Supporting Information for

A new perspective for evaluating photoelectric performance of organic-inorganic hybrid perovskites based on DFT calculations of excited states

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Table S1 Calculation results for the electron-hole distribution index from the ground state to the first singlet state, *D* index means the centroid distance between holes and electrons. *Sr* index means the overlap between holes and electrons. *T* index measures the degree of separation of holes and electrons. *Ec* and *Es* are exciton binding energy and excited energy respectively. *Q* is the amount of net charge transfer. *G* and *S* are the HOMO-LUMO gap and score index, respectively.

Clusters	*D* (Å)	*Sr* (a.u.)	*t* (Å)	*Ec* (eV)	*Es* (eV)	*Q* (e)	*G* (eV)	S
$FAGeCl_3$	0.12	0.71	-1.05	6.61	5.59	0.14	6.76	0.20
$FAGeBr_3$	0.26	0.69	-1.15	5.90	5.25	0.15	6.65	0.33
$FAGeI_3$	0.37	0.67	-1.16	5.48	4.08	0.28	6.30	0.67
$FASnCl_3$	0.37	0.70	-0.88	6.21	5.43	0.16	7.12	0.31
$FASnBr_3$	0.71	0.60	-0.91	5.21	4.86	0.33	6.94	0.75
$FASnI_3$	0.45	0.64	-1.11	5.20	4.28	0.38	6.52	0.78
$FAPbCl_3$	0.88	0.65	-0.41	5.73	5.91	0.62	7.98	0.73
$FAPbBr_3$	0.65	0.58	-0.79	5.29	5.19	0.60	7.57	0.82
$FAPbI_3$	0.93	0.61	-0.56	4.93	4.44	0.57	6.77	1.22
$JAGeCl_3$	0.17	0.70	-1.03	6.73	5.52	0.13	6.85	0.20
$JAGeBr_3$	0.40	0.65	-0.90	6.17	4.93	0.16	6.50	0.41
$JAGeI_3$	0.68	0.62	-0.86	5.23	4.03	0.41	6.08	1.00
$JASnCl_3$	1.01	0.60	-0.84	5.54	5.31	0.42	7.15	0.38
$JASnBr_3$	0.25	0.70	-1.29	5.12	5.29	0.32	6.78	0.42
$JASnI_3$	0.52	0.61	-1.06	5.09	4.20	0.48	6.31	0.93
$JAPbCl_3$	0.33	0.55	-0.97	5.63	5.63	0.67	7.97	0.59
$JAPbBr_3$	0.47	0.54	-0.99	5.27	5.12	0.66	7.43	0.79
$JAPbI_3$	0.82	0.58	-0.76	4.95	4.42	0.60	6.71	1.15
$MAGeCl_3$	0.10	0.74	-1.17	6.64	5.78	0.35	8.30	0.16
$MAGeBr_3$	0.22	0.69	-1.10	6.08	5.20	0.20	7.84	0.27
$MAGeI_3$	0.02	0.70	-1.35	5.56	4.21	0.22	6.68	0.44
$MASnCl_3$	0.33	0.71	-0.99	6.28	5.52	0.37	8.23	0.32
$MASnBr_3$	0.39	0.73	-1.00	5.88	5.11	0.41	7.76	0.47
$MASnI_3$	0.15	0.70	-1.36	5.28	4.50	0.29	6.88	0.53
$MAPbCl_3$	0.87	0.67	-0.41	5.78	6.01	0.61	8.69	0.66
$MAPbBr_3$	0.96	0.71	-0.35	5.43	5.49	0.66	7.97	0.90
$MAPbI_3$	1.18	0.42	0.07	4.88	4.57	0.75	6.95	1.83
$EAGeCl_3$	0.12	0.71	-1.01	6.59	5.50	0.38	7.80	0.24
$EAGeBr_3$	0.30	0.67	-0.96	6.09	4.93	0.13	7.57	0.32
$EAGeI_3$	0.40	0.67	-1.04	5.51	4.05	0.16	6.55	0.58
$EASnCl_3$	0.31	0.69	-0.96	6.24	5.28	0.16	8.02	0.29
$EASnBr_3$	0.42	0.69	-0.90	5.82	4.88	0.21	7.55	0.47
$EASnI_3$	0.52	0.66	-0.94	5.28	4.26	0.21	6.69	0.72
$EAPbCl_3$	0.89	0.61	-0.40	5.81	5.74	0.37	8.43	0.69
$EAPbBr_3$	1.06	0.59	-0.36	5.42	5.15	0.39	7.67	0.99
$EAPbI_3$	1.21	0.59	-0.28	4.97	4.35	0.41	6.71	1.41
$BAGeCl_3$	0.11	0.73	-1.12	6.64	5.70	0.13	8.44	0.15
$BAGeBr_3$	0.37	0.67	-0.97	6.13	5.16	0.15	7.85	0.34
$BAGeI_3$	0.23	0.70	-1.28	5.53	4.24	0.13	6.73	0.45
$BASnCl_3$	0.27	0.72	-1.10	6.29	5.49	0.16	8.20	0.25
$BASnBr_3$	0.44	0.70	-0.89	5.86	5.05	0.21	7.72	0.46
$BASnI_3$	0.56	0.66	-0.95	5.35	4.47	0.22	6.95	0.69
$BAPbCl_3$	0.82	0.66	-0.53	5.82	6.00	0.37	8.68	0.60
$BAPbBr_3$	0.97	0.65	-0.43	5.47	5.44	0.41	8.02	0.86
$BAPbI_3$	1.35	0.48	0.12	4.85	4.63	0.59	7.00	1.80
$DAGeCl_3$	0.27	0.69	-1.14	6.19	5.51	0.16	7.17	0.22
$DAGeBr_3$	0.38	0.65	-0.95	5.96	4.95	0.15	7.07	0.37
$DAGeI_3$	0.29	0.68	-1.19	5.44	4.08	0.16	6.55	0.54
$DASnCl_3$	0.25	0.69	-1.15	6.04	5.30	0.17	7.49	0.29
$DASnBr_3$	0.36	0.68	-1.05	5.69	4.91	0.20	7.32	0.45
$DASnI_3$	0.48	0.64	-1.02	5.19	4.30	0.20	6.70	0.70
$DAPbCl_3$	0.83	0.59	-0.58	5.62	5.75	0.37	8.29	0.67
$DAPbBr_3$	0.92	0.59	-0.56	5.28	5.17	0.39	7.66	0.90
$DAPbI_3$	1.00	0.61	-0.58	4.91	4.40	0.41	6.73	1.20
$KBGeCl_3$	0.12	0.72	-1.10	6.55	5.68	0.13	8.16	0.09
$KBGeBr_3$	0.38	0.66	-0.96	6.00	5.15	0.14	7.80	0.28
$KBGeI_3$	0.12	0.70	-1.33	5.49	4.19	0.14	6.67	0.39
$KBSnCl_3$	0.30	0.70	-1.02	6.18	5.37	0.16	8.09	0.22
$KBSnBr_3$	0.40	0.70	-0.99	5.74	5.03	0.21	7.67	0.38
$KBSnI_3$	0.55	0.66	-0.84	5.27	4.46	0.22	6.87	0.67
$KBPbCl_3$	0.86	0.63	-0.47	5.72	5.85	0.37	8.52	0.56
$KBPbBr_3$	1.00	0.61	-0.40	5.34	5.32	0.39	7.81	0.84
$KBPbI_3$	1.32	0.44	-0.23	4.83	4.60	0.61	6.94	1.57
$KCGeCl_3$	0.09	0.72	-1.17	6.46	5.58	0.13	7.90	0.04
$KCGeBr_3$	0.39	0.66	-0.96	6.03	5.14	0.15	7.79	0.22
$KCGeI_3$	0.14	0.70	-1.31	5.48	4.19	0.14	6.66	0.35
$KCSnCl_3$	0.28	0.70	-1.04	6.12	5.36	0.16	8.07	0.17
$KCSnBr_3$	0.40	0.70	-0.99	5.74	5.03	0.21	7.67	0.32
$KCSnI_3$	0.52	0.65	-0.87	5.28	4.46	0.21	6.87	0.59
$KCPbCl_3$	0.87	0.63	-0.47	5.71	5.84	0.37	8.51	0.49
$KCPbBr_3$	1.01	0.60	-0.42	5.33	5.31	0.39	7.80	0.76

