Supplementary Information for:

Small Practical Cluster Models for Perovskites Based on the Similarity Criterion of Central Location Environment and Their Applications

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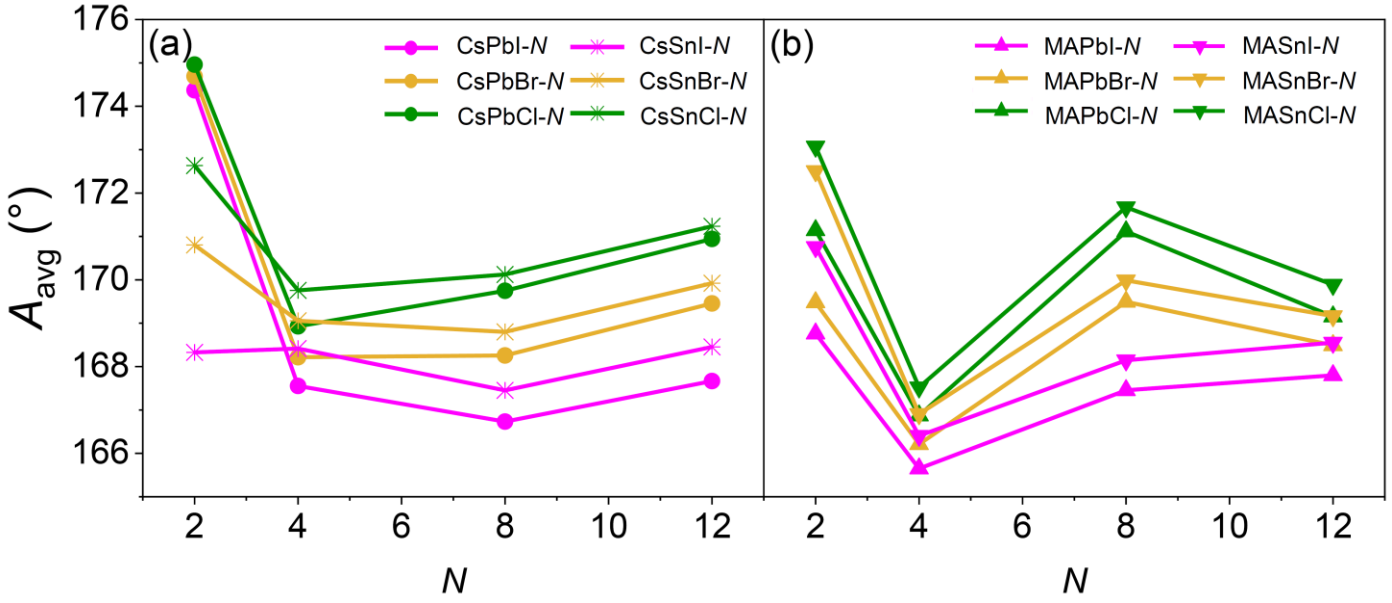

Fig. S1. The average angle of B-X_b-B (A_{avg}, °) in (a) CsBX-*N* and (b) MABX-*N* (B = Pb and Sn; X = Cl, Br, and I; *N* = 2, 4, 8, and 12).

