Fd\bar{3}m$	2.42	3.15	0.17	3.81
$CuRhO_2$	29214	$R\bar{3}m$	2.22	2.96	0.06	2.23
$ZnPt_3O_6$	35339	*Cmmm*	1.26	1.26	0.01	0.90
$CdPt_3O_6$	35407	*Cmmm*	1.16	1.16	0.01	0.99
Li_2PdO_2	61199	*Immm*	3.35	3.85	-0.02	2.49
$AgRhO_2$	261561	$R\bar{3}m$	2.27	2.62	-0.10	2.03
$NaRhO_2$	66280	$R\bar{3}m$	3.32	3.39	-0.28	6.25
Rh_2O_3	9206	*Pbca*	2.43	2.43	-0.32	6.29
Rh_2O_3	33645	$R\bar{3}c$	2.54	2.70	-0.41	3.21
$CdRh_2O_4$	28954	*Amm2*	2.75	2.75	-0.48	3.29
$MgRh_2O_4$	109299	$Fd\bar{3}m$	3.11	3.11	-0.48	8.12
$ZnRh_2O_4$	109298	$Fd\bar{3}m$	2.90	2.91	-0.53	4.55
$PdBi_2O_4$	200145	$P4/ncc$	1.59	2.24	-0.57	1.13
K_2PdO_2	6158	*Immm*	3.56	3.79	-0.62	2.62
$CaRh_2O_4$	170597	*Pnma*	2.77	2.79	-0.66	11.17
KPd_2O_3	248051	$R\bar{3}m$	1.90	2.18	-0.67	2.28
Na_2PtO_3	25020	*Fddd*	3.29	3.36	-0.93	2.13
$LiRhO_2$	59179	$Fd\bar{3}m$	3.51	3.51	-0.97	16.95

Table S4. Names, ICSD numbers, space groups, fundamental and optical band gaps and hole effective masses of Group I: closed shell d^{10} (Cu^{1+} & Ag^{1+}) in Figure 5d.

Name	ICSD	Space group	E_g (eV)	E_g^{opt} (eV)	FEH (eV)	m_h^* (m_e)
LiCuO	40156	$I4/mmm$	2.59	3.10	0.88	2.77
CuLaOTe	154591	$P4/nmm$	2.24	2.24	0.52	0.53
Cu_2O	63281	$Pn\bar{3}m$	2.04	2.04	0.28	1.36
$CuAlO_2$	25593	$R\bar{3}m$	3.48	4.15	0.19	2.73
$CuAlO_2$	95661	$P6_3/mmc$	3.58	3.94	0.18	3.64
CuBiOSe	74475	$P4/nmm$	1.15	1.28	0.18	0.79
$CuCrO_2$	82065	$P6_3/mmc$	2.86	3.71	0.11	3.65
$CuCrO_2$	26676	$I4/mmm$	2.90	3.63	0.10	4.43
NaCuO	15099	$I\bar{4}$	2.79	2.97	0.08	9.01
CuLaOSe	96758	$P4/nmm$	2.84	2.84	-0.02	0.78
$CuGaO_2$	95664	$P6_3/mmc$	2.41	3.78	-0.06	3.41
$CuGaO_2$	188625	$R\bar{3}m$	2.38	4.04	-0.08	2.26
Cu_2BaO_2	9456	$I4_1/amd$	2.75	2.75	-0.12	2.34
CuLaOS	86249	$P4/nmm$	3.02	3.02	-0.30	1.02
$CuLa_3O_2S_3$	96438	$Pnma$	1.87	1.87	-0.31	0.67
$CuInO_2$	95670	$P6_3/mmc$	1.65	2.62	-0.32	3.10
$CuInO_2$	91855	$R\bar{3}m$	1.60	2.85	-0.36	2.62
$CuFeO_2$	246912	$R\bar{3}m$	1.54	1.54	-0.50	1.97
$NaCu_2O_2$	169713	$Pnma$	2.67	2.83	-0.51	2.19
$AgCrO_2$	25624	$R\bar{3}m$	2.92	3.46	-0.53	2.58
$CuMnO_2$	30379	$Fd\bar{3}m$	1.88	2.21	-0.54	1.31
$LiCu_2O_2$	69051	$P4_2/nmc$	2.19	2.79	-0.62	2.06
$CuInW_2O_8$	74944	$C2/c$	1.54	1.68	-0.67	3.70
$LiAg_3O_2$	4204	$Ibam$	1.97	1.97	-0.68	0.75
$CuScO_2$	151929	$P6_3/mmc$	3.96	3.78	-0.68	4.35
$AgAlO_2$	300020	$P6_3/mmc$	2.98	4.33	-0.68	2.38
$CuScO_2$	65547	$R\bar{3}m$	3.68	3.70	-0.69	2.65
KCuO	25695	$I\bar{4}$	2.94	2.99	-0.69	5.67
$CuReO_4$	416510	$R\bar{3}m$	2.71	2.71	-0.75	5.84
RbCuO	15100	$I\bar{4}$	2.78	2.81	-0.78	6.04
Cu_2PbO_2	400657	$C2/c$	1.65	1.77	-0.78	1.98
NaAgO	40153	$I4/mmm$	2.47	3.73	-0.80	5.13
Cu_2SrO_2	25002	$I4_1/amd$	3.15	3.15	-0.80	1.58