$KCPbI_3$	1.15	0.62	-0.43	4.94	4.49	0.41	6.82	1.12
$RAGeCl_3$	0.18	0.73	-1.11	6.27	5.62	0.15	6.91	0.19
$RAGeBr_3$	0.20	0.69	-1.15	5.97	5.00	0.16	6.77	0.31
$RAGeI_3$	0.17	0.67	-1.30	5.37	4.06	0.18	6.38	0.55
$RASnCl_3$	0.28	0.70	-1.03	6.11	5.41	0.16	7.24	0.29
$RASnBr_3$	0.19	0.68	-1.43	5.42	4.95	0.32	7.03	0.46
$RASnI_3$	0.20	0.66	-1.30	5.17	4.30	0.22	6.56	0.61
$RAPbCl_3$	0.48	0.62	-1.01	5.60	5.78	0.40	8.08	0.49
$RAPbBr_3$	0.48	0.60	-1.09	5.26	5.18	0.43	7.56	0.67
$RAPbI_3$	0.74	0.62	-0.89	4.93	4.40	0.42	6.70	1.02
$TAGeCl_3$	0.12	0.72	-1.14	6.51	5.68	0.12	8.22	0.11
$TAGeBr_3$	0.37	0.66	-0.97	5.98	5.14	0.13	7.79	0.30
$TAGeI_3$	0.12	0.70	-1.33	5.49	4.20	0.13	6.67	0.40
$TASnCl_3$	0.30	0.71	-1.09	6.17	5.45	0.16	8.15	0.23
$TASnBr_3$	0.40	0.71	-1.06	5.75	5.05	0.20	7.69	0.38
$TASnI_3$	0.47	0.66	-0.94	5.24	4.47	0.19	6.86	0.63
$TAPbCl_3$	0.84	0.65	-0.56	5.70	5.94	0.37	8.59	0.55
$TAPbBr_3$	0.93	0.64	-0.57	5.37	5.42	0.40	7.92	0.75
$TAPbI_3$	1.24	0.44	-0.29	4.81	4.58	0.60	6.93	1.57
$UAGeCl_3$	0.09	0.73	-1.22	6.47	5.71	0.13	8.44	0.11
$UAGeBr_3$	0.22	0.73	-1.12	5.98	5.21	0.18	7.88	0.24
$UAGeI_3$	0.07	0.69	-1.31	5.50	4.24	0.13	6.70	0.40
$UASnCl_3$	0.33	0.71	-1.03	6.18	5.46	0.16	8.14	0.24
$UASnBr_3$	0.42	0.72	-1.02	5.74	5.06	0.21	7.69	0.39
$UASnI_3$	0.47	0.73	-1.04	5.26	4.50	0.23	6.91	0.59
$UAPbCl_3$	0.92	0.67	-0.40	5.69	5.92	0.39	8.58	0.62
$UAPbBr_3$	0.98	0.69	-0.37	5.36	5.42	0.43	7.98	0.82
$UAPbI_3$	1.28	0.43	-0.21	4.80	4.62	0.61	6.97	1.63

Table S2 Effective radii of molecular cations and anions and the tolerance factor (TF) of perovskites. Ionic radii of FA, MA, EA, BA, DA, and RA were used according to ref. 1. Ionic radii of TA and UA were used according to ref. 2. Ionic radii of JA, KB, KC was estimated because the large A makes the three-dimensional structure of the perovskite change to the two-dimensional structure[4-6]. Ionic radii of B and X were used according to ref. 3. TFs in the range of 0.78-1.05 have been bolded.