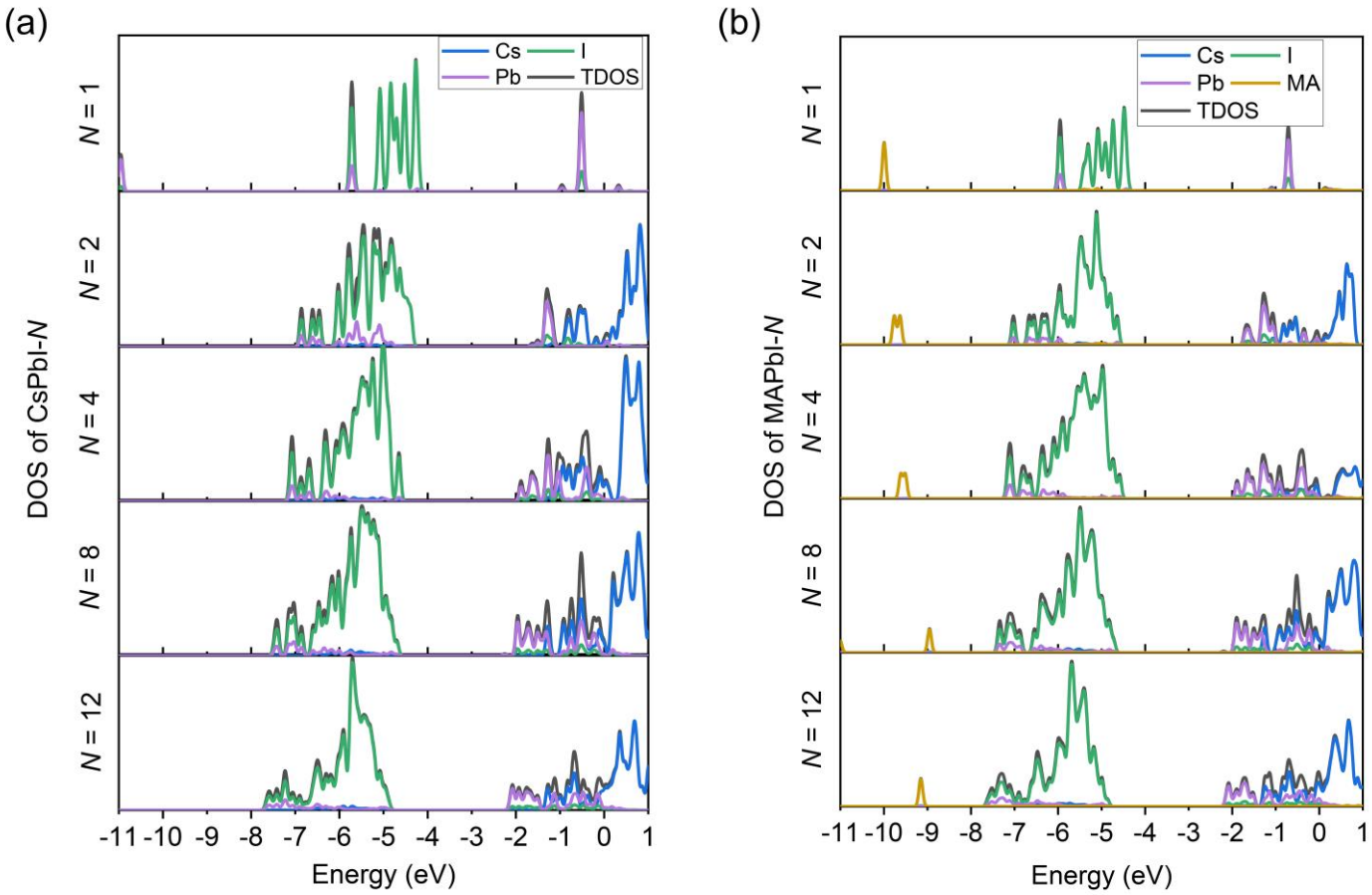

Fig. S2. The partial density of states (PDOS) and total density of states (TDOS) of CsBX-*N* and MABX-*N* (*N* = 1, 2, 4, 8, and 12). The full width at half maximum is set as 0.1 eV.