Name	ICSD	Space group	E_g (eV)	E_g^{opt} (eV)	FEH (eV)	m_h^* (m_e)
$CuYW_2O_8$	36622	$P1$	2.33	2.52	-0.84	2.74
$CuVO_3$	19046	$R\bar{3}$	1.56	1.63	-0.89	3.59
$CuYO_2$	60848	$R\bar{3}m$	4.17	4.06	-0.92	3.21
$AgFeO_2$	242114	$R\bar{3}m$	1.96	2.28	-0.92	0.79
$AgFeO_2$	242115	$P6_3/mmc$	2.10	2.10	-0.94	1.02
$CuYO_2$	35580	$P6_3/mmc$	4.20	4.48	-0.95	3.97
Na_3AgO_2	24817	$Ibam$	2.34	3.69	-0.97	0.93
K_3CoO_2	73212	$Pnma$	2.52	2.52	-0.97	117.33
$NaAg_3O_2$	9627	$Ibam$	1.82	1.82	-0.97	0.96
$CuMnVO_4$	170136	$Cmcm$	2.25	2.43	-0.98	2.42

Table S5. Names, ICSD numbers, space groups, fundamental and optical band gaps and hole effective masses of Group II: s in Figure 5e.

Name	ICSD	Space group	E_g (eV)	E_g^{opt} (eV)	FEH (eV)	m_h^* (m_e)
SnO	15516	$P\bar{3}m1$	0.71	2.79	0.65	1.25
$K_2Sn_2O_3$	40463	$I2_13$	1.85	1.89	0.20	0.32
$Rb_2Sn_2O_3$	24816	$R\bar{3}m$	1.66	1.66	-0.17	0.28
$K_2Sn_2O_3$	2216	$R3$	1.76	1.76	-0.37	0.26
In_6PtGa_2O	411505	$Fm\bar{3}m$	1.66	1.67	-0.70	7.13
In_7IrGeO_8	417829	$F\bar{4}3m$	1.42	1.46	-0.85	6.94
SnO	20624	$Pmn2_1$	1.95	2.70	-0.92	0.99
In_6PtGe_2O	170897	$Fm\bar{3}m$	2.56	2.78	-0.93	3.11

Table S6. Names, ICSD numbers, space groups, fundamental and optical band gaps and hole effective masses of Group III: oxychalcogenides in Figure 5f.