Clusters	r_A (Å)	r_B (Å)	r_X (Å)	TF	Clusters	r_A (Å)	r_B (Å)	r_X (Å)	TF
$FAGeCl_3$	2.53	1.2	1.02	1.13	**$DASnBr_3$**	2.92	1.39	1.2	1.12
$FAGeBr_3$	2.53	1.2	1.2	1.10	**$DASnI_3$**	2.92	1.39	1.39	1.10
$FAGeI_3$	2.53	1.2	1.39	1.07	**$DAPbCl_3$**	2.92	1.46	1.02	1.12
$FASnCl_3$	2.53	1.39	1.02	**1.04**	**$DAPbBr_3$**	2.92	1.46	1.2	1.10
$FASnBr_3$	2.53	1.39	1.2	**1.02**	**$DAPbI_3$**	2.92	1.46	1.39	1.07
$FASnI_3$	2.53	1.39	1.39	**1.00**	**$KBGeCl_3$**	3.31	1.2	1.02	1.38
$FAPbCl_3$	2.53	1.46	1.02	**1.01**	**$KBGeBr_3$**	3.31	1.2	1.2	1.33
$FAPbBr_3$	2.53	1.46	1.2	**0.99**	**$KBGeI_3$**	3.31	1.2	1.39	1.28
$FAPbI_3$	2.53	1.46	1.39	**0.97**	**$KBSnCl_3$**	3.31	1.39	1.02	1.27
$JAGeCl_3$	2.73	1.2	1.02	1.19	**$KBSnBr_3$**	3.31	1.39	1.2	1.23
$JAGeBr_3$	2.73	1.2	1.2	1.16	**$KBSnI_3$**	3.31	1.39	1.39	1.20
$JAGeI_3$	2.73	1.2	1.39	1.12	**$KBPbCl_3$**	3.31	1.46	1.02	1.23
$JASnCl_3$	2.73	1.39	1.02	1.10	**$KBPbBr_3$**	3.31	1.46	1.2	1.20
$JASnBr_3$	2.73	1.39	1.2	1.07	**$KBPbI_3$**	3.31	1.46	1.39	1.17
$JASnI_3$	2.73	1.39	1.39	**1.05**	**$KCGeCl_3$**	3.88	1.2	1.02	1.56
$JAPbCl_3$	2.73	1.46	1.02	**1.07**	**$KCGeBr_3$**	3.88	1.2	1.2	1.50
$JAPbBr_3$	2.73	1.46	1.2	**1.04**	**$KCGeI_3$**	3.88	1.2	1.39	1.44
$JAPbI_3$	2.73	1.46	1.39	**1.02**	**$KCSnCl_3$**	3.88	1.39	1.02	1.44
$MAGeCl_3$	2.17	1.2	1.02	**1.02**	**$KCSnBr_3$**	3.88	1.39	1.2	1.39
$MAGeBr_3$	2.17	1.2	1.2	**0.99**	**$KCSnI_3$**	3.88	1.39	1.39	1.34
$MAGeI_3$	2.17	1.2	1.39	**0.97**	**$KCPbCl_3$**	3.88	1.46	1.02	1.40
$MASnCl_3$	2.17	1.39	1.02	**0.94**	**$KCPbBr_3$**	3.88	1.46	1.2	1.35
$MASnBr_3$	2.17	1.39	1.2	**0.92**	**$KCPbI_3$**	3.88	1.46	1.39	1.31
$MASnI_3$	2.17	1.39	1.39	**0.91**	**$RAGeCl_3$**	2.58	1.2	1.02	1.15
$MAPbCl_3$	2.17	1.46	1.02	**0.91**	**$RAGeBr_3$**	2.58	1.2	1.2	1.11
$MAPbBr_3$	2.17	1.46	1.2	**0.90**	**$RAGeI_3$**	2.58	1.2	1.39	1.08
$MAPbI_3$	2.17	1.46	1.39	**0.88**	**$RASnCl_3$**	2.58	1.39	1.02	1.06
$EAGeCl_3$	2.74	1.2	1.02	1.20	**$RASnBr_3$**	2.58	1.39	1.2	**1.03**
$EAGeBr_3$	2.74	1.2	1.2	1.16	**$RASnI_3$**	2.58	1.39	1.39	**1.01**
$EAGeI_3$	2.74	1.2	1.39	1.13	**$RAPbCl_3$**	2.58	1.46	1.02	**1.03**
$EASnCl_3$	2.74	1.39	1.02	1.10	**$RAPbBr_3$**	2.58	1.46	1.2	**1.00**
$EASnBr_3$	2.74	1.39	1.2	1.08	**$RAPbI_3$**	2.58	1.46	1.39	**0.98**
$EASnI_3$	2.74	1.39	1.39	**1.05**	**$TAGeCl_3$**	3.07	1.2	1.02	1.30
$EAPbCl_3$	2.74	1.46	1.02	1.07	**$TAGeBr_3$**	3.07	1.2	1.2	1.26
$EAPbBr_3$	2.74	1.46	1.2	**1.05**	**$TAGeI_3$**	3.07	1.2	1.39	1.22
$EAPbI_3$	2.74	1.46	1.39	**1.02**	**$TASnCl_3$**	3.07	1.39	1.02	1.20
$BAGeCl_3$	2.16	1.2	1.02	**1.01**	**$TASnBr_3$**	3.07	1.39	1.2	1.17
$BAGeBr_3$	2.16	1.2	1.2	**0.99**	**$TASnI_3$**	3.07	1.39	1.39	1.13
$BAGeI_3$	2.16	1.2	1.39	**0.97**	**$TAPbCl_3$**	3.07	1.46	1.02	1.17
$BASnCl_3$	2.16	1.39	1.02	**0.93**	**$TAPbBr_3$**	3.07	1.46	1.2	1.14
$BASnBr_3$	2.16	1.39	1.2	**0.92**	**$TAPbI_3$**	3.07	1.46	1.39	1.11
$BASnI_3$	2.16	1.39	1.39	**0.90**	**$UAGeCl_3$**	3.04	1.2	1.02	1.29
$BAPbCl_3$	2.16	1.46	1.02	**0.91**	**$UAGeBr_3$**	3.04	1.2	1.2	1.25
$BAPbBr_3$	2.16	1.46	1.2	**0.89**	**$UAGeI_3$**	3.04	1.2	1.39	1.21
$BAPbI_3$	2.16	1.46	1.39	**0.88**	**$UASnCl_3$**	3.04	1.39	1.02	1.19
$DAGeCl_3$	2.92	1.2	1.02	1.25	**$UASnBr_3$**	3.04	1.39	1.2	1.16
$DAGeBr_3$	2.92	1.2	1.2	1.21	**$UASnI_3$**	3.04	1.39	1.39	1.13
$DAGeI_3$	2.92	1.2	1.39	1.18	**$UAPbCl_3$**	3.04	1.46	1.02	1.16
$DASnCl_3$	2.92	1.39	1.02	1.16	**$UAPbBr_3$**	3.04	1.46	1.2	1.13
$DASnBr_3$	2.92	1.39	1.2	1.12	**$UAPbI_3$**	3.04	1.46	1.39	1.10

Table S3 The binding energy table which is calculated by the formula $\Delta E = E_{ABX_3} - E_A - E_{BX_3}$. M06-2X-D3, M06-2X, B3LYP-D3, and B3LYP are the testing functionals. Error is the difference between the binding energy calculated by other functionals and M06-2X-D3. (all energies are in eV) Time is job cpu time which is exported by Gaussian 09.

Cluster	M06-2X-D3			M06-2X		
	Binding energy	**Error**	**Time (hours)**	**Binding energy**	**Error**	**Time (hours)**
$MAPbF_3$	5.886	0.000	0.640	5.881	0.005	0.628
$MAPbCl_3$	4.989	0.000	0.602	4.982	0.007	0.559
$MAPbBr_3$	4.770	0.000	0.871	4.763	0.007	0.992
$MAPbI_3$	4.524	0.000	1.003	4.518	0.007	1.064
Cluster	**B3LYP-D3**			**B3LYP**		
	Binding energy	**Error**	**Time (hours)**	**Binding energy**	**Error**	**Time (hours)**
$MAPbF_3$	5.866	0.020	0.444	5.684	0.201	0.402
$MAPbCl_3$	5.100	0.112	0.381	4.819	0.169	0.373
$MAPbBr_3$	4.888	0.118	0.710	4.579	0.191	0.606
$MAPbI_3$	4.673	0.149	0.732	4.327	0.198	0.792

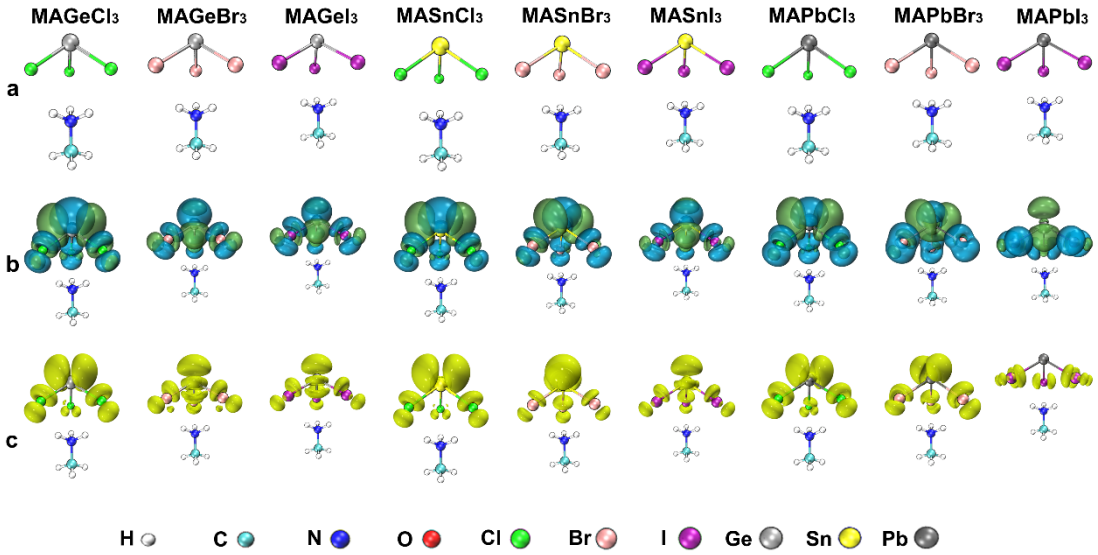


Figure S1. a) Optimized structures of $MABX_3$ (B = Ge^{2+}, Sn^{2+}, Pb^{2+}, and X = Cl^-, Br^-, I^-). b) The electron-hole distribution chart. Green and blue isosurfaces represent the distribution of electrons and holes, respectively. c) The *s*(r) distribution charts. The yellow isosurface represents the overlap of electrons and holes. The isosurfaces were uniformly selected as 0.002, respectively.