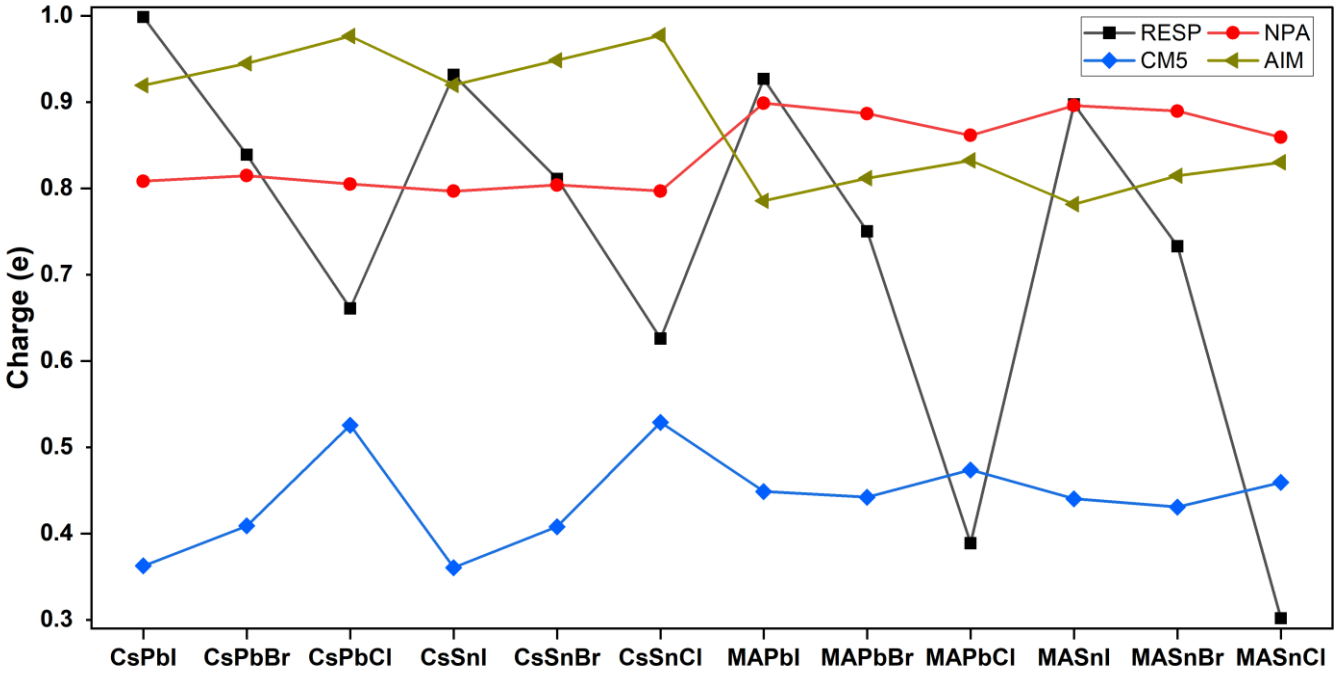

Fig. S3. The average charge on each central A sites of ABX-12 systems (A = Cs and MA; B = Pb and Sn; X = I, Br, and Cl) with different calculated methods.

