Supplementary Information

Transport properties of doped wide band gap layered oxychalcogenide semiconductors $Sr_2GaO_3Cu\mathit{Ch}$, $Sr_2ScO_3Cu\mathit{Ch}$ and $Sr_2InO_3Cu\mathit{Ch}$ (*Ch* = S or Se)

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Section A: Rietveld refinement fits to X-ray diffraction data for all six Sr_2MO_3CuCh materials

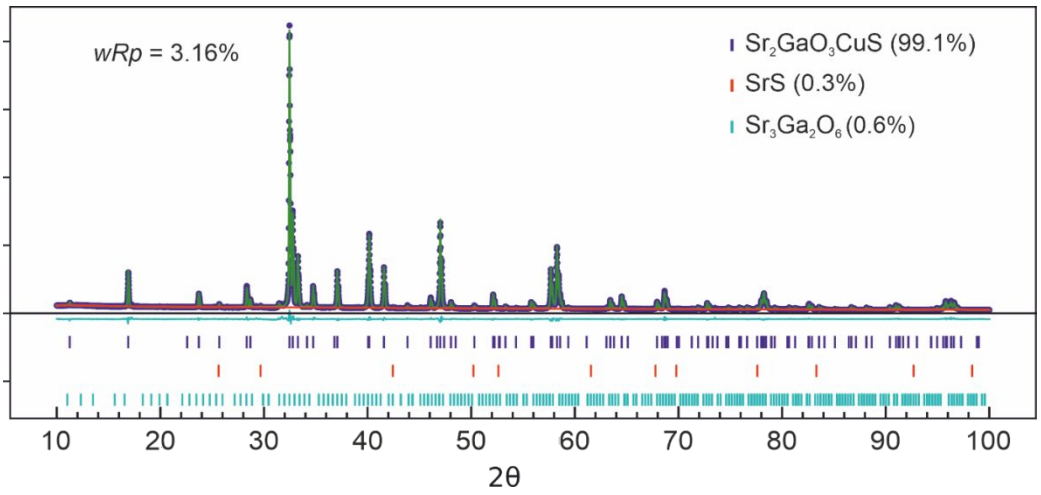

Figure S1. Rietveld refinement of Sr_2GaO_3CuS, data in blue, refinement fit in green.

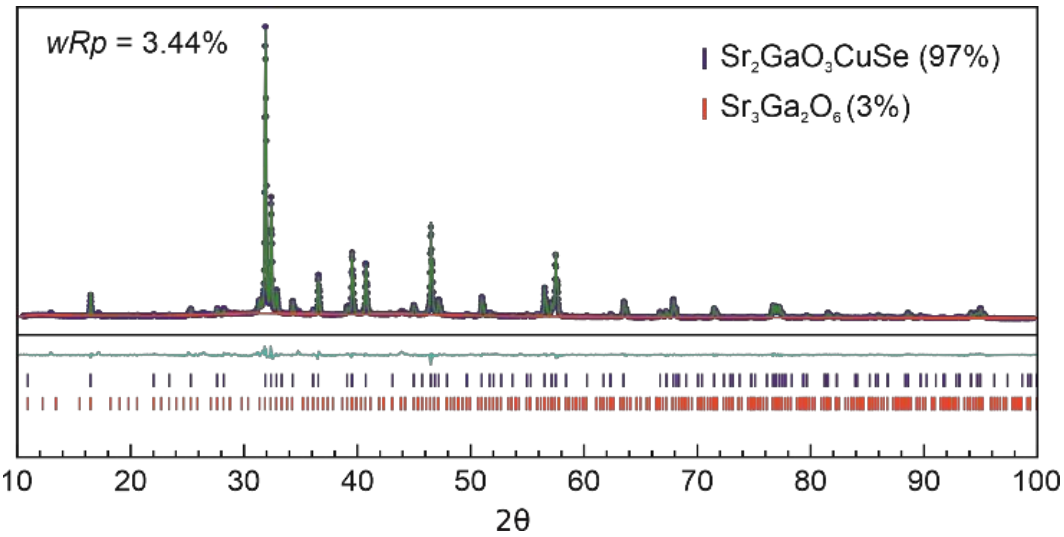

Figure S2. Rietveld refinement of Sr_2GaO_3CuSe, data in blue, refinement fit in green.

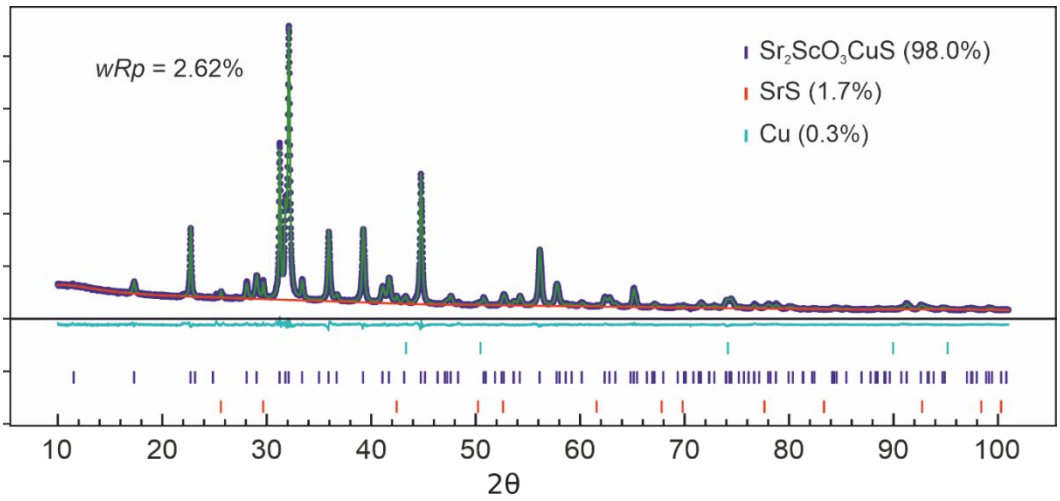

Figure S3. Rietveld refinement of Sr_2ScO_3CuS, data in blue, refinement fit in green.

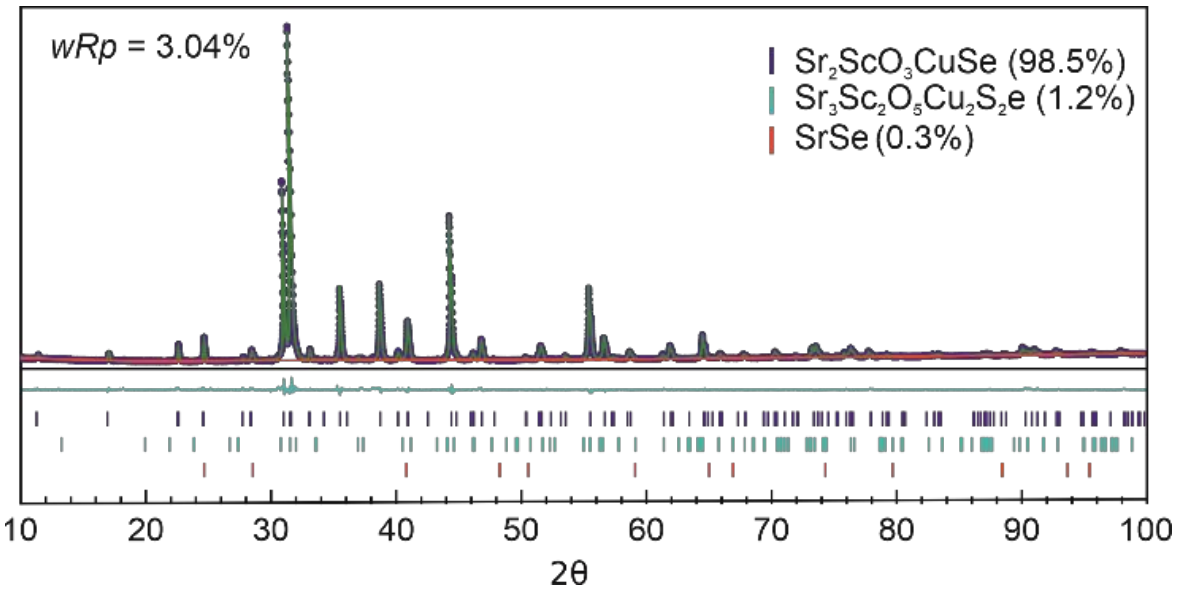

Figure S4. Rietveld refinement of Sr_2ScO_3CuSe, data in blue, refinement fit in green.