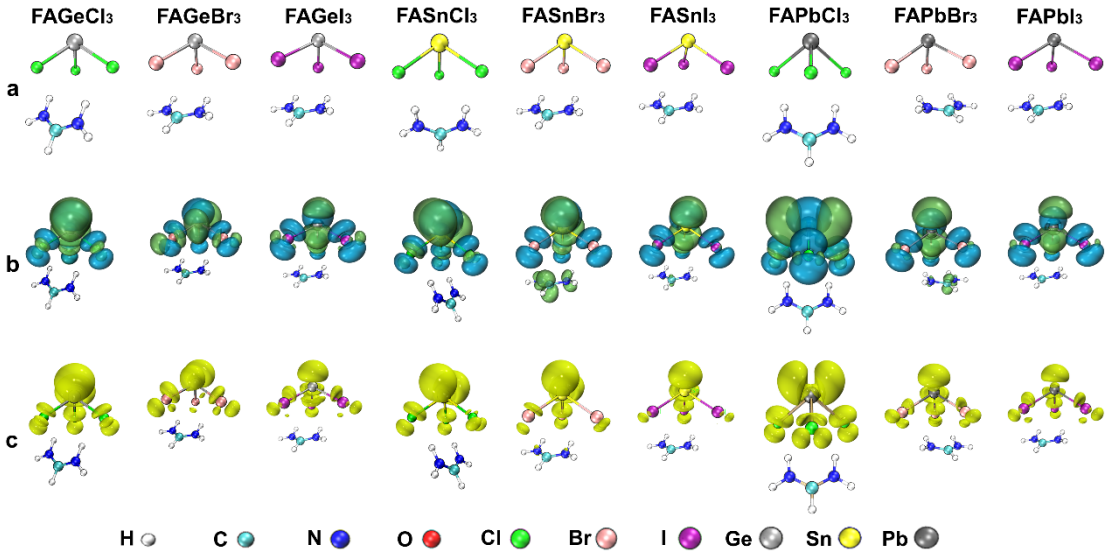


Figure S2. a) Optimized structures of $FABX_3$ (B = Ge^{2+}, Sn^{2+}, Pb^{2+}, and X = Cl^-, Br^-, I^-). b) The electron-hole distribution chart. Green and blue isosurfaces represent the distribution of electrons and holes, respectively. c) The *s*(r) distribution charts. The yellow isosurface represents the overlap of electrons and holes. The isosurfaces were uniformly selected as 0.002, respectively.

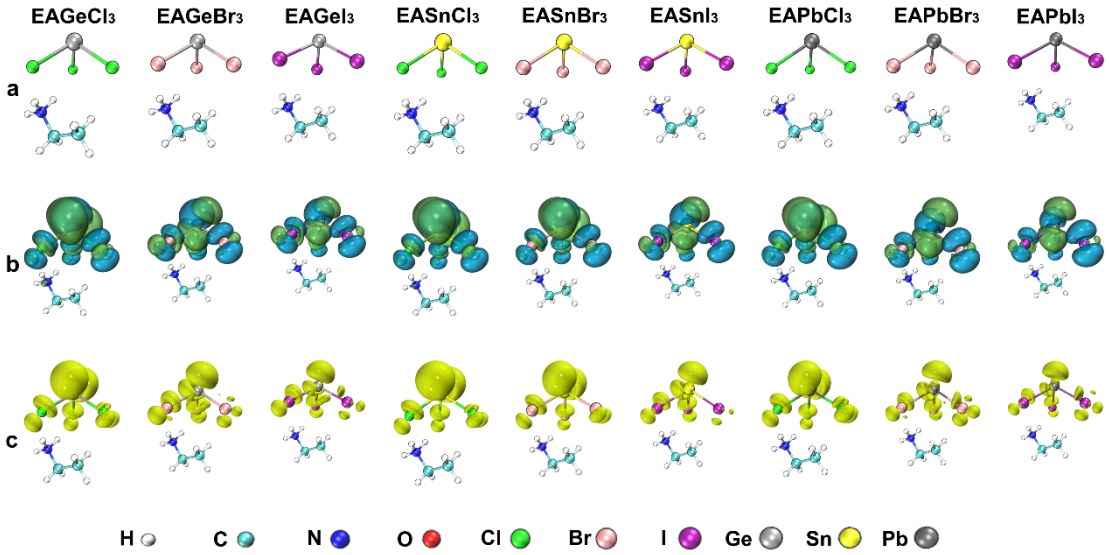


Figure S3. a) Optimized structures of $EABX_3$ (B = Ge^{2+}, Sn^{2+}, Pb^{2+}, and X = Cl^-, Br^-, I^-). b) The electron-hole distribution chart. Green and blue isosurfaces represent the distribution of electrons and holes, respectively. c) The *s*(r) distribution charts. The yellow isosurface represents the overlap of electrons and holes. The isosurfaces were uniformly selected as 0.002, respectively.

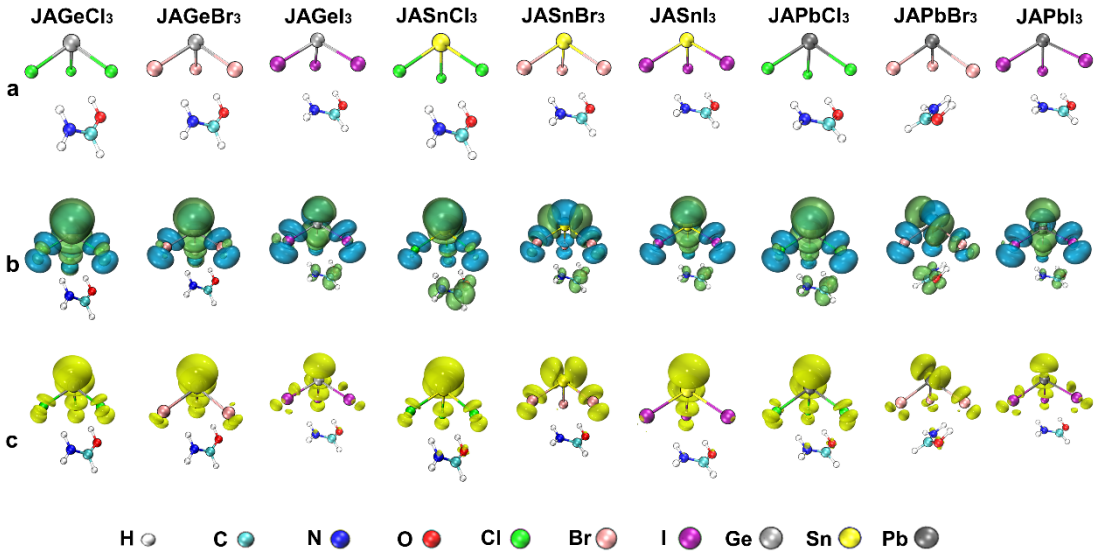


Figure S4. a) Optimized structures of $JABX_3$ (B = Ge^{2+}, Sn^{2+}, Pb^{2+}, and X = Cl^-, Br^-, I^-). b) The electron-hole distribution chart. Green and blue isosurfaces represent the distribution of electrons and holes, respectively. c) The *s*(r) distribution charts. The yellow isosurface represents the overlap of electrons and holes. The isosurfaces were uniformly selected as 0.002, respectively.