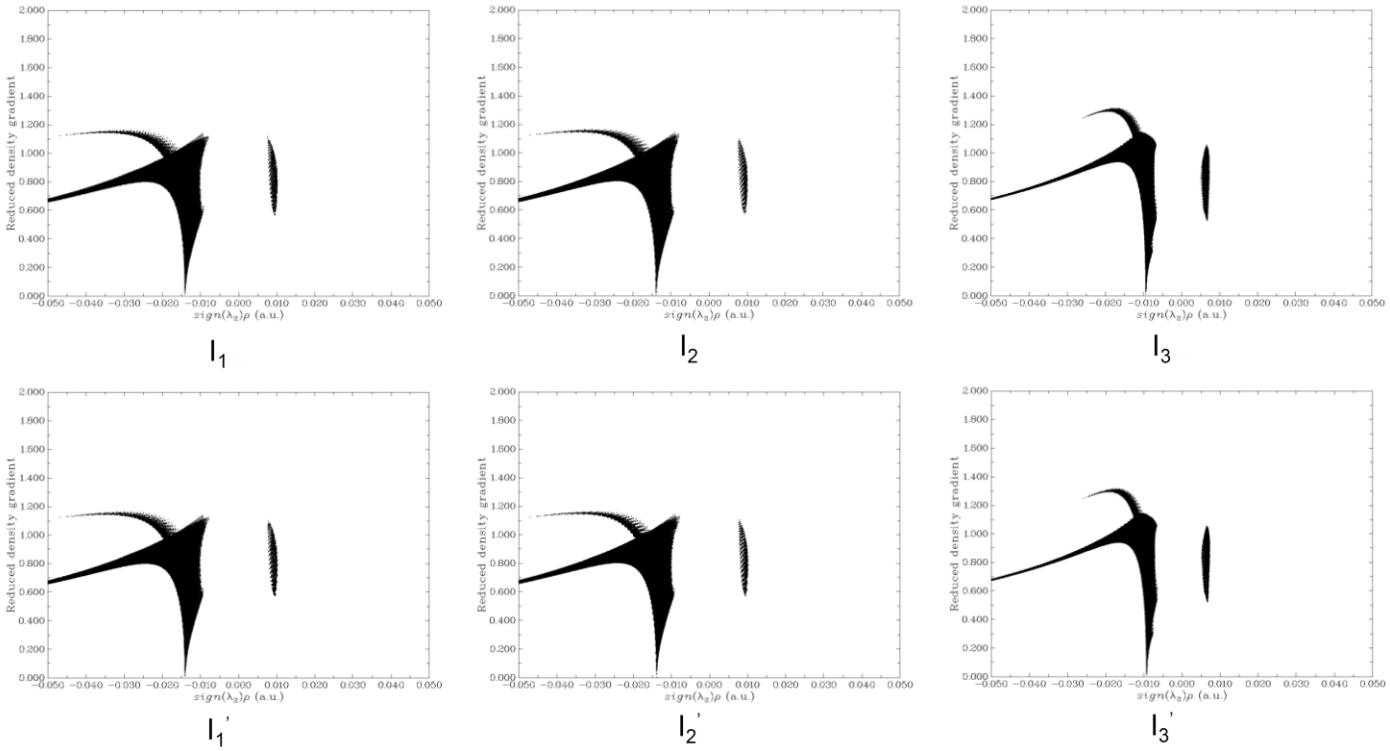

Fig. S4. The specific RDG analyses between each pair of (N)H-X atoms for MAPbI-12. I_n and I_n' correspond to I_n in Figure 8 since the position of them are the same.

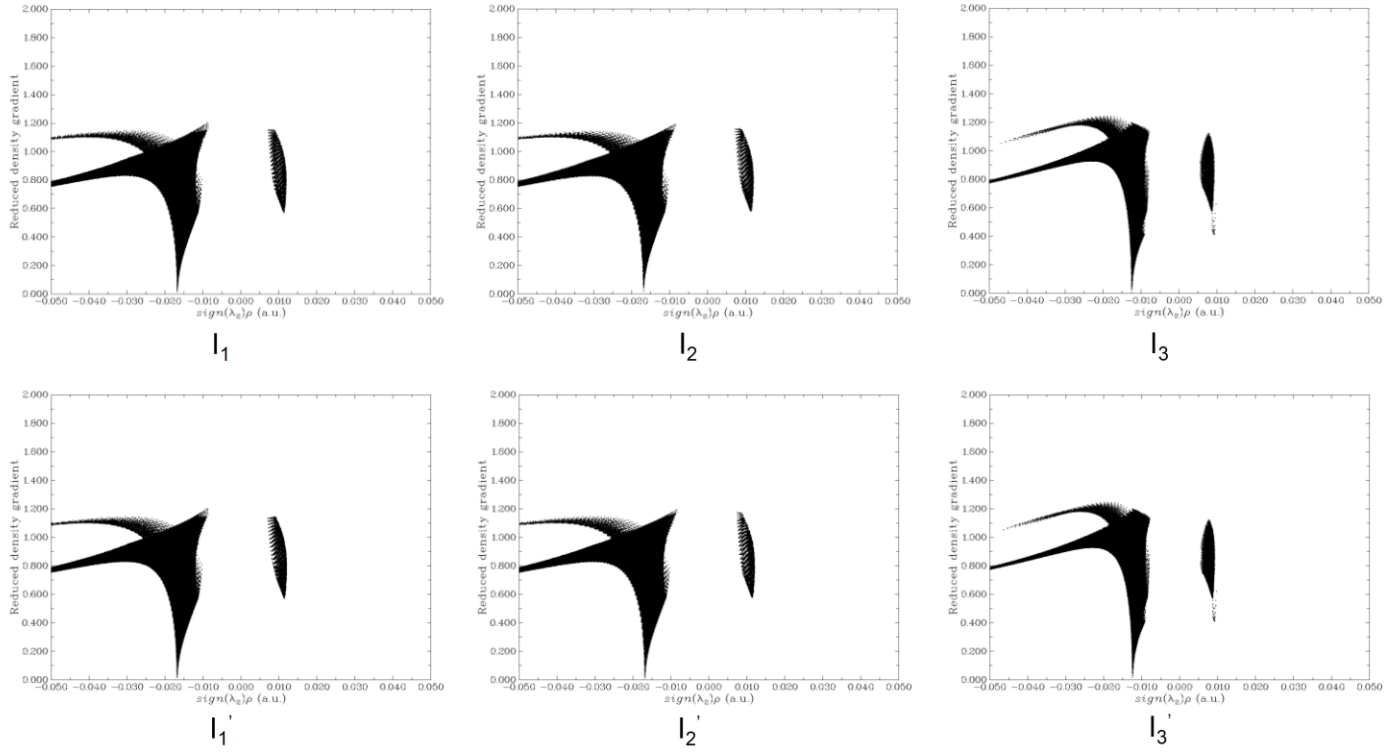

Fig. S5. The specific RDG analyses between each pair of (N)H-X atoms for MAPbBr-12. I_n and I_n' correspond to I_n in Figure 8 since the position of them are the same.