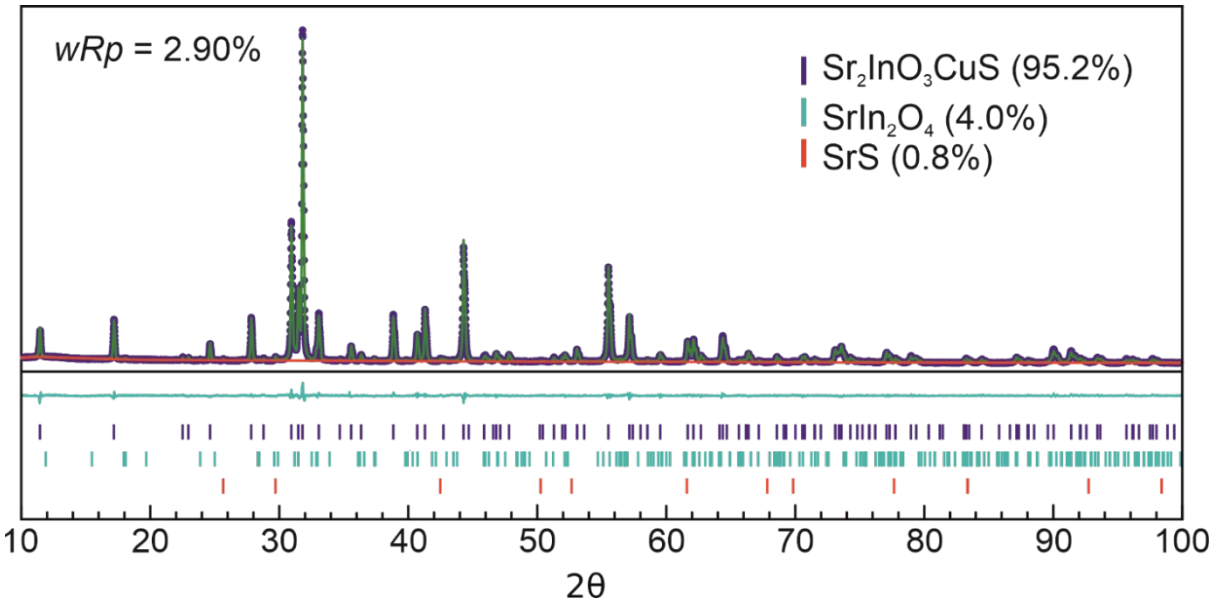

Figure S5. Rietveld refinement of Sr_2InO_3CuS, data in blue, refinement fit in green.

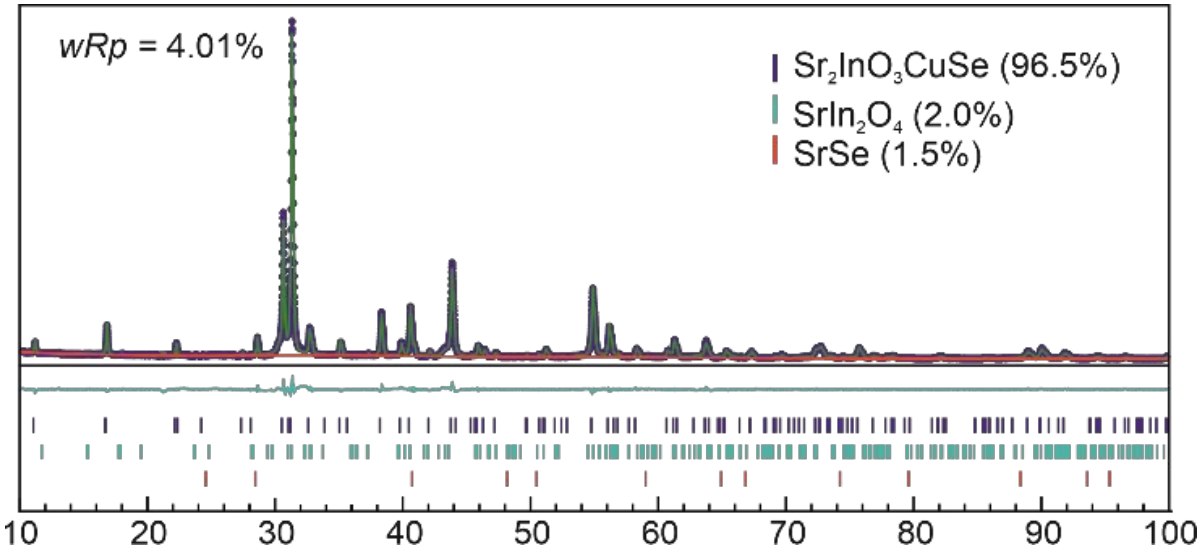

Figure S6. Rietveld refinement of Sr_2InO_3CuSe, data in blue, refinement fit in green.

Section B: Tables comparing our refined structural models to prior literature, where available

	$Sr_2Ga_2O_3CuS$, This work	$Sr_2Ga_2O_3CuS$, from reference 1
Lattice parameter *a* / Å	3.864026(13)	3.8606(4)
Lattice parameter *c* / Å	15.74911(6)	15.730(2)
Data Points	8887	N/A
Reflections (main phase)	104	N/A
Parameters	46	N/A
Purity	99.1	N/A
wRp	3.156	6.14
R_f^2	1.818	3.12
GoF	2.28	1.11
Sr1 (0.75, 0.75, *z*)	0.18435(5)	0.1842(2)
Sr2 (0.75, 0.75, *z*)	0.41401(5)	0.4140(1)
Ga (0.25, 0.25, *z*)	0.31210(7)	0.3144(2)
O1 (0.25, 0.75, *z*)	0.28940(16)	0.2899(4)
O2 (0.25, 0.25, *z*)	0.42975(22)	0.4270(6)
Cu (0.25, 0.75, *z*)	0	0
S (0.25, 0.25, *z*)	0.09413(15)	0.0940(3)

Table S1. Comparison of our refined model of Sr_3GaO_3CuS to prior literature data.

	Sr_2ScO_3CuS, this work	Sr_2ScO_3CuS, from reference 2
Lattice parameter *a* / Å	4.04780(4)	4.045
Lattice parameter *c* / Å	15.37012(20)	15.359
Data Points	8985	N/A
Reflections (main phase)	111	N/A
Parameters	44	N/A
Purity	98%	N/A
wRp	2.617	7.54
Rf2	2.476	2.88
GoF	1.61	N/A
Sr1 (0.75, 0.75, *z*)	0.17947(5)	0.181
Sr2 (0.75, 0.75, *z*)	0.41286(5)	0.415
Sc (0.25, 0.25, *z*)	0.30250(14)	0.305
O1 (0.25, 0.75, *z*)	0.28218(22)	0.283
O2 (0.25, 0.25, *z*)	0.43048(27)	0.429
Cu (0.25, 0.75, *z*)	0	0
S (0.25, 0.25, *z*)	0.08830(13)	0.09

Table S2. Comparison of our refined model of Sr_3ScO_3CuS to prior literature data.

	Sr_2InO_3CuS, this work	Sr_2InO_3CuS, from reference 3
Lattice parameter *a* / Å	4.092392 (20)	4.092009(38)
Lattice parameter *c* / Å	15.52813 (9)	15.51559(19)
Data Points	8887	N/A
Reflections (main phase)	111	N/A
Parameters	43	N/A
Purity	95.2%	100%
wRp	2.81	6.28
R_f^2	1.86	3.39
GoF	2.09	1.85
Sr1 (0.75, 0.75, *z*)	0.17706(5)	0.17598(19
Sr2 (0.75, 0.75, *z*)	0.41351(5)	0.41390(17)
In (0.25, 0.25, *z*)	0.30135(5)	0.30163(13)
O1 (0.25, 0.75, *z*)	0.27842(18)	0.28362(74)
O2 (0.25, 0.25, *z*)	0.4401(3)	0.4451(12)
Cu (0.25, 0.75, *z*)	0	0
S (0.25, 0.25, *z*)	0.08644(11)	0.08496(47)

Table S3. Comparison of the refined model of Sr_3InO_2CuS to prior literature data.