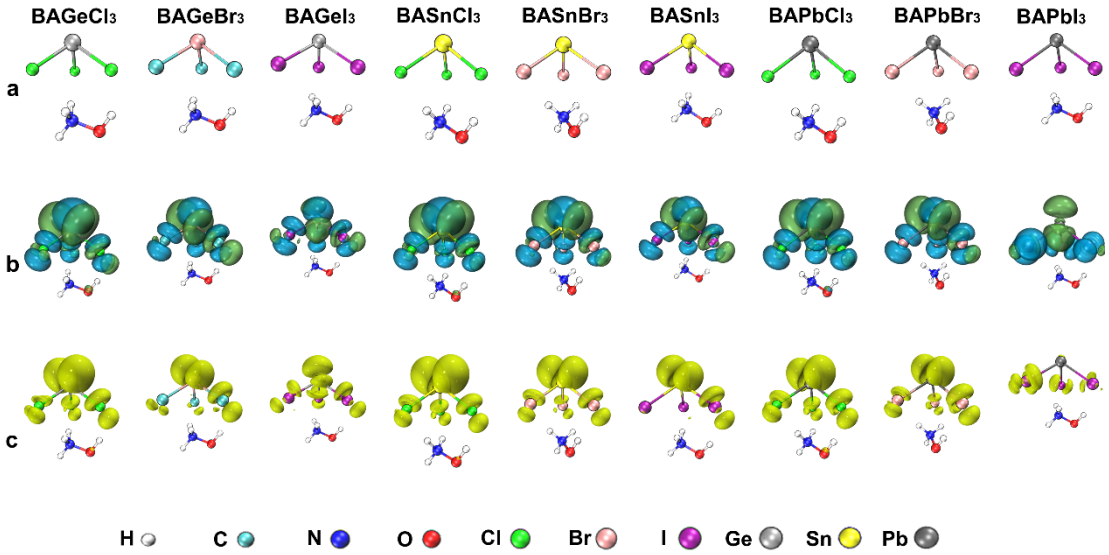


Figure S5. a) Optimized structures of $BABX_3$ (B = Ge^{2+}, Sn^{2+}, Pb^{2+}, and X = Cl^-, Br^-, I^-). b) The electron-hole distribution chart. Green and blue isosurfaces represent the distribution of electrons and holes, respectively. c) The *s*(r) distribution charts. The yellow isosurface represents the overlap of electrons and holes. The isosurfaces were uniformly selected as 0.002, respectively.

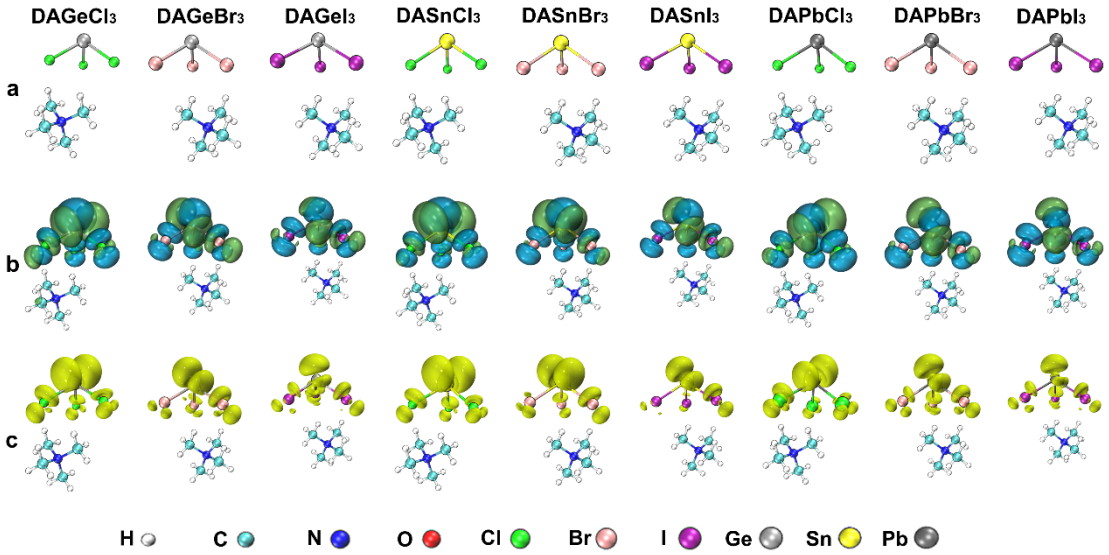


Figure S6. a) Optimized structures of $DABX_3$ (B = Ge^{2+}, Sn^{2+}, Pb^{2+}, and X = Cl^-, Br^-, I^-). b) The electron-hole distribution chart. Green and blue isosurfaces represent the distribution of electrons and holes, respectively. c) The *s*(r) distribution charts. The yellow isosurface represents the overlap of electrons and holes. The isosurfaces were uniformly selected as 0.002, respectively.

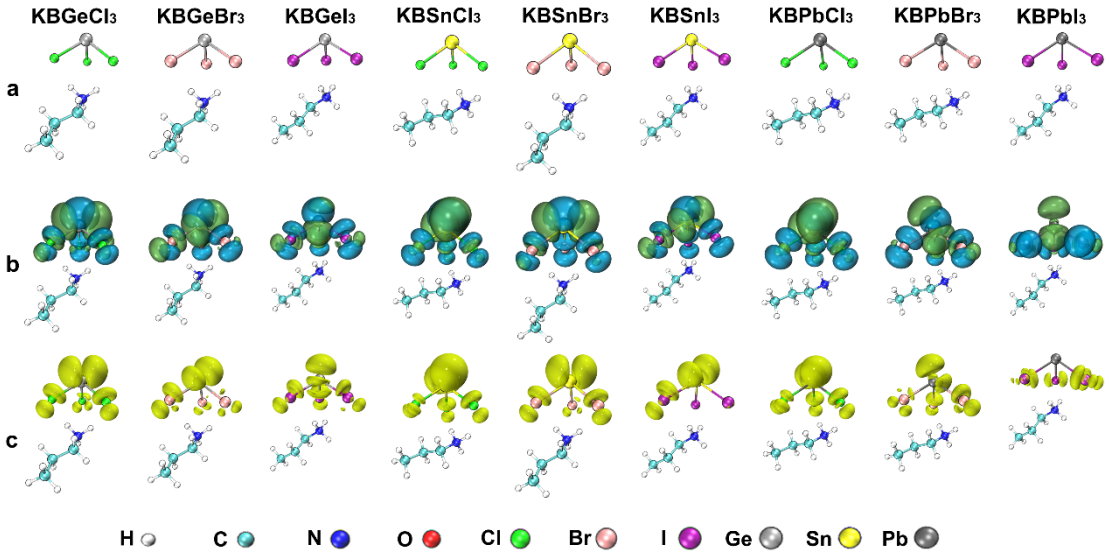


Figure S7. a) Optimized structures of $KBBX_3$ (B = Ge^{2+}, Sn^{2+}, Pb^{2+}, and X = Cl^-, Br^-, I^-). b) The electron-hole distribution chart. Green and blue isosurfaces represent the distribution of electrons and holes, respectively. c) The *s*(r) distribution charts. The yellow isosurface represents the overlap of electrons and holes. The isosurfaces were uniformly selected as 0.002, respectively.