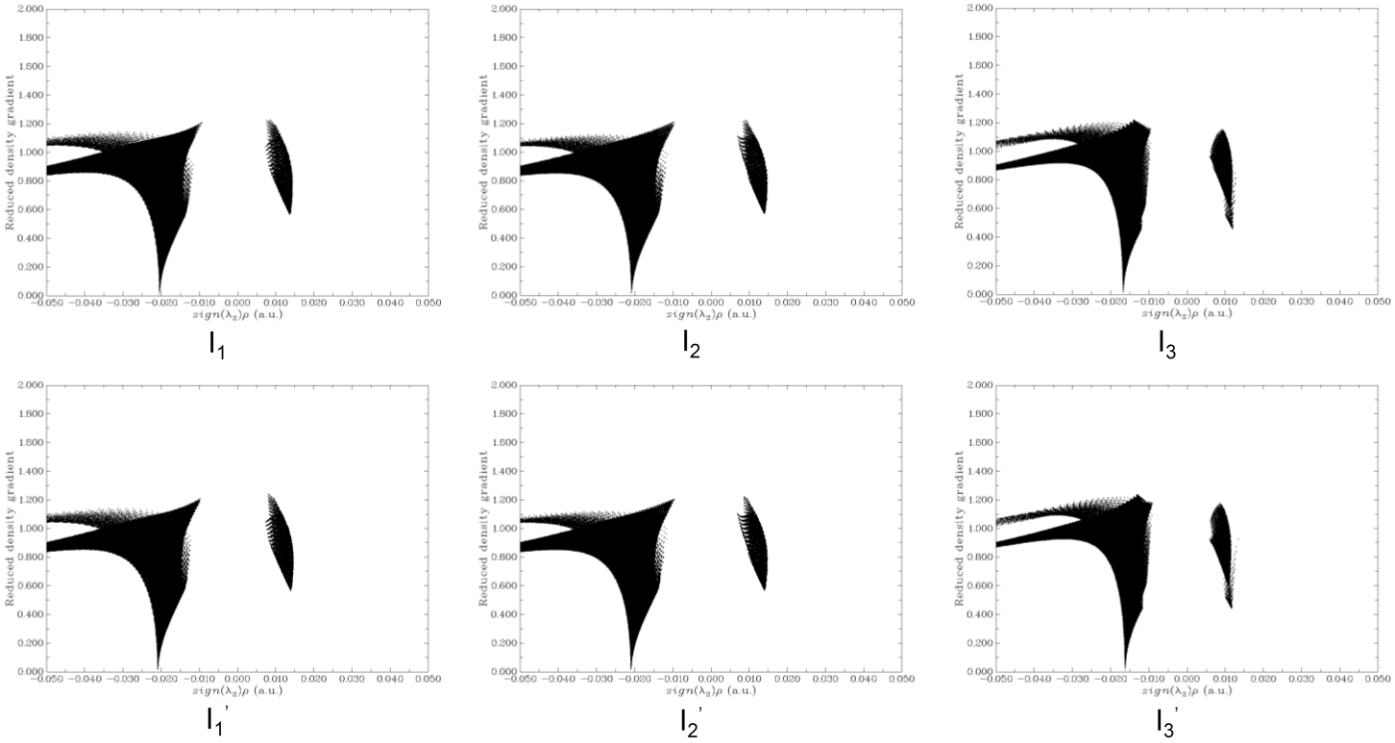

Fig. S6. The specific RDG analyses between each pair of (N)H-X atoms for MAPbCl-12. I_n and I_n' correspond to I_n in Figure 8 since the position of them are the same.

