Electronic Supplementary Information (ESI)

Title: Crystal Structure, Bandgap, Photoluminescence and Resistivity Properties of Double Perovskite $Cs_2AgBiCl_6$ Single Crystal and its Thin Film

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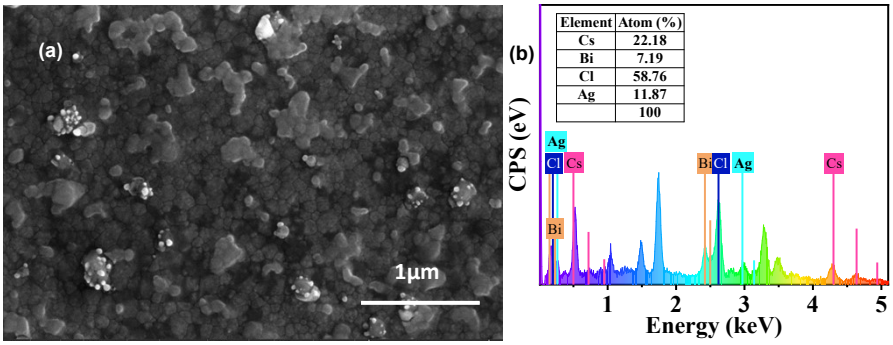
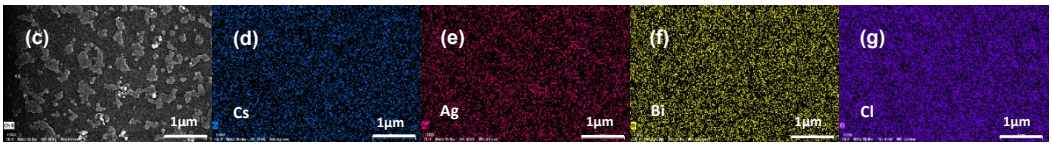
Supplementary Figures





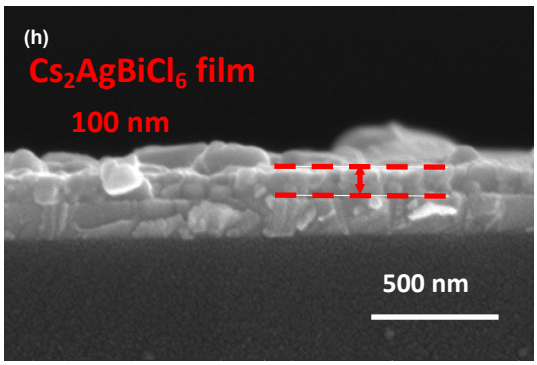


Figure S1 Vapor deposited $Cs_2AgBiCl_6$-DP thin film for studying resistance characteristics. (a) SEM image of $Cs_2AgBiCl_6$-DP thin film; (b) EDS spectrum and element content of $Cs_2AgBiCl_6$-DP thin film; the region (c) Corresponding to element mapping of Cs (d), Ag (e), Bi (f) and Cl (g) in $Cs_2AgBiCl_6$-DP thin film; (h) The SEM image of the cross-sectional morphology of the $Cs_2AgBiCl_6$-DP thin film.

Supplementary Tables

Table S1 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for $Cs_2AgBiCl_6$. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
Bi(1)	5000	10000	5000	20(3)
Ag(1)	5000	10000	0	37(5)
Cs(1)	2500	7500	2500	49(4)
Cl(1)	5000	10000	2522(13)	29(5)

Table S2 Bond lengths [Å] and angles [deg] for $Cs_2AgBiCl_6$.