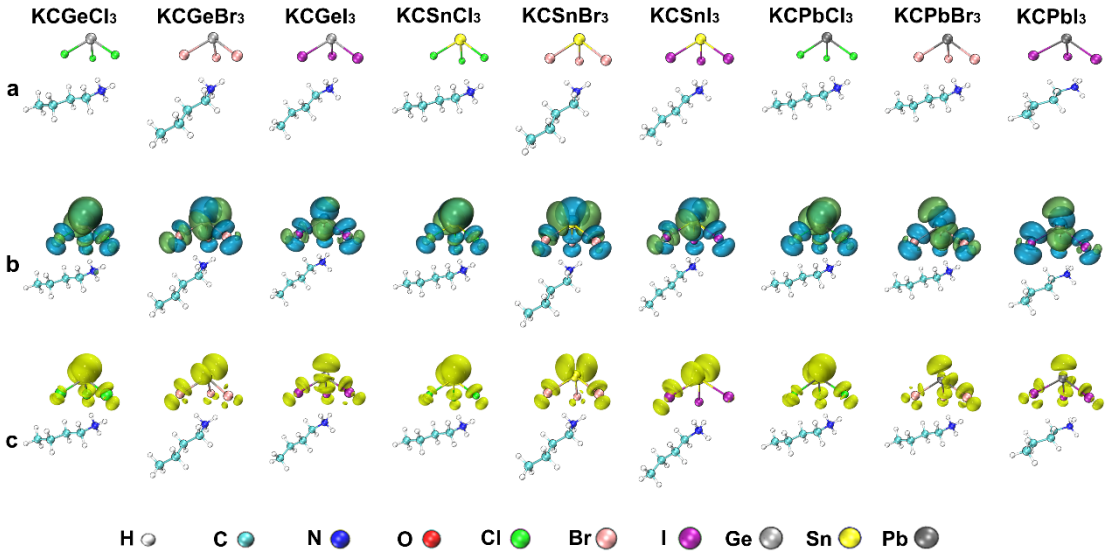


Figure S8. a) Optimized structures of $KCBX_3$ (B = Ge^{2+}, Sn^{2+}, Pb^{2+}, and X = Cl^-, Br^-, I^-). b) The electron-hole distribution chart. Green and blue isosurfaces represent the distribution of electrons and holes, respectively. c) The *s*(r) distribution charts. The yellow isosurface represents the overlap of electrons and holes. The isosurfaces were uniformly selected as 0.002, respectively.

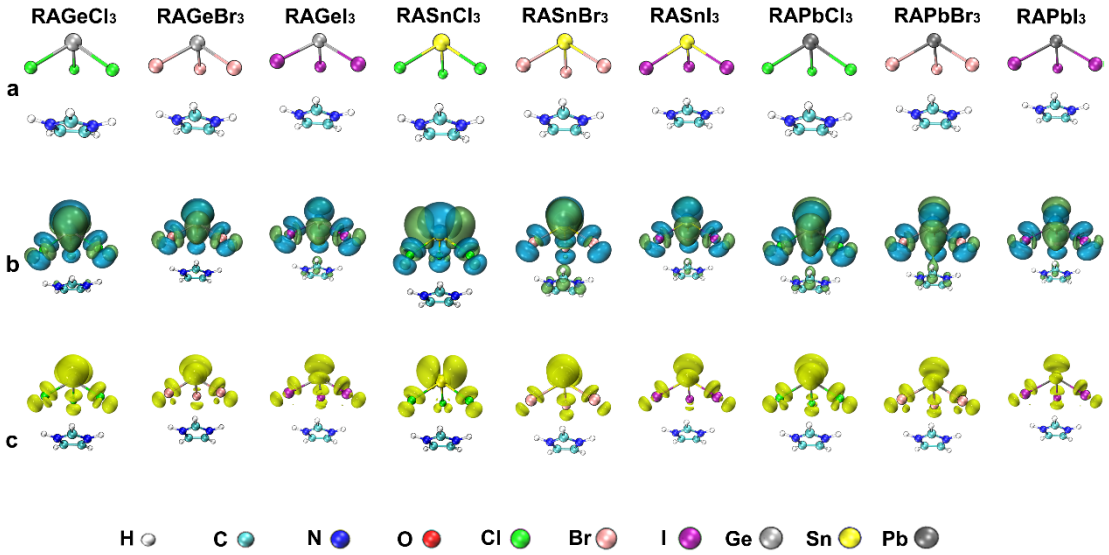


Figure S9. a) Optimized structures of $RABX_3$ (B = Ge^{2+}, Sn^{2+}, Pb^{2+}, and X = Cl^-, Br^-, I^-). b) The electron-hole distribution chart. Green and blue isosurfaces represent the distribution of electrons and holes, respectively. c) The *s*(r) distribution charts. The yellow isosurface represents the overlap of electrons and holes. The isosurfaces were uniformly selected as 0.002, respectively.

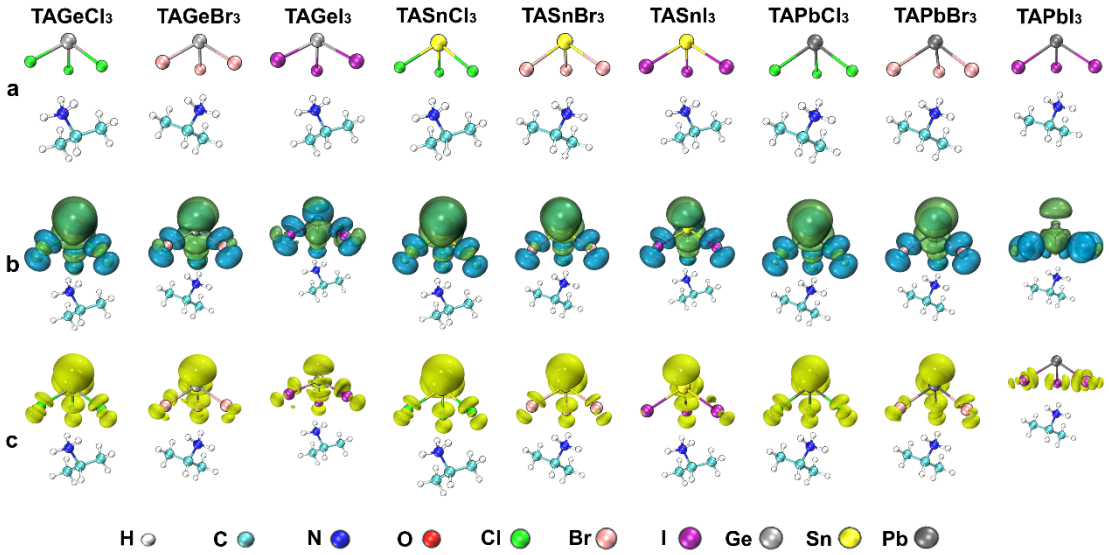


Figure S10. a) Optimized structures of $TABX_3$ (B = Ge^{2+}, Sn^{2+}, Pb^{2+}, and X = Cl^-, Br^-, I^-). b) The electron-hole distribution chart. Green and blue isosurfaces represent the distribution of electrons and holes, respectively. c) The *s*(r) distribution charts. The yellow isosurface represents the overlap of electrons and holes. The isosurfaces were uniformly selected as 0.002, respectively.

