Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

$A_2AgCrCl_6$ (A = Li, Na, K, Rb, Cs) Halide Double Perovskites: A Transition Metal-based Semiconducting Material Series with Appreciable Optical Characteristics

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Table S1: SCAN-*rVV*10 relaxed coordinates of cubic-$Cs_2AgCrCl_6$ and the normalized absolute contributions of each atom type to its HOMO and LUMO bands.

No	Atom Type	x	y	z
1	Cs1	0.25000	0.25000	0.25000
2	Cs2	0.75000	0.75000	0.75000
3	Ag1	0.50000	0.50000	0.50000
4	Cr1	0.00000	0.00000	0.00000
5	Cl1	0.23373	0.23373	0.76627
6	Cl2	0.76627	0.76627	0.23373
7	Cl3	0.76627	0.23373	0.76627
8	Cl4	0.23373	0.76627	0.23373
9	Cl5	0.76627	0.23373	0.23373
10	Cl6	0.23373	0.76627	0.76627

SUM OF ABSOLUTE CONTRIBUTIONS OF EACH ORBITAL FOR HOMO BAND 40

atom	s	py	pz	px	dxy	dyz	dz2	dxz	dx2	tot
1	0.000	0.108	0.010	0.106	0.000	0.000	0.000	0.000	0.000	0.224
2	0.000	0.108	0.010	0.106	0.000	0.000	0.000	0.000	0.000	0.224
3	0.000	0.000	0.000	0.000	0.082	0.444	0.015	0.476	0.105	1.122
4	0.000	0.002	0.000	0.003	1.035	13.064	0.001	24.352	0.005	38.462
5	0.000	0.863	0.004	1.577	0.000	0.000	0.000	0.000	0.000	2.444
6	0.000	0.864	0.004	1.575	0.000	0.000	0.000	0.000	0.000	2.443
7	0.000	0.020	0.702	0.055	0.000	0.000	0.000	0.000	0.000	0.777
8	0.000	0.020	0.703	0.055	0.000	0.000	0.000	0.000	0.000	0.778
9	0.000	0.069	1.389	0.030	0.000	0.000	0.000	0.000	0.000	1.488

10 0.000 0.069 1.389 0.030 0.000 0.000 0.000 0.000 0.000 1.488

AVERAGE OCCUPATION OF BAND 40 is 1.000000
NORMALIZED CONTRIBUTION OF EACH TYPE (HOMO BAND)
atom Cs_sv -> s=0.00 % p=0.91 % d=0.00 %
atom Ag -> s=0.00 % p=0.00 % d=2.27 %
atom Cr -> s=0.00 % p=0.01 % d=77.77 %
atom Cl -> s=0.00 % p=19.05 % d=0.00 %

SUM OF ABSOLUTE CONTRIBUTIONS OF EACH ORBITAL FOR (LUMO) BAND 41

atom	s	py	pz	px	dxy	dyz	dz2	dxz	dx2	tot
1	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
2	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
3	2.711	0.183	0.314	0.189	0.001	0.000	1.241	0.000	0.934	5.573
4	0.113	0.173	0.101	0.059	0.023	0.004	23.304	0.003	7.634	31.414
5	0.248	0.023	1.960	0.014	0.000	0.000	0.000	0.000	0.000	2.245
6	0.248	0.023	1.960	0.014	0.000	0.000	0.000	0.000	0.000	2.245
7	0.206	1.371	0.025	0.031	0.000	0.000	0.000	0.000	0.000	1.633
8	0.206	1.371	0.025	0.031	0.000	0.000	0.000	0.000	0.000	1.633
9	0.212	0.052	0.015	1.280	0.000	0.000	0.000	0.000	0.000	1.559
10	0.212	0.052	0.015	1.280	0.000	0.000	0.000	0.000	0.000	1.559

AVERAGE OCCUPATION OF BAND 41 is 0.000000

NORMALIZED CONTRIBUTION OF EACH TYPE (LUMO BAND)
atom Cs -> s=0.00 % p=0.00 % d=0.00 %
atom Ag -> s=5.66 % p=1.43 % d=4.55 %
atom Cr -> s=0.24 % p=0.70 % d=64.70 %
atom Cl -> s=2.78 % p=19.94 % d=0.00 %