	Sr_2InO_3CuSe, this work	Sr_2InO_3CuSe from reference 3 [3]
Lattice parameter *a* / Å	4.12638(4)	4.125381(91)
Lattice parameter *c* / Å	15.82112(18)	15.81973(46)
Data Points	8887	N/A
Reflections (main phase)	115	N/A
Parameters	51	N/A
Purity	96.5%	93.6%
wRp	4.01	5.53
R_f^2	4.15	3.72
GoF	3.07	1.48
Sr1 (0.75, 0.75, *z*)	0.18483(16)	0.18464(24)
Sr2 (0.75, 0.75, *z*)	0.41576(14)	0.41492(20)
In (0.25, 0.25, *z*)	0.30547(15)	.30504(22
O1 (0.25, 0.75, *z*)	0.2843(4)	0.28354(86)
O2 (0.25, 0.25, *z*)	0.4397(7)	0.4409(14)
Cu (0.25, 0.75, *z*)	0	0
Se (0.25, 0.25, *z*)	0.09303(17)	0.09114(30)

Table S4. Comparison of the refined model of Sr_3InO_2CuSe to prior literature data.

Section C. Full structural details of all six Sr_2MO_3CuCh compounds, derived from samples and diffraction data prepared for this work

Atom Site	x	y	z	Uiso (Å^2)
Sr1	0.75	0.75	0.18435(5)	0.02885(27)
Sr2	0.75	0.75	0.41401(5)	0.02931(26)
Ga	0.25	0.25	0.31210(7)	0.02741(29)
O1	0.25	0.75	0.28940(16)	0.0571(11)
O2	0.25	0.25	0.42975(22)	0.0366(13)
Cu	0.25	0.75	0	0.0387(4)
S	0.25	0.25	0.09413(15)	0.0296(6)

Table S5. Structural parameters of the refined model of Sr_2GaO_3CuS. Sample refined in the *P*4/*nmm* space group, with a =3.864023(13) Å , c =15.74911(6) Å, vol =235.145(2) Å^3 , GOF = 2.28, Wrp = 3.16% and R_f^2=1.82% for 46 variables at room temperature.

Atom Site	x	y	z	Uiso (Å^2)
Sr1	0.75	0.75	0.17947(5)	0.0563(5)
Sr2	0.75	0.75	0.41286(5)	0.0553(5)
Sc	0.25	0.25	0.30250(14)	0.0430(5)
O1	0.25	0.75	0.28218(22)	0.0919(14)
O2	0.25	0.25	0.43048(27)	0.0430(14)
Cu	0.25	0.75	0	0.0785(6)
S	0.25	0.25	0.08830(13)	0.0593(9)

Table S6. Structural parameters of the refined model of Sr_2ScO_3CuS. Sample refined in the *P*4/*nmm* space group, with a =4.04780(4) Å c =15.37012(20) Å, vol =251.835(6) Å^3, GOF = 1.61, Wrp = 2.62% and R_f^2=2.48% for 46 variables at room temperature.

Atom Site	x	y	z	Uiso (Å^2)
Sr1	0.75	0.75	0.17706(5)	0.0110(4)
Sr2	0.75	0.75	0.41351(5)	0.0183(4)
In	0.25	0.25	0.30135(5)	0.00804(26)
O1	0.25	0.75	0.27842(18)	0.0272(12)
O2	0.25	0.25	0.4401(3)	0.0467(15)
Cu	0.25	0.75	0	0.0234(4)
S	0.25	0.25	0.08644(11)	0.0094(8)

Table S7. Structural parameters of the refined model of Sr_2InO_3CuS. Sample refined in the *P*4/*nmm* space group, with a = 4.092392 (20) Å, c = 15.52813 (9) Å, vol = 260.060(3) Å^3 , GOF = 2.09, Wrp = 2.811% and R_f^2=1.857% for 43 variables at room temperature.

Atom Site	x	y	z	Uiso (Å^2)
Sr1	0.75	0.75	0.19312(13)	0.0284(7)
Sr2	0.75	0.75	0.41598(11)	0.0323(9)
In	0.25	0.25	0.31667(14)	0.0275(10)
O1	0.25	0.75	0.2923(4)	0.0367(25)
O2	0.25	0.25	0.4334(6)	0.052(4)
Cu	0.25	0.75	0	0.0395(10)
Se	0.25	0.25	0.09785(12)	0.0268(9)

Table S8. Structural parameters of the refined model of Sr_2GaO_3CuSe. Sample refined in the *P*4/*nmm* space group, with a = 3.89988(4) Å, c = 16.09379(17) Å, vol = 244.771(6) Å^3, GOF = 3.72, Wrp = 3.30% and R_f^2=2.704% for 48 variables at room temperature.

Atom Site	x	y	z	Uiso (Å^2)
Sr1	0.75	0.75	0.18840(9)	0.0449(4)
Sr2	0.75	0.75	0.41500(7)	0.0431(4)
Sc	0.25	0.25	0.30730(18)	0.0344(6)
O1	0.25	0.75	0.28796(23)	0.0731(16)
O2	0.25	0.25	0.43136(28)	0.0636(19)
Cu	0.25	0.75	0	0.0567(5)
Se	0.25	0.25	0.09413(9)	0.0465(5)

Table S9. Structural parameters of the refined model of Sr_2ScO_3CuSe. Sample refined in the *P*4/*nmm* space group, with a = 4.076704(24) Å, c = 15.70839(13) Å, vol = 261.065(4) Å^3, GOF =2.25, Wrp = 3.23% and R_f^2=3.017% for 37 variables at room temperature.

Atom Site	x	y	z	Uiso (Å^2)
Sr1	0.75	0.75	0.18483(16)	0.0224(8)
Sr2	0.75	0.75	0.41576(14)	0.0396(10)
In	0.25	0.25	0.30547(15)	0.0247(6)
O1	0.25	0.75	0.2843(4)	0.0619(31)
O2	0.25	0.25	0.4397(7)	0.066(4)
Cu	0.25	0.75	0	0.0363(9)
Se	0.25	0.25	0.09303(17)	0.0211(9)

Table S10. Structural parameters of the refined model of Sr_2InO_3CuSe. Sample refined in the *P*4/*nmm* space group, with a = 4.12638(4) Å, c = 15.82112(18) Å, vol = 269.386(6) Å^3, GOF = 3.07, Wrp = 4.01% and R_f^2=4.153% for 51 variables at room temperature.

Bond / angle	Sr_2GaO_3CuS	Sr_2ScO_3CuS	Sr_2InO_3CuS	Sr_2GaO_3CuSe	Sr_2ScO_3CuSe	Sr_2InO_3CuSe
M-O1 eq / Å	1.96481(50)	2.04786(61)	2.07694(50)	1.9890(13)	2.06087(68)	2.0902(11)
M-O2 ax/ Å	1.8529(36)	1.9671(47)	2.1545(47)	1.8786(99)	1.9488(52)	2.124(11)
M-*X*/ Å	3.4328(26)	3.2923(29)	3.3372(19)	3.5216(30)	3.3486(32)	3.3610(36)
O1-*B*-O2 / °	100.484(87)	98.77(12)	99.871(87)	101.37(22)	98.48(13)	99.22(20)
*M*O5 block/ Å	2.2104(43)	2.2794(54)	2.5106(54)	2.271(12)	2.2526(57)	2.459(13)
Sr1-O1/ Å	2.5436(17)	2.5668(21)	2.5815(18)	2.5199(43)	2.5692(24)	2.5949(41)
Sr1-X / Å	3.0797(11)	3.18684(94)	3.21775(82)	3.1552(14)	3.24077(91)	3.2593(16)
O1_*A*1_X / °	79.839(42)	76.684(44)	76.266(37)	80.188(85)	77.240(48)	76.523(83)
Sr1 Block / Å	3.0753(35)	2.9800(39)	2.9811(33)	3.1294(67)	3.0448(39)	3.0261(69)
Sr2-O2 eq / Å	2.74350(32)	2.87501(40)	2.92307(67)	2.77185(99)	2.89410(40)	2.9423(15)
Sr2-O2-ax / Å	2.4606(36)	2.4079(42)	2.2732(47)	2.4240(98)	2.4134(45)	2.287(11)
Sr2 Block / Å	1.1064(35)	1.0685(42)	0.9301(47)	1.0718(97)	1.0782(44)	0.954(11)
Cu-*X* / Å	2.4352(14)	2.4368(11)	2.44715(94)	2.5064(12)	2.51818(83)	2.5344(16)
X-Cu-*X* / °	105.001(72)	112.310(61)	113.472(51)	102.151(58)	108.085(42)	108.993(79)
CuCh block / Å	2.9649(33)	2.7144(28)	2.6845(24)	3.1496(27)	2.9573(20)	2.9437(38)

Table S11. Summary of all major bond angles, bond lengths and 'block' heights for the Sr_2MO_3CuCh phases, where *M* = Sc, Ga or In, and *Ch* =S or Se. Graphical representation of the location of the different atom sites (*eg.* Sr1, Sr2) and 'blocks' please refer to figure 2 in the main paper.