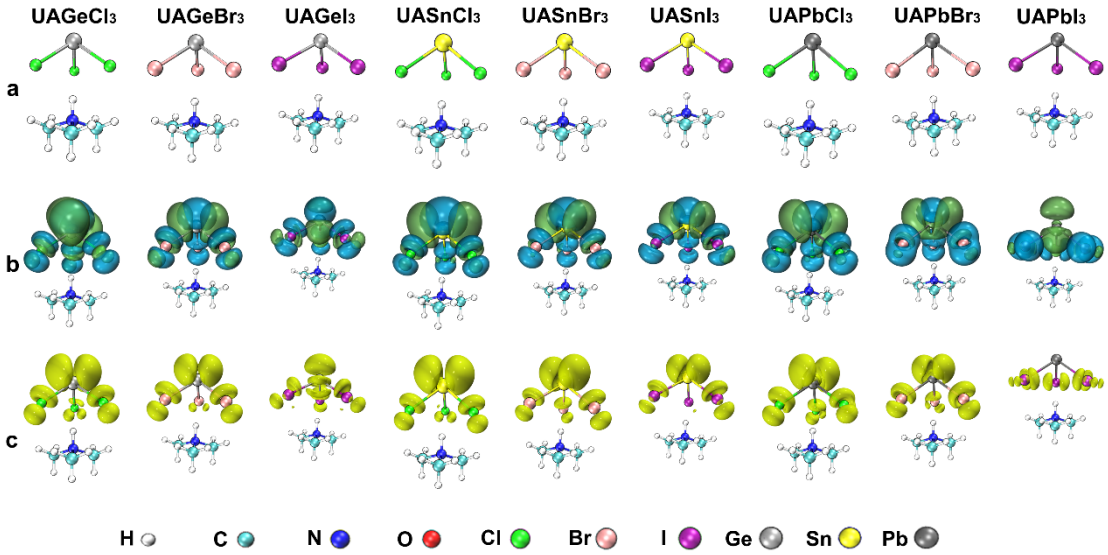
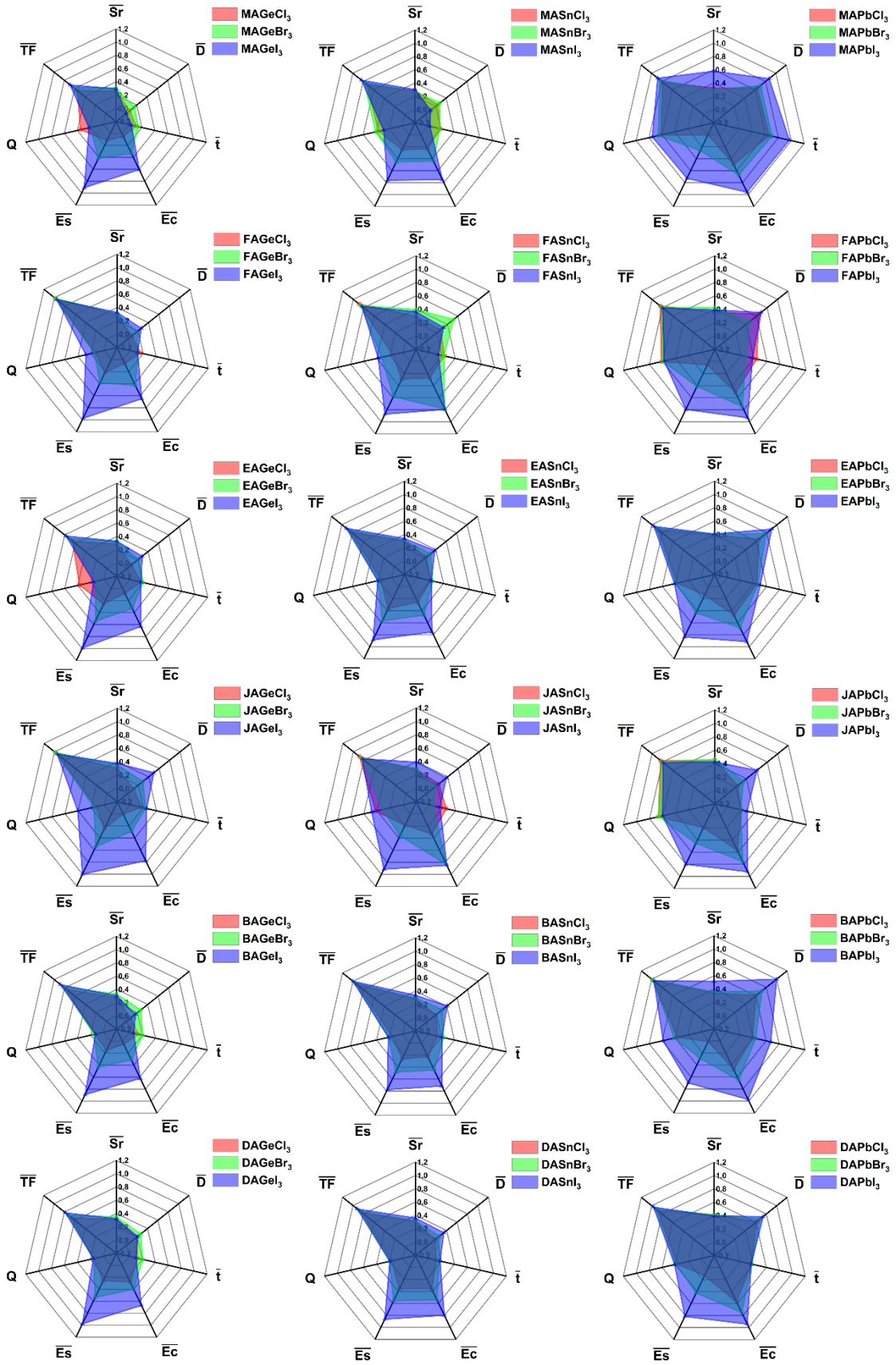


Figure S11. a) Optimized structures of $UABX_3$ (B = Ge^{2+}, Sn^{2+}, Pb^{2+}, and X = Cl^-, Br^-, I^-). b) The electron-hole distribution chart. Green and blue isosurfaces represent the distribution of electrons and holes, respectively. c) The *s*(r) distribution charts. The yellow isosurface represents the overlap of electrons and holes. The isosurfaces were uniformly selected as 0.002, respectively.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MAGeBr3
MAGeI3
MASnCl3
MASnBr3
MASnI3
MAPbCl3
MAPbBr3
MAPbI3
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FAGeBr3
FAGeI3
FASnCl3
FASnBr3
FASnI3
FAPbCl3
FAPbBr3
FAPbI3
EAGeCl3
EAGeBr3
EAGeI3
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BASnBr3
BASnI3
BAPbCl3
BAPbBr3
BAPbI3
DAGeCl3
DAGeBr3
DAGeI3
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Sr
D
t
Ec
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Q
TF