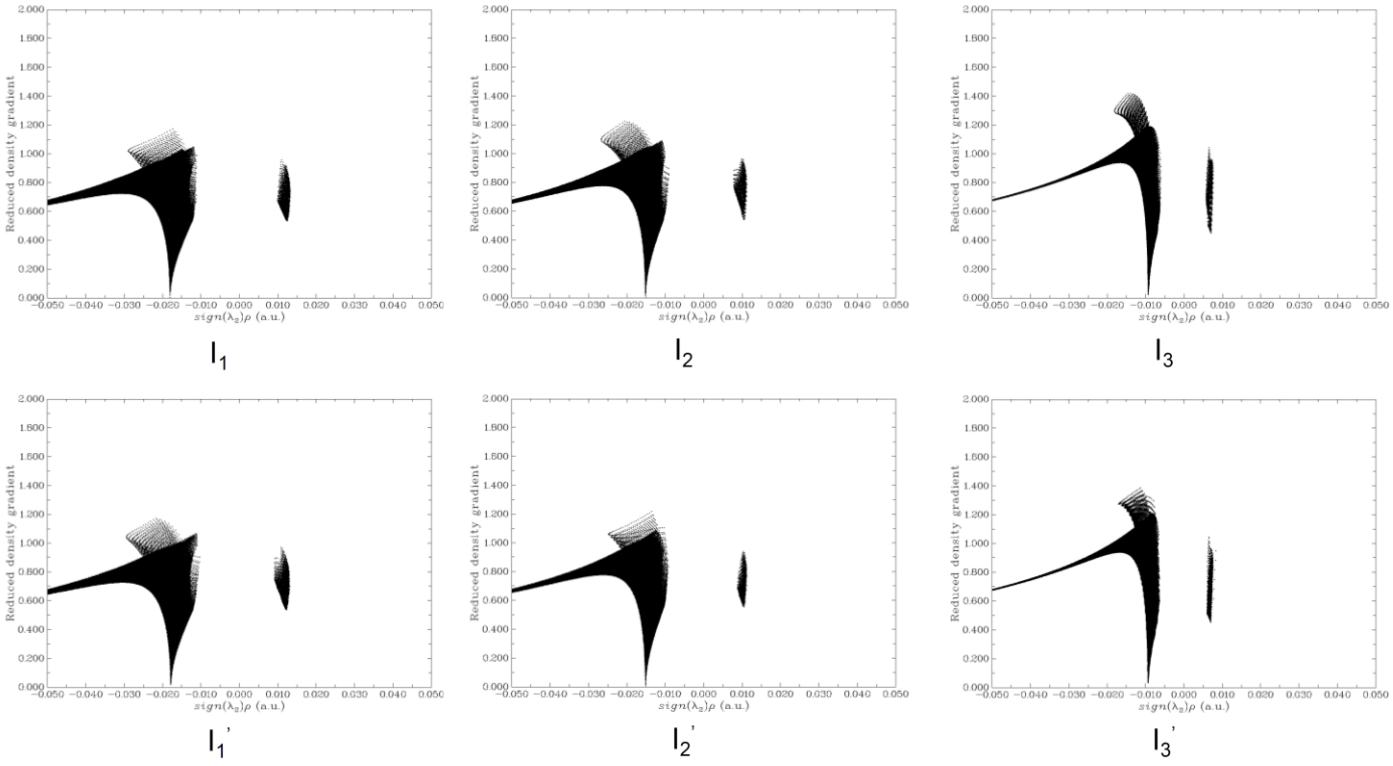

Fig. S7. The specific RDG analyses between each pair of (N)H-X atoms for EAPbI-12. I_n and I_n' correspond to I_n in Figure 8 since the position of them are the same.