Section D. Rietveld refinement fits and summary for sodium and potassium doped $A_{0.05}Sr_{1.95}MO_3CuCh$ samples

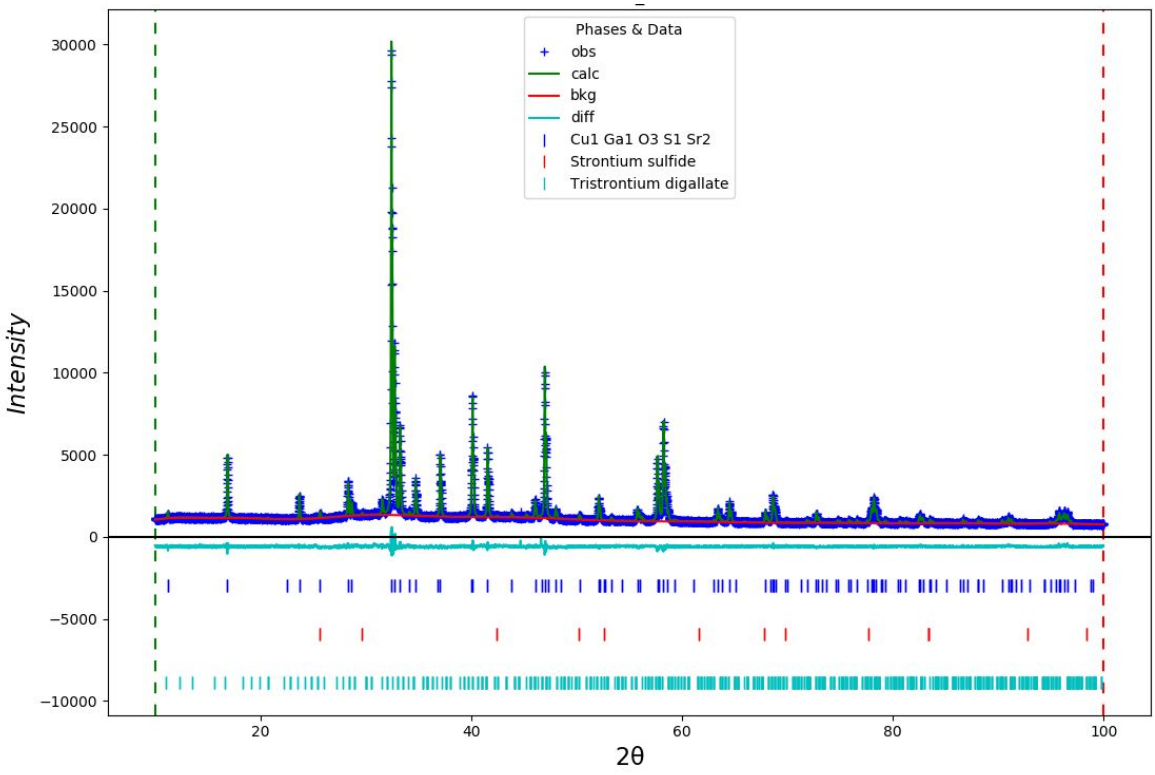

Figure S7. Refinement of sodium doped nominal $Na_{0.05}Sr_{195}GaO_3CuS$

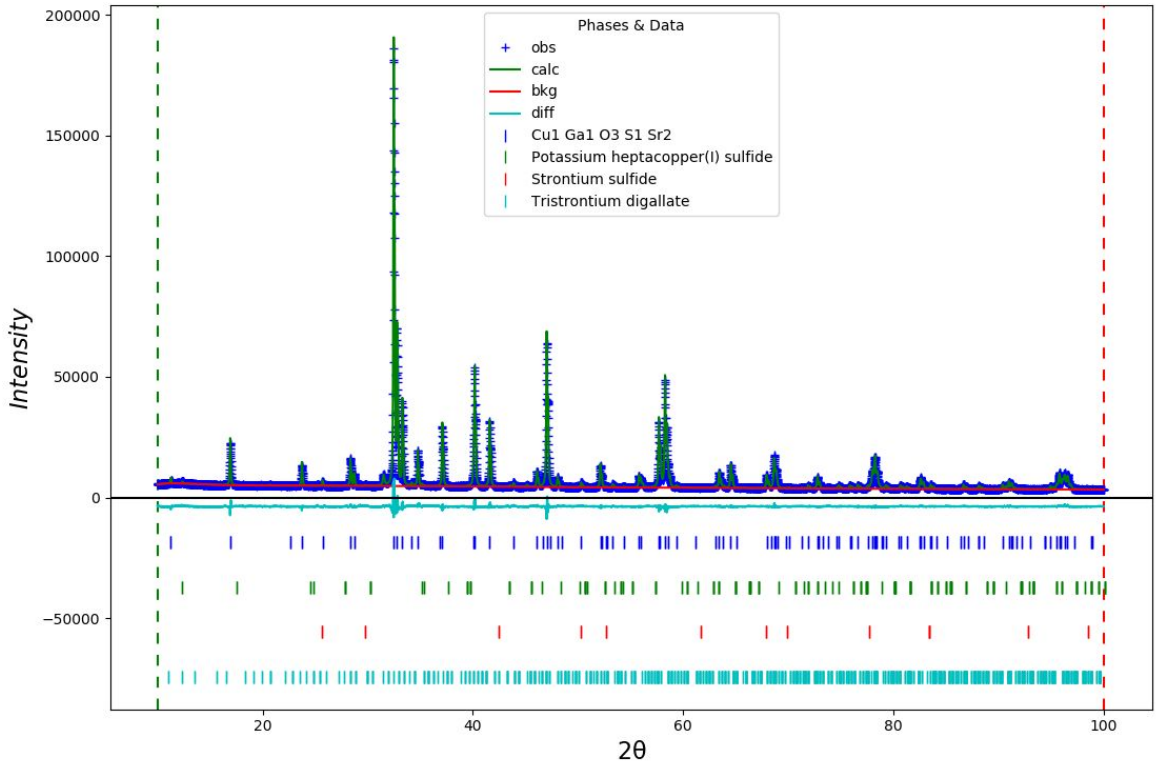

Figure S8. Refinement of potassium doped nominal $K_{0.05}Sr_{1.95}GaO_3CuS$