Bond	Bond lengths [Å] and angles [deg]
Bi(1)-Cl(1)#1	2.675(14)
Bi(1)-Cl(1)#2	2.675(14)
Bi(1)-Cl(1)#3	2.675(14)
Bi(1)-Cl(1)#4	2.675(14)
Bi(1)-Cl(1)#5	2.675(14)
Bi(1)-Cl(1)	2.675(14)
Bi(1)-Cs(1)#5	4.6735(3)
Bi(1)-Cs(1)#6	4.6735(3)
Bi(1)-Cs(1)#7	4.6735(3)
Bi(1)-Cs(1)#8	4.6735(3)
Bi(1)-Cs(1)#9	4.6735(3)
Bi(1)-Cs(1)#10	4.6735(3)
Ag(1)-Cl(1)#11	2.722(14)
Ag(1)-Cl(1)	2.722(14)
Ag(1)-Cl(1)#12	2.722(14)
Ag(1)-Cl(1)#13	2.722(14)
Ag(1)-Cl(1)#14	2.722(14)
Ag(1)-Cl(1)#15	2.722(14)
Cs(1)-Cl(1)#1	3.8160(3)
Cs(1)-Cl(1)#4	3.8160(3)
Cs(1)-Cl(1)	3.8160(3)
Cs(1)-Cl(1)#16	3.8160(3)
Cs(1)-Cl(1)#17	3.8160(3)
Cs(1)-Cl(1)#18	3.8160(3)
Cs(1)-Cl(1)#13	3.8160(3)
Cs(1)-Cl(1)#19	3.8160(3)

Cs(1)-Cl(1)#14	3.8160(3)
Cs(1)-Cl(1)#20	3.8160(3)
Cs(1)-Cl(1)#7	3.8160(3)
Cs(1)-Cl(1)#6	3.8160(3)
Cl(1)-Cs(1)#9	3.8160(3)
Cl(1)-Cs(1)#7	3.8160(3)
Cl(1)-Cs(1)#6	3.8160(3)

Cl(1)#1-Bi(1)-Cl(1)#2	180.000(2)
Cl(1)#1-Bi(1)-Cl(1)#3	90.000(1)
Cl(1)#2-Bi(1)-Cl(1)#3	90.000(4)
Cl(1)#1-Bi(1)-Cl(1)#4	90.000(4)
Cl(1)#2-Bi(1)-Cl(1)#4	90.000(3)
Cl(1)#3-Bi(1)-Cl(1)#4	180
Cl(1)#1-Bi(1)-Cl(1)#5	90.000(1)
Cl(1)#2-Bi(1)-Cl(1)#5	90
Cl(1)#3-Bi(1)-Cl(1)#5	90.000(1)
Cl(1)#4-Bi(1)-Cl(1)#5	90.000(1)
Cl(1)#1-Bi(1)-Cl(1)	90.000(1)
Cl(1)#2-Bi(1)-Cl(1)	90
Cl(1)#3-Bi(1)-Cl(1)	90.000(1)
Cl(1)#4-Bi(1)-Cl(1)	90.000(2)
Cl(1)#5-Bi(1)-Cl(1)	180.000(1)
Cl(1)#1-Bi(1)-Cs(1)#5	125.264(1)
Cl(1)#2-Bi(1)-Cs(1)#5	54.736(1)
Cl(1)#3-Bi(1)-Cs(1)#5	54.7
Cl(1)#4-Bi(1)-Cs(1)#5	125.264(1)
Cl(1)#5-Bi(1)-Cs(1)#5	54.736(2)
Cl(1)-Bi(1)-Cs(1)#5	125.264(1)
Cl(1)#1-Bi(1)-Cs(1)#6	54.736(1)
Cl(1)#2-Bi(1)-Cs(1)#6	125.264(1)
Cl(1)#3-Bi(1)-Cs(1)#6	54.7
Cl(1)#4-Bi(1)-Cs(1)#6	125.264(1)
Cl(1)#5-Bi(1)-Cs(1)#6	125.264(1)
Cl(1)-Bi(1)-Cs(1)#6	54.736(1)
Cs(1)#5-Bi(1)-Cs(1)#6	109.5
Cl(1)#1-Bi(1)-Cs(1)#7	125.264(1)
Cl(1)#2-Bi(1)-Cs(1)#7	54.736(1)
Cl(1)#3-Bi(1)-Cs(1)#7	125.3
Cl(1)#4-Bi(1)-Cs(1)#7	54.7
Cl(1)#5-Bi(1)-Cs(1)#7	125.264(1)
Cl(1)-Bi(1)-Cs(1)#7	54.736(1)
Cs(1)#5-Bi(1)-Cs(1)#7	109.5
Cs(1)#6-Bi(1)-Cs(1)#7	109.5