Name	ICSD	Space group	E_g (eV)	E_g^{opt} (eV)	FEH (eV)	m_h^* (m_e)
$Na_2Fe_2OSe_2$	186502	*I*4/*mmm*	1.48	1.51	1.98	1.04
ZrOS	36111	*P*4/*nmm*	1.57	1.57	0.67	0.54
CuLaOTe	154591	*P*4/*nmm*	2.24	2.24	0.52	0.53
La_2O_2Te	27004	*I*4/*mmm*	3.03	3.12	0.20	0.65
CuBiOSe	74475	*P*4/*nmm*	1.15	1.28	0.18	0.79
Na_5CoO_2S	412978	*P*4/*mmm*	1.89	2.53	0.16	2.28
$La_2Mn_2O_3Se_2$	181385	*I*4/*mmm*	2.30	2.62	0.01	2.35
CuLaOSe	96758	*P*4/*nmm*	2.84	2.84	-0.02	0.78
$La_2O_2S_2$	68498	*Cmce*	2.50	3.12	-0.06	0.86
$La_2O_2S_2$	2455	*Pbcm*	2.59	3.21	-0.10	0.86
La_2SiO_4Se	59941	*Pbcm*	3.75	3.82	-0.15	1.07
CuLaOS	86249	*P*4/*nmm*	3.02	3.02	-0.30	1.02
$CuLa_3O_2S_3$	96438	*Pnma*	1.87	1.87	-0.31	0.67
$La_4O_4Se_3$	419128	*Amm*2	1.63	1.68	-0.42	0.32
Sc_2O_2S	2450	*P*6$_3$/*mmc*	3.25	3.83	-0.64	1.00
$Ba_3V_2O_3S_4$	279607	*I*4/*mmm*	2.02	2.03	-0.66	4.88
$K_3Sb_7O_9S_3$	4215	*P*6$_3$	2.34	2.53	-0.70	5.37
Bi_2O_2S	29451	*Pnnm*	1.51	1.98	-0.88	1.12
Y_2OS_2	67503	*P*2$_1$/*c*	3.56	3.67	-0.89	1.49
AgLaOS	89020	*P*4/*nmm*	2.48	2.48	-0.90	0.82

Table S7. Names, ICSD numbers, space groups, fundamental and optical band gaps and hole effective masses of Group III: oxypnictides in Figure 5g.

Name	ICSD	Space group	E_g (eV)	E_g^{opt} (eV)	FEH (eV)	m_h^* (m_e)
AlScOC	419683	$R\bar{3}m$	1.21	2.48	1.68	0.43
La_3SbO_3	380456	$C2/m$	1.28	1.33	1.09	0.48
Ca_4Sb_2O	16353	$I4/mmm$	1.59	1.89	1.09	0.52
Ca_4As_2O	68203	$I4/mmm$	1.81	2.06	0.89	0.54
Ca_4Bi_2O	416137	$I4/mmm$	1.33	1.67	0.88	0.51
Ba_3TaAs_3O	280155	$Pnma$	1.62	1.63	0.64	0.88
Sr_3TaAs_3O	409567	$Pnma$	1.87	1.90	0.63	1.00
ZnYAsO	163780	$P4/nmm$	1.84	1.85	0.57	0.55
Ba_3NbAs_3O	408853	$Pnma$	1.60	1.65	0.46	0.91
ZnYOP	418523	$R\bar{3}m$	2.04	2.10	0.44	0.44
Ba_3BPO_3	402017	$P6_3/mmc$	2.21	2.51	0.42	0.80
Ca_4OP_2	68202	$I4/mmm$	2.04	2.28	0.41	0.80
ZnLaAsO	420204	$P4/nmm$	1.35	1.35	0.29	0.55
Sr_4As_2O	33904	$I4/mmm$	1.79	1.83	0.25	0.85
Sr_3BPO_3	401207	$P6_3/mmc$	3.01	3.27	0.14	1.15
Ba_3BAsO_3	402682	$P6_3/mmc$	2.24	2.47	0.08	0.78
ZnLaOP	85777	$P4/nmm$	1.45	1.45	-0.02	0.72
Sr_4OP_2	33903	$I4/mmm$	1.91	1.95	-0.10	1.36
Ba_3ZnON_2	55536	$P4/mmm$	1.19	1.23	-0.24	0.75
K_6NbAs_3O	409630	$P2_13$	1.70	1.76	-0.28	18.53
Ba_4Sb_2O	402284	$I4/mmm$	1.09	1.09	-0.50	0.34
KBa_4Sb_3O	410747	$I4/mcm$	1.69	1.74	-0.55	2.18
$LaTaON_2$	411138	$C2/m$	1.60	1.60	-0.94	0.50
Ba_4As_2O	33905	$I4/mmm$	1.21	1.21	-1.00	0.40