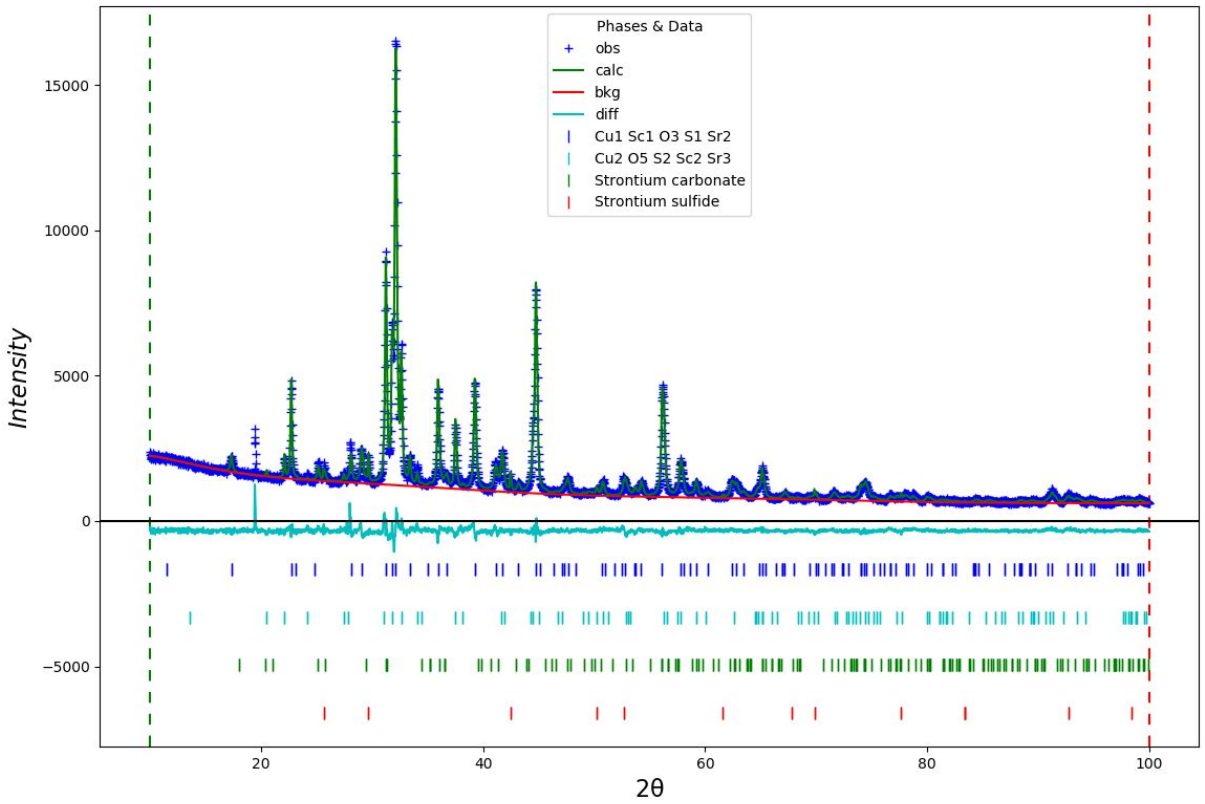

Figure S9. Refinement of sodium doped nominal $Na_{0.05}Sr_{1.95}ScO_3CuS$

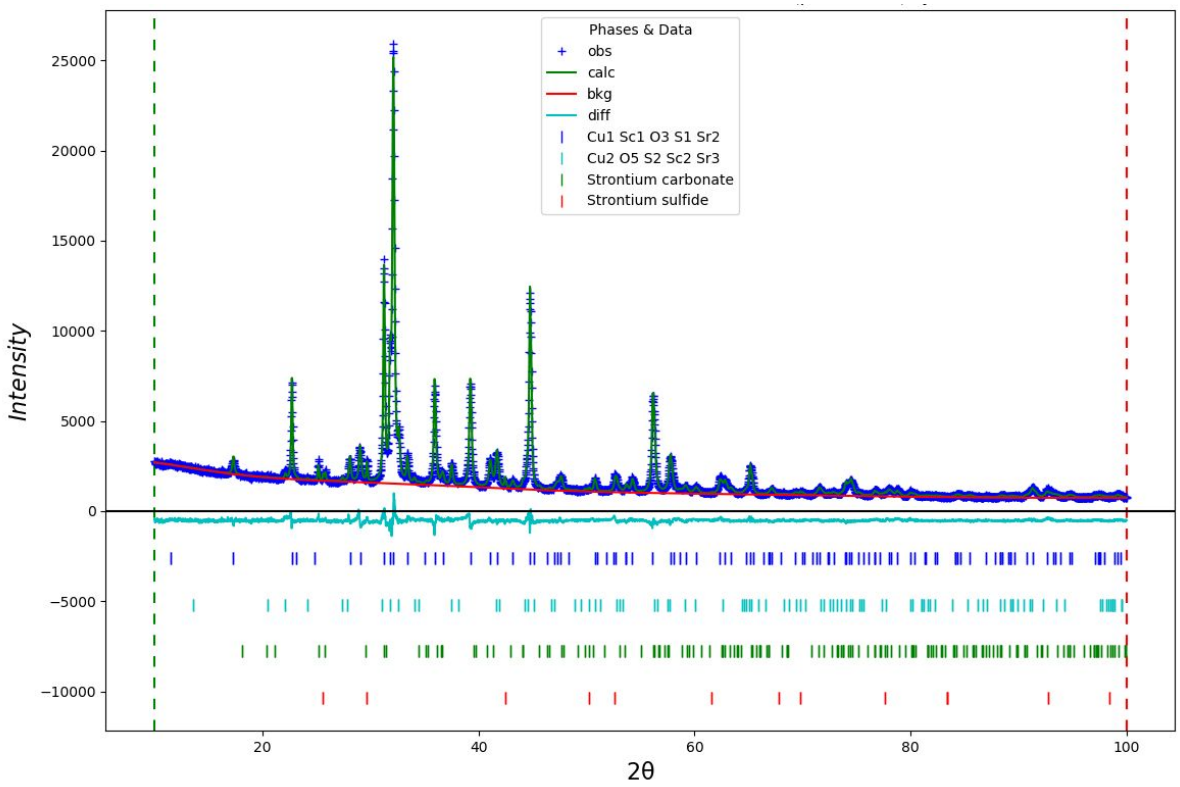

Figure S10. Refinement of potassium doped nominal $K_{0.05}Sr_{1.95}ScO_3CuS$

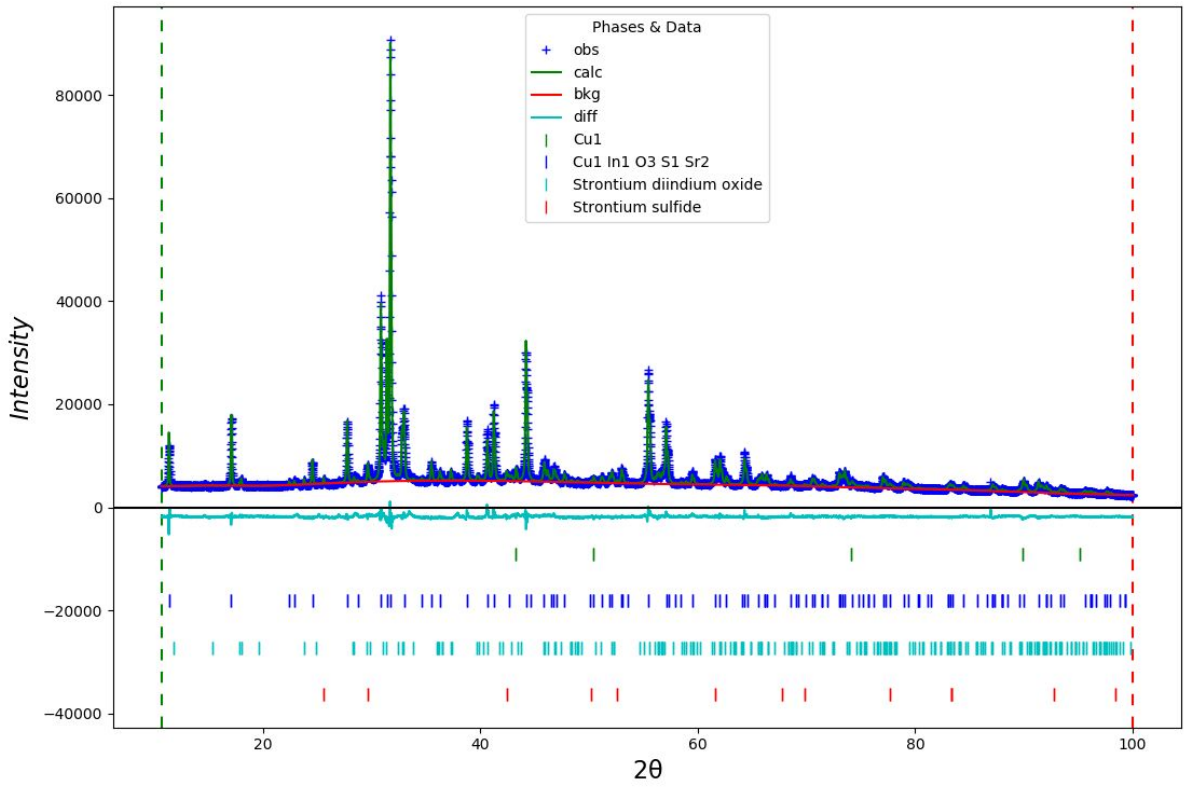