Cl(1)#1-Bi(1)-Cs(1)#8	54.736(1)
Cl(1)#2-Bi(1)-Cs(1)#8	125.264(1)
Cl(1)#3-Bi(1)-Cs(1)#8	125.3
Cl(1)#4-Bi(1)-Cs(1)#8	54.7
Cl(1)#5-Bi(1)-Cs(1)#8	54.736(2)
Cl(1)-Bi(1)-Cs(1)#8	125.264(1)
Cs(1)#5-Bi(1)-Cs(1)#8	109.5
Cs(1)#6-Bi(1)-Cs(1)#8	109.5
Cs(1)#7-Bi(1)-Cs(1)#8	109.5
Cl(1)#1-Bi(1)-Cs(1)#9	125.264(1)
Cl(1)#2-Bi(1)-Cs(1)#9	54.736(1)
Cl(1)#3-Bi(1)-Cs(1)#9	54.7
Cl(1)#4-Bi(1)-Cs(1)#9	125.3
Cl(1)#5-Bi(1)-Cs(1)#9	125.264(2)
Cl(1)-Bi(1)-Cs(1)#9	54.736(1)
Cs(1)#5-Bi(1)-Cs(1)#9	70.5
Cs(1)#6-Bi(1)-Cs(1)#9	70.5
Cs(1)#7-Bi(1)-Cs(1)#9	70.5
Cs(1)#8-Bi(1)-Cs(1)#9	180
Cl(1)#1-Bi(1)-Cs(1)#10	54.736(1)
Cl(1)#2-Bi(1)-Cs(1)#10	125.264(1)
Cl(1)#3-Bi(1)-Cs(1)#10	54.7
Cl(1)#4-Bi(1)-Cs(1)#10	125.3
Cl(1)#5-Bi(1)-Cs(1)#10	54.736(1)
Cl(1)-Bi(1)-Cs(1)#10	125.264(1)
Cs(1)#5-Bi(1)-Cs(1)#10	70.5
Cs(1)#6-Bi(1)-Cs(1)#10	70.5
Cs(1)#7-Bi(1)-Cs(1)#10	180
Cs(1)#8-Bi(1)-Cs(1)#10	70.5
Cs(1)#9-Bi(1)-Cs(1)#10	109.5
Cl(1)#11-Ag(1)-Cl(1)	90.000(1)
Cl(1)#11-Ag(1)-Cl(1)#12	90.000(1)
Cl(1)-Ag(1)-Cl(1)#12	180.000(1)
Cl(1)#11-Ag(1)-Cl(1)#13	90.000(1)
Cl(1)-Ag(1)-Cl(1)#13	90
Cl(1)#12-Ag(1)-Cl(1)#13	90
Cl(1)#11-Ag(1)-Cl(1)#14	180
Cl(1)-Ag(1)-Cl(1)#14	90
Cl(1)#12-Ag(1)-Cl(1)#14	90.000(2)
Cl(1)#13-Ag(1)-Cl(1)#14	90.000(2)
Cl(1)#11-Ag(1)-Cl(1)#15	90.000(1)
Cl(1)-Ag(1)-Cl(1)#15	90
Cl(1)#12-Ag(1)-Cl(1)#15	90
Cl(1)#13-Ag(1)-Cl(1)#15	180.000(1)