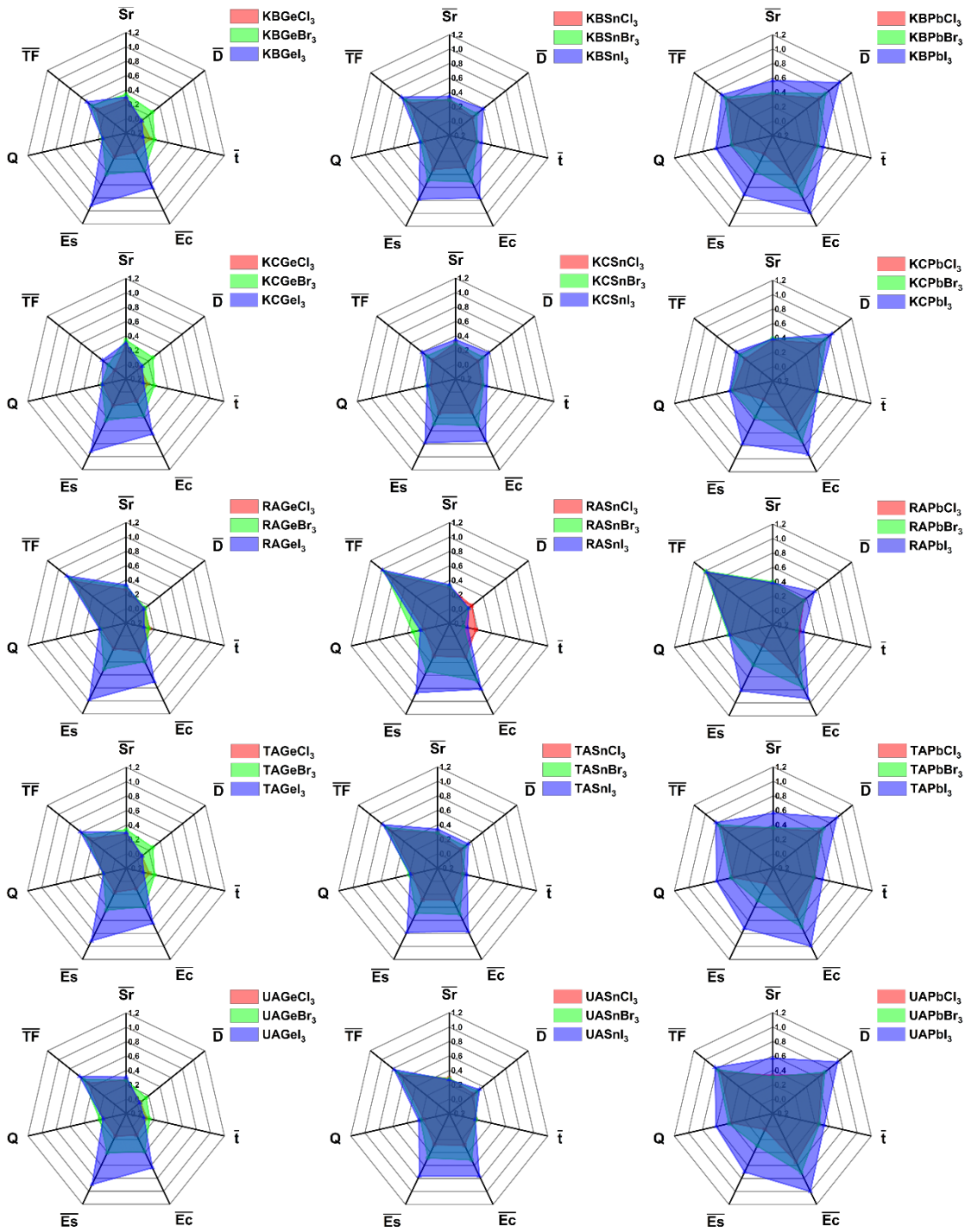

Figure S12. Radar chart of the normalized electronic excitation characteristic index. $\overline{D}$ index means the centroid distance between holes and electrons. $\overline{Sr}$ index means the separation between holes and electrons. $\overline{TF}$ means the normalized tolerance factor. The Q index represents the net charge transfer. $\overline{Ec}$ and $\overline{Es}$ respectively represent the relative magnitude of exciton binding energy and excitation energy. $\bar{t}$ index measures the degree of separation of holes and electrons.

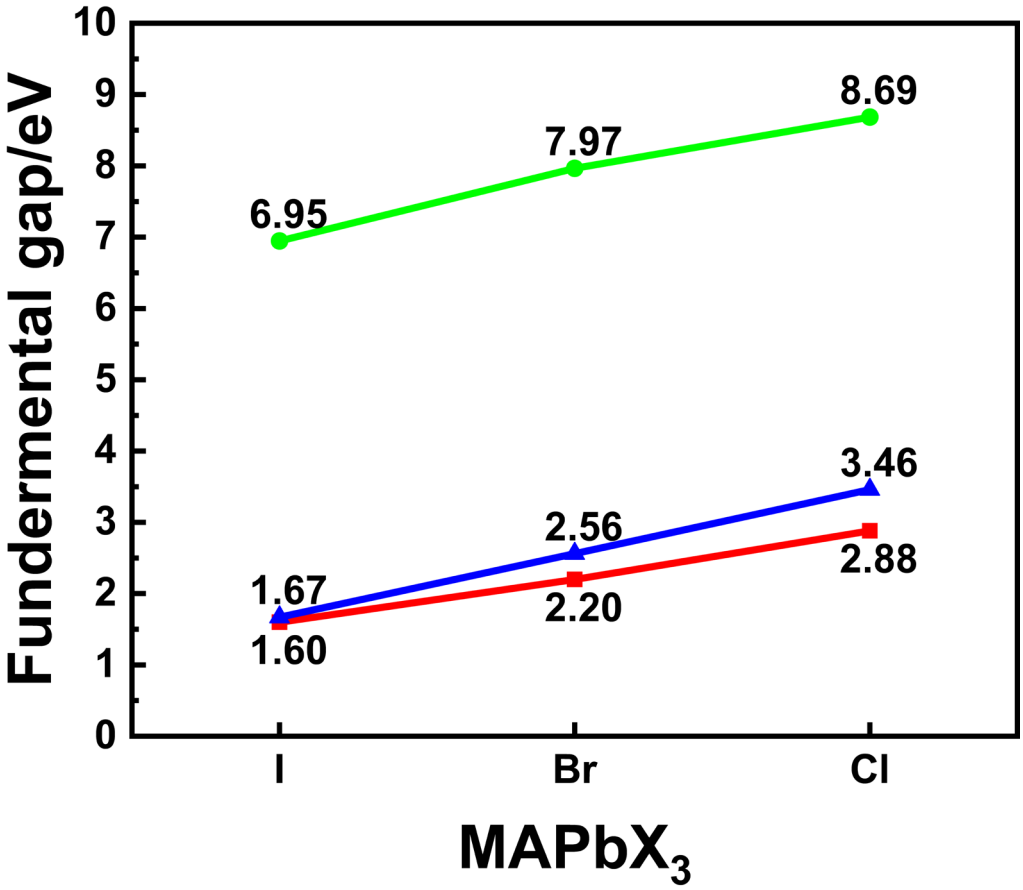

Figure S13. The DFT-M06-2X calculated HOMO-LUMO gaps (green) of the molecules compared to band gaps (blue) calculated by the DFT-GGA-GW with SOC and the experimental values (red).

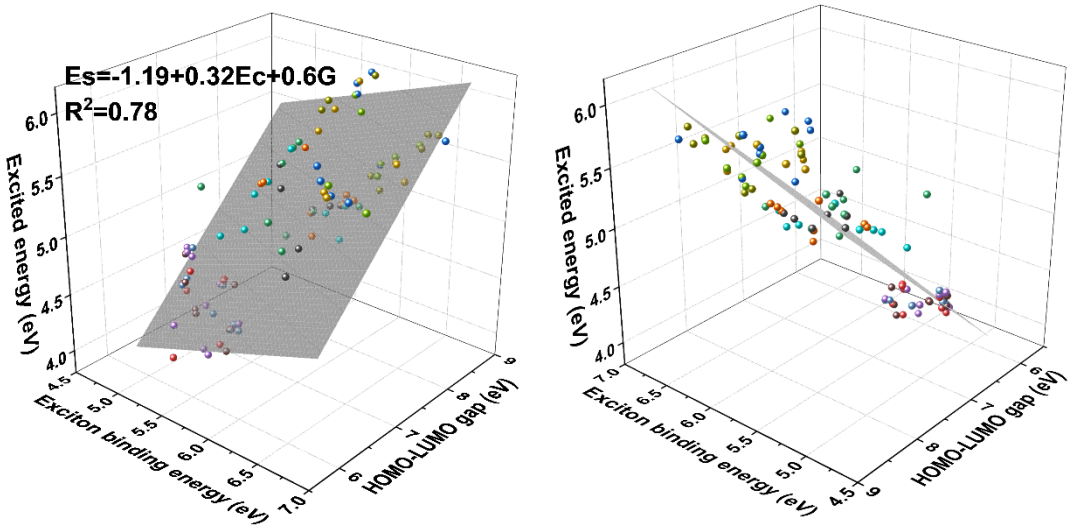

Figure S14 Two-dimensional plane fitting diagram between exciton binding energy, HOMO-LUMO gap, and excitation energy. *Es* means the excited energy. *Ec* means the exciton binding energy and *G* represents the HOMO-LUMO gap.

Notes and references

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