Figure S11. Refinement of sodium doped nominal $Na_{0.05}Sr_{1.95}InO_3CuS$

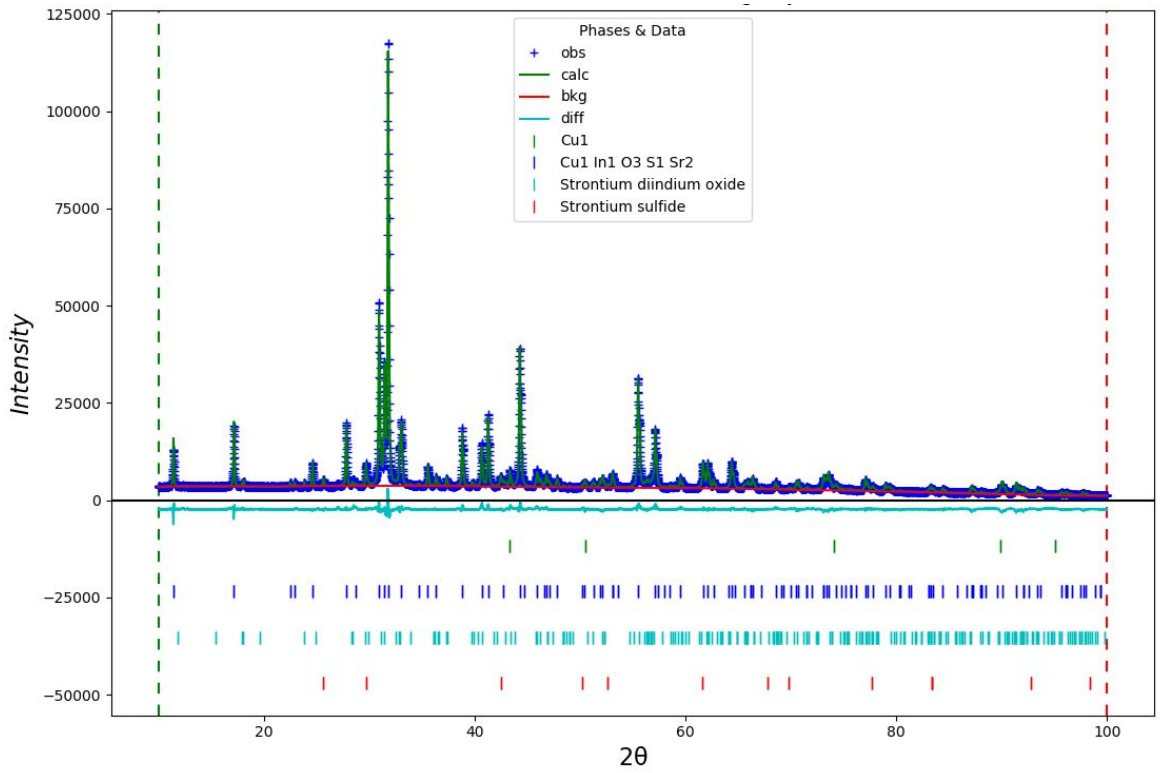

Figure S12. Refinement of potassium doped nominal $K_{0.05}Sr_{1.95}InO_3CuS$

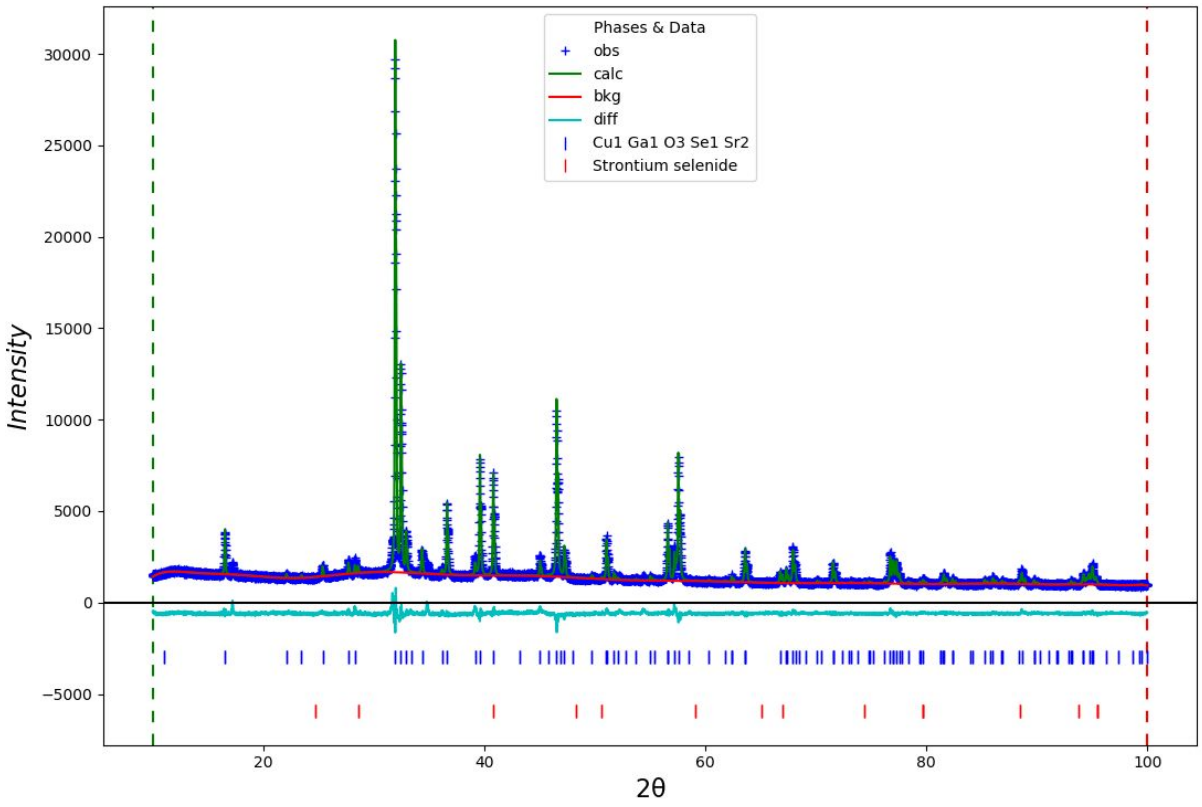

Figure S13. Refinement of sodium doped nominal $Na_{0.05}Sr_{1.95}GaO_3CuSe$

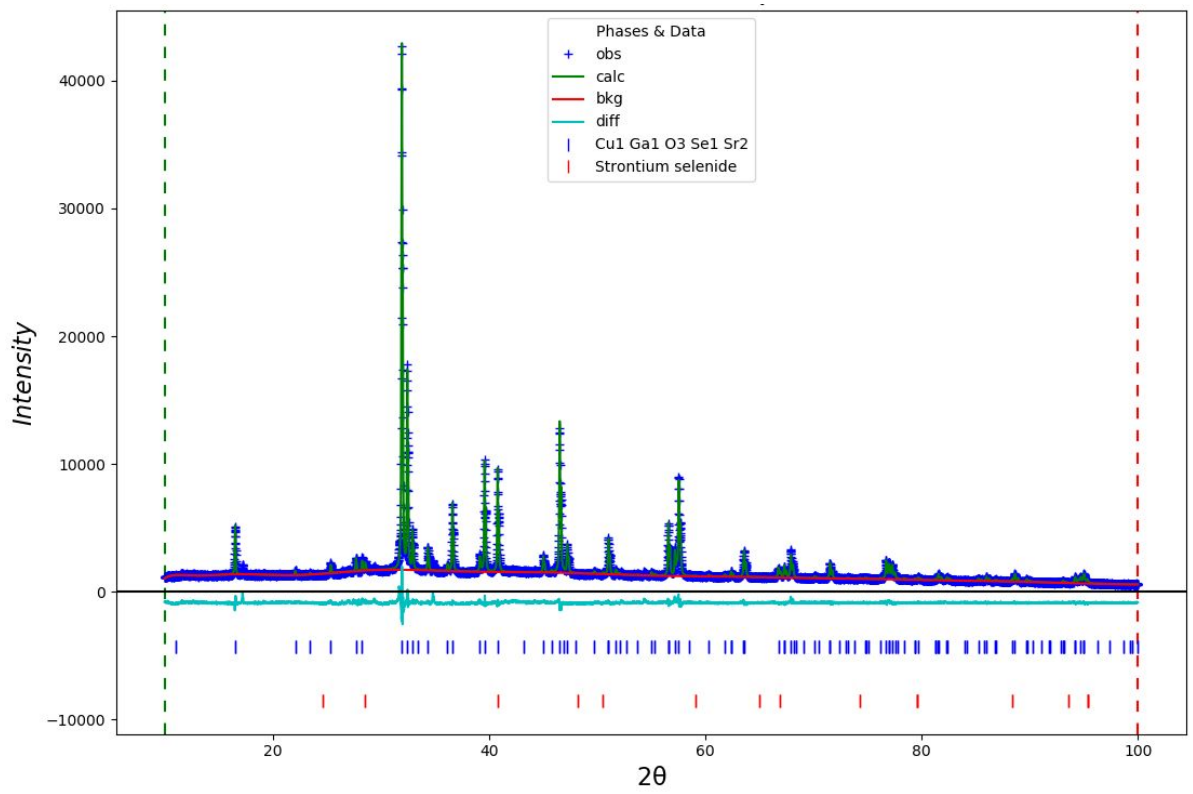