Cl(1)#14-Ag(1)-Cl(1)#15	90.000(1)
Cl(1)#1-Cs(1)-Cl(1)#4	59.4(3)
Cl(1)#1-Cs(1)-Cl(1)	59.4(3)
Cl(1)#4-Cs(1)-Cl(1)	59.4(3)
Cl(1)#1-Cs(1)-Cl(1)#16	179.3(4)
Cl(1)#4-Cs(1)-Cl(1)#16	119.999(2)
Cl(1)-Cs(1)-Cl(1)#16	119.999(2)
Cl(1)#1-Cs(1)-Cl(1)#17	119.999(2)
Cl(1)#4-Cs(1)-Cl(1)#17	179.3(4)
Cl(1)-Cs(1)-Cl(1)#17	119.999(2)
Cl(1)#16-Cs(1)-Cl(1)#17	60.6(3)
Cl(1)#1-Cs(1)-Cl(1)#18	119.999(1)
Cl(1)#4-Cs(1)-Cl(1)#18	119.999(2)
Cl(1)-Cs(1)-Cl(1)#18	179.3(4)
Cl(1)#16-Cs(1)-Cl(1)#18	60.6(3)
Cl(1)#17-Cs(1)-Cl(1)#18	60.6(3)
Cl(1)#1-Cs(1)-Cl(1)#13	90.002(4)
Cl(1)#4-Cs(1)-Cl(1)#13	119.999(1)
Cl(1)-Cs(1)-Cl(1)#13	60.6(3)
Cl(1)#16-Cs(1)-Cl(1)#13	90.002(3)
Cl(1)#17-Cs(1)-Cl(1)#13	59.4(3)
Cl(1)#18-Cs(1)-Cl(1)#13	119.999(2)
Cl(1)#1-Cs(1)-Cl(1)#19	90.002(3)
Cl(1)#4-Cs(1)-Cl(1)#19	60.6(3)
Cl(1)-Cs(1)-Cl(1)#19	119.999(2)
Cl(1)#16-Cs(1)-Cl(1)#19	90.002(4)
Cl(1)#17-Cs(1)-Cl(1)#19	119.999(2)
Cl(1)#18-Cs(1)-Cl(1)#19	59.4(3)
Cl(1)#13-Cs(1)-Cl(1)#19	179.3(4)
Cl(1)#1-Cs(1)-Cl(1)#14	119.999(1)
Cl(1)#4-Cs(1)-Cl(1)#14	90.002(3)
Cl(1)-Cs(1)-Cl(1)#14	60.6(3)
Cl(1)#16-Cs(1)-Cl(1)#14	59.4(3)
Cl(1)#17-Cs(1)-Cl(1)#14	90.002(3)
Cl(1)#18-Cs(1)-Cl(1)#14	119.999(2)
Cl(1)#13-Cs(1)-Cl(1)#14	60.6(3)
Cl(1)#19-Cs(1)-Cl(1)#14	119.999(2)
Cl(1)#1-Cs(1)-Cl(1)#20	60.6(3)
Cl(1)#4-Cs(1)-Cl(1)#20	90.002(3)
Cl(1)-Cs(1)-Cl(1)#20	119.999(1)
Cl(1)#16-Cs(1)-Cl(1)#20	119.999(2)
Cl(1)#17-Cs(1)-Cl(1)#20	90.002(3)
Cl(1)#18-Cs(1)-Cl(1)#20	59.4(3)
Cl(1)#13-Cs(1)-Cl(1)#20	119.999(1)