Figure S14. Refinement of potassium doped nominal $K_{0.05}Sr_{1.95}GaO_3CuSe$

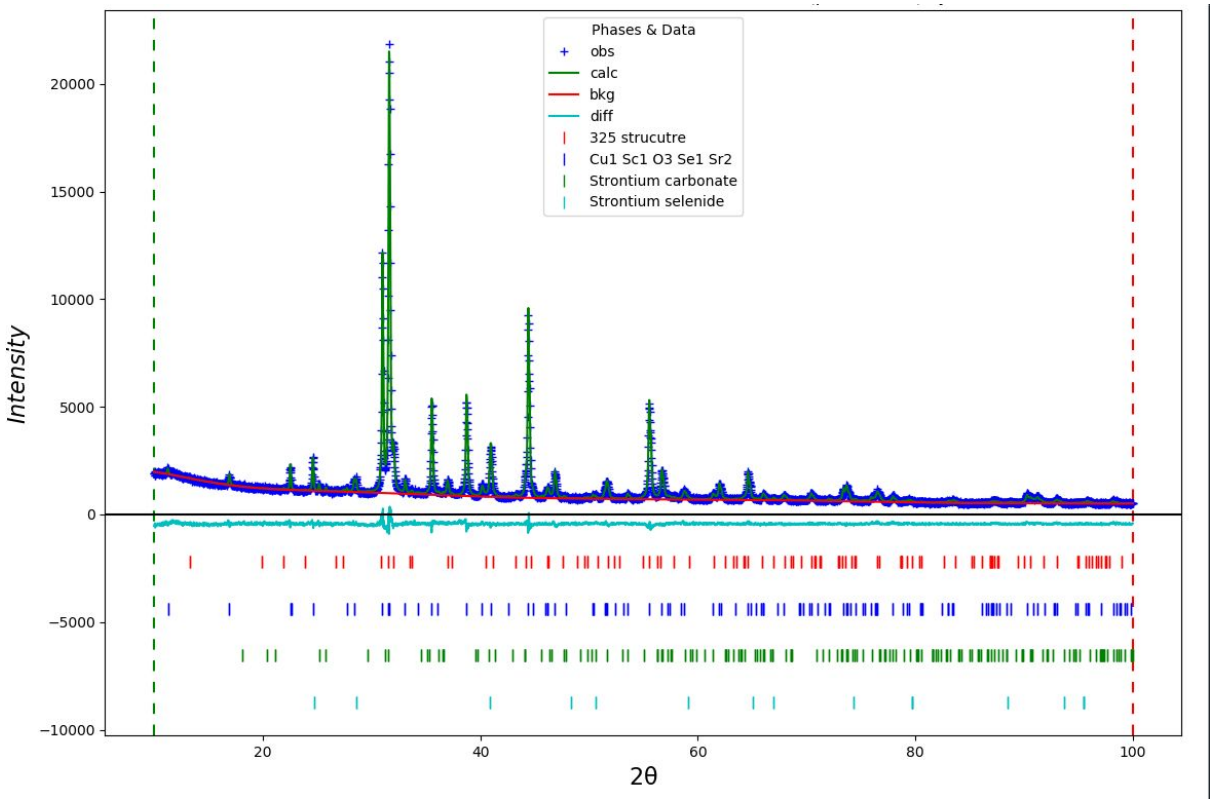

Figure S15. Refinement of sodium doped nominal $Na_{0.05}Sr_{1.95}ScO_3CuSe$.

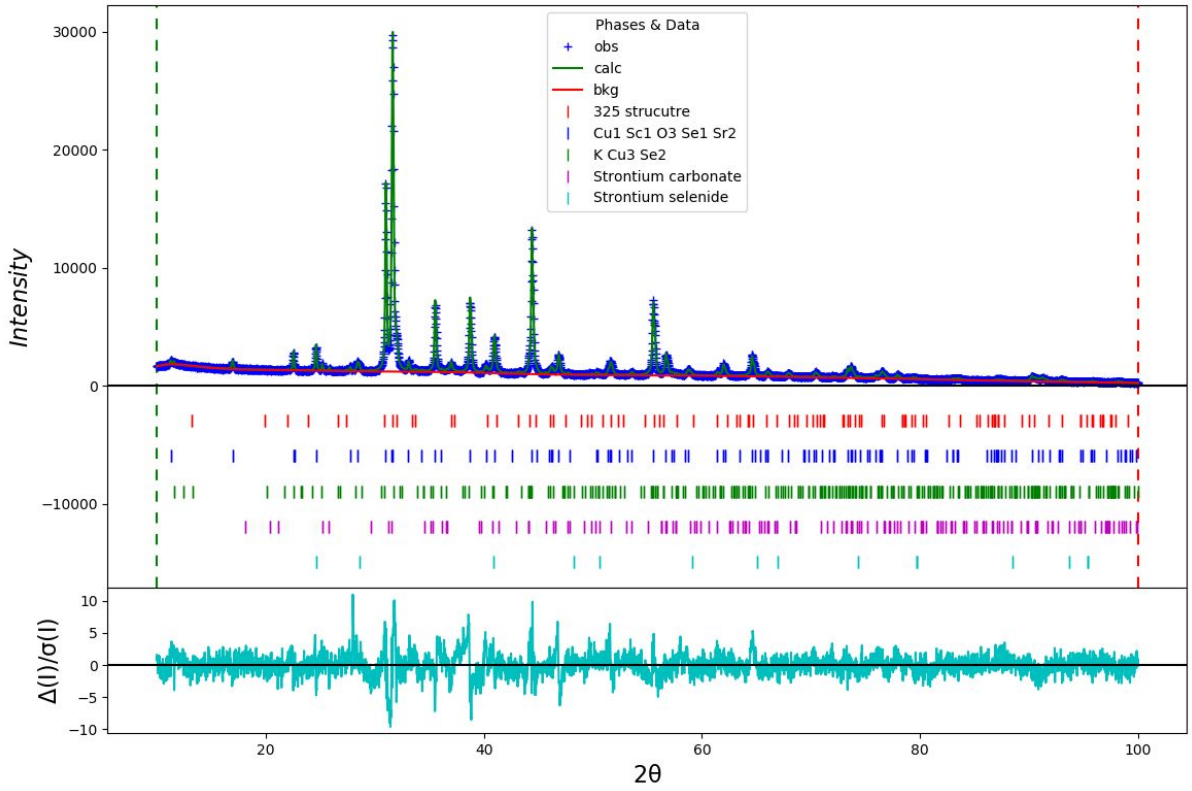

Figure S16. Refinement of potassium doped nominal $K_{0.05}Sr_{1.95}ScO_3CuSe$.

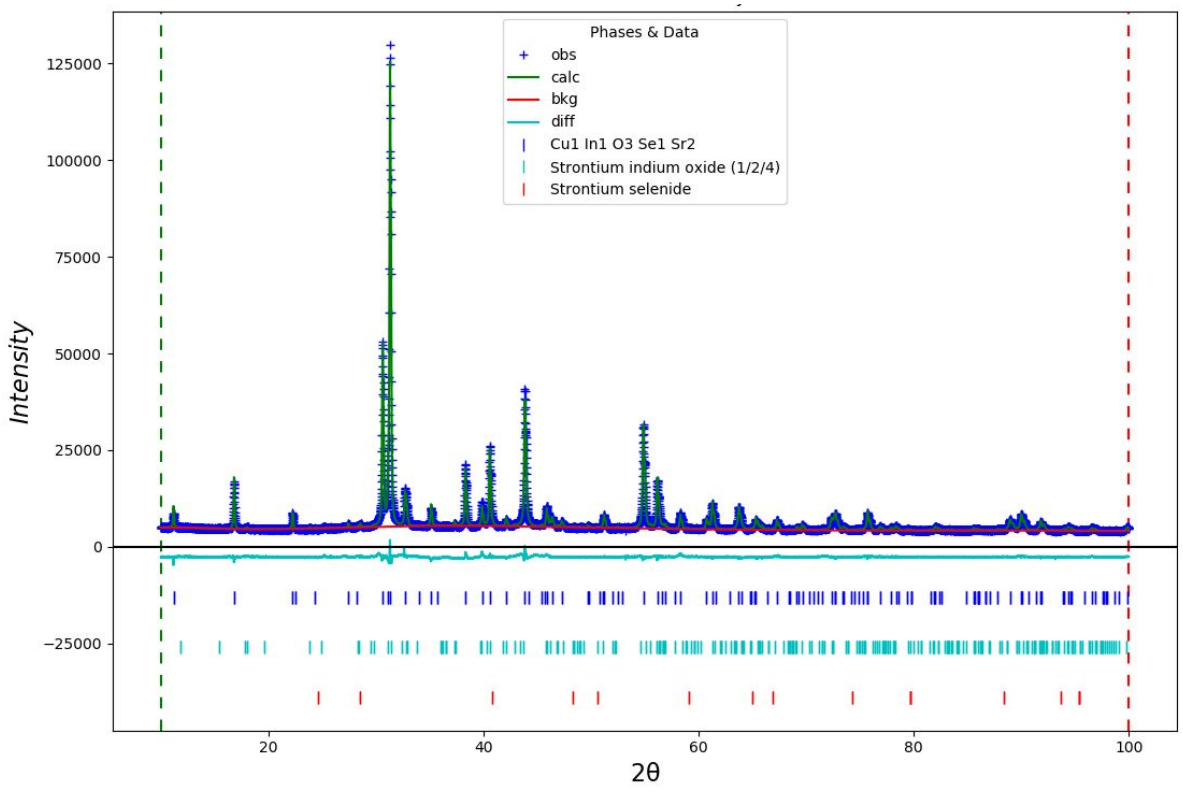

Figure S17. Refinement of sodium doped nominal $Na_{0.05}Sr_{1.95}InO_3CuSe$.

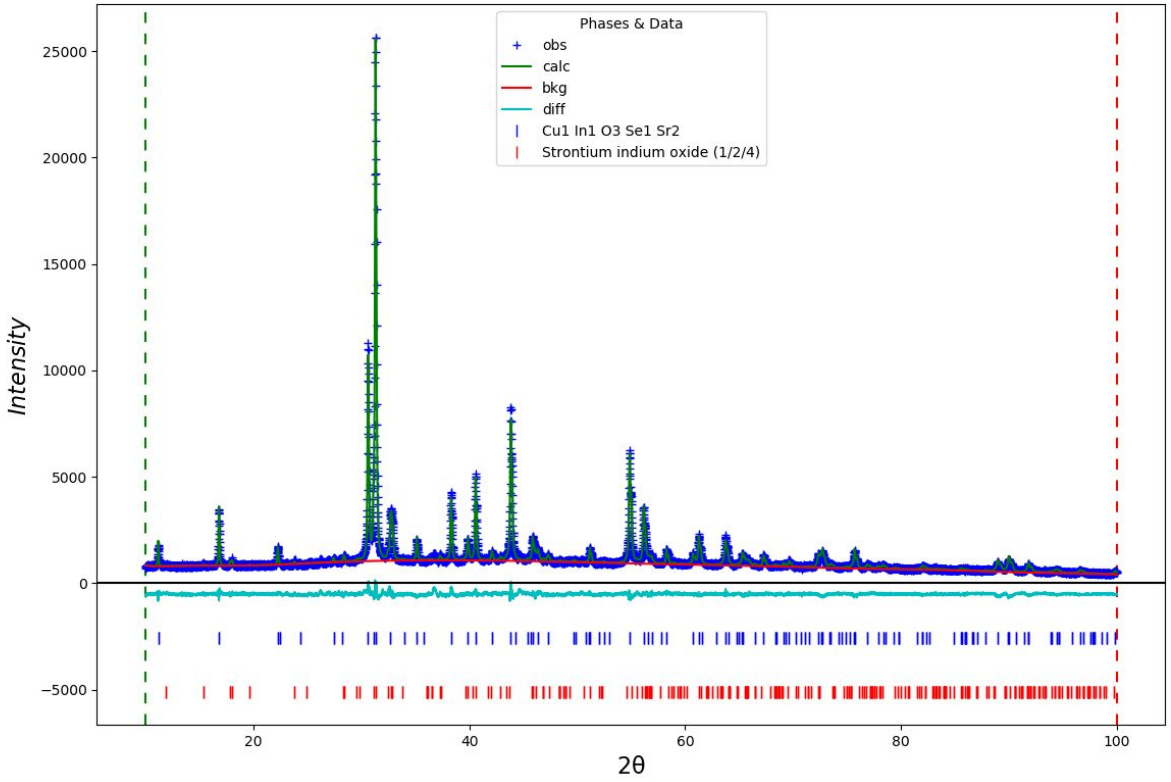

Figure S18. Refinement of potassium doped nominal $K_{0.05}Sr_{1.95}InO_3CuSe$.

Sample	Band Gap / eV	Results of refinement
Sr_2GaO_3CuS	2.43	wRp = 3.16%. 99.1 wt% main phase; 0.3 wt% SrS; 0.6wt% $Sr_3Ga_2O_6$
$Na_{0.05}Sr_{1.95}GaO_3CuS$	2.42	wRp = 3.62%. 98.1 wt% main phase; 0.3 wt% SrS ; 1.6 wt% $Sr_3Ga_2O_6$
$K_{0.05}Sr_{1.95}GaO_3CuS$	2.43	wRp 3.40%. 98.0 wt% main; 0.1 wt% SrS; 1. 7 wt% $Sr_3Ga_2O_6$; 0.7 wt% KCu_7S_4
Sr_2ScO_3CuS	3.15	wRp = 3.71%. 99.4 wt% main; 0.6 wt% $SrSO_4$
$Na_{0.05}Sr_{1.95}ScO_3CuS$	3.08	wRp = 5.01%. 83.1 wt% main; 0.8 wt% SrS; 13.7wt % $Sr_3Sc_2O_5Cu_2S_2$; 2.3wt % $SrCO_3$.
$K_{0.05}Sr_{1.95}ScO_3CuS$	3.11	wRp = 4.34%. 90.9 wt% main; 0.8 wt% SrS; 6.5 wt% $Sr_3Sc_2O_5Cu_2S_2$; 1.8w% $SrCO_3$
Sr_2InO_3CuS	2.29	wRp = 2.81%. 95.2 wt% main; 0.8 wt% SrS; 4 wt% $SrIn_2O_4$
$Na_{0.05}Sr_{1.95}InO_3CuS$	2.24	wRp = 3.57%. 83.1% main phase; 2.2 wt% SrS; 13.3 wt% $SrIn_2O_4$; **1.5 wt% Cu**
$K_{0.05}Sr_{1.95}InO_3CuS$	2.26	wRp = 4.59%. 84.8% main phase; 3.2% SrS; 10.1% $SrIn_2O_4$; **1.8% Cu**
Sr_2GaO_3CuSe	1.85	wRp = 3.3%. 97wt% main; 3 wt% $Sr_3Ga_2O_6$
$Na_{0.05}Sr_{1.95}GaO_3CuSe$	1.86	wRp = 4.6%. 99.1 wt% main; 0.4 wt% SrSe; 0.5 wt% $SrGa_2O_4$
$K_{0.05}Sr_{1.95}GaO_3CuSe$	1.85	wRp = 4.75%. 99.4 wt% main; 0.6 wt% SrSe
Sr_2ScO_3CuSe	2.95	wRp = 3.23%. 98.5 wt% main; 1.2 wt% $Sr_3Sc_2O_5Cu_2Se_2$; 0.3 w% SrSe.
$Na_{0.05}Sr_{1.95}ScO_3CuSe$	2.88	wRp = 4.1%. 90.3 wt% main; 8.2 wt% $Sr_3Sc_2O_5Cu_2Se_2$; 0.5 wt% SrSe; 1 wt% $SrCO_3$
$K_{0.05}Sr_{1.95}ScO_3CuSe$	2.94	wRp = 4.62%; 90.3 wt% main; 8.0 wt% $Sr_3Sc_2O_5Cu_2Se_2$; 0.3 wt% SrSe; 1.1 wt% $SrCO_3$; 0.3 wt% KCu_3Se_2
Sr_2InO_3CuSe	1.88	wRp = 4.01%. 96.5% wt% main; 1.5 wt% SrSe; 2 wt% $SrIn_2O_4$
$Na_{0.05}Sr_{1.95}InO_3CuSe$	1.87	wRp = 3.04%. 95.2 wt% main; 0.2 wt% SrSe; 4.6 wt% $SrIn_2O_4$
$K_{0.05}Sr_{1.95}InO_3CuSe$	1.84	wRp = 4.76%. 86.3 wt% main; 13.7 wt% $SrIn_2O_4$

Table S12. Summary of the band gaps and refinements on the doped layered oxychalcogenide phases. Data for undoped samples also provided.

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