Cl(1)#19-Cs(1)-Cl(1)#20	59.4(3)
Cl(1)#14-Cs(1)-Cl(1)#20	179.3(4)
Cl(1)#1-Cs(1)-Cl(1)#7	119.999(2)
Cl(1)#4-Cs(1)-Cl(1)#7	60.6(3)
Cl(1)-Cs(1)-Cl(1)#7	90.002(3)
Cl(1)#16-Cs(1)-Cl(1)#7	59.4(3)
Cl(1)#17-Cs(1)-Cl(1)#7	119.999(2)
Cl(1)#18-Cs(1)-Cl(1)#7	90.002(4)
Cl(1)#13-Cs(1)-Cl(1)#7	119.999(1)
Cl(1)#19-Cs(1)-Cl(1)#7	60.6(3)
Cl(1)#14-Cs(1)-Cl(1)#7	59.4(3)
Cl(1)#20-Cs(1)-Cl(1)#7	119.999(1)
Cl(1)#1-Cs(1)-Cl(1)#6	60.6(3)
Cl(1)#4-Cs(1)-Cl(1)#6	119.999(1)
Cl(1)-Cs(1)-Cl(1)#6	90.002(4)
Cl(1)#16-Cs(1)-Cl(1)#6	119.999(2)
Cl(1)#17-Cs(1)-Cl(1)#6	59.4(3)
Cl(1)#18-Cs(1)-Cl(1)#6	90.002(3)
Cl(1)#13-Cs(1)-Cl(1)#6	59.4(3)
Cl(1)#19-Cs(1)-Cl(1)#6	119.999(1)
Cl(1)#14-Cs(1)-Cl(1)#6	119.999(2)
Cl(1)#20-Cs(1)-Cl(1)#6	60.6(3)
Cl(1)#7-Cs(1)-Cl(1)#6	179.3(4)
Bi(1)-Cl(1)-Ag(1)	180
Bi(1)-Cl(1)-Cs(1)	90.3(2)
Ag(1)-Cl(1)-Cs(1)	89.7(2)
Bi(1)-Cl(1)-Cs(1)#9	90.3(2)
Ag(1)-Cl(1)-Cs(1)#9	89.7(2)
Cs(1)-Cl(1)-Cs(1)#9	179.3(4)
Bi(1)-Cl(1)-Cs(1)#7	90.3(2)
Ag(1)-Cl(1)-Cs(1)#7	89.7(2)
Cs(1)-Cl(1)-Cs(1)#7	89.998(3)
Cs(1)#9-Cl(1)-Cs(1)#7	89.998(3)
Bi(1)-Cl(1)-Cs(1)#6	90.3(2)
Ag(1)-Cl(1)-Cs(1)#6	89.7(2)
Cs(1)-Cl(1)-Cs(1)#6	89.998(3)
Cs(1)#9-Cl(1)-Cs(1)#6	89.998(3)
Cs(1)#7-Cl(1)-Cs(1)#6	179.3(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,z+1/2,y-1/2 #2 x,-z+3/2,-y+3/2

#3 -z+1,-x+3/2,-y+3/2 #4 z,x+1/2,y-1/2

#5 -x+1,-y+2,-z+1 #6 -x+1,-y+3/2,-z+1/2

#7 -x+1/2,-y+2,-z+1/2 #8 -x+1/2,-y+3/2,-z+1

#9 x+1/2,y+1/2,z #10 x+1/2,y,z+1/2

#11 z+1/2,x+1/2,y-1 #12 -x+1,-y+2,-z
#13 x,-z+1,-y+1 #14 -z+1/2,-x+3/2,-y+1
#15 -x+1,z+1,y-1 #16 -x+1/2,z+1/2,y-1
#17 z,x,y-1 #18 x-1/2,y-1/2,z #19 x-1/2,-z+1,-y+3/2
#20 -z+1/2,-x+1,-y+3/2

Table S3 Anisotropic displacement parameters (A^2 x 10^3) for $Cs_2AgBiCl_6$. The anisotropic displacement factor exponent takes the form: $-2\ pi^2\ [h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U12]$.

	U11	**U22**	**U33**	**U23**	**U13**	**U12**
Bi(1)	20(3)	20(3)	20(3)	0	0	0
Ag(1)	37(5)	37(5)	37(5)	0	0	0
Cs(1)	49(4)	49(4)	49(4)	0	0	0
Cl(1)	37(7)	37(7)	11(7)	0	0	0