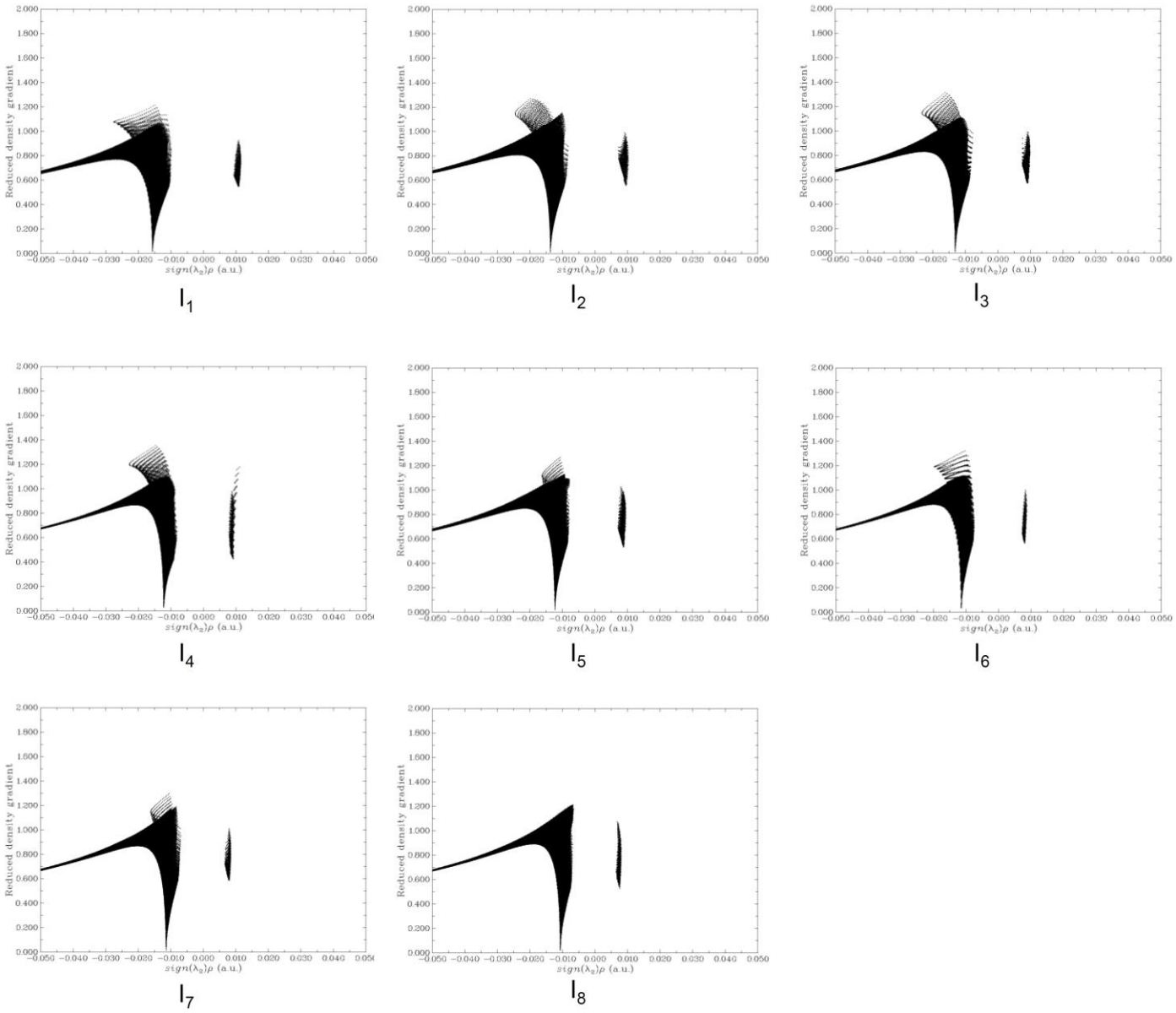

Fig. S8. The specific RDG analyses between each pair of (N)H-X atoms for FAPbI-12.

Table S1. The binding energies ΔE_1, ΔE_1', ΔE_2, and ΔE_2' (in eV) between A and BX part in ABX-12 (A = Cs and MA; B = Pb and Sn; X = Cl, Br, and I) calculated by equations (1), (2), (3), and (4), respectively.

	ΔE_1	ΔE_1'	ΔE_2	ΔE_2'		ΔE_1	ΔE_1'	ΔE_2	ΔE_2'
CsSnI-12	5.27	5.64	5.26	6.40	MASnI-12	5.44	5.74	5.41	6.58
CsSnBr-12	5.26	5.93	5.23	6.72	MASnBr-12	5.38	6.06	5.32	6.84
CsSnCl-12	5.23	6.26	5.19	7.09	MASnCl-12	5.26	6.31	5.19	7.12
CsPbI-12	5.80	5.66	5.80	6.40	MAPbI-12	5.97	5.87	5.96	6.59
CsPbBr-12	5.84	5.94	5.83	6.71	MAPbBr-12	5.98	6.09	5.95	6.86
CsPbCl-12	5.87	6.25	5.87	7.07	MAPbCl-12	5.95	6.33	5.91	7.14

Table S2. Frequencies of main vibrational modes (cm^{-1}) of organic cations for both isolated ones and those in cage structures.

	MA	MAPbI-12	MAPbBr-12	MAPbCl-12	EA	EAPbI-12	FA	FAPbI-12
C-N stretch	916	973 973	984 985	997 998	804	864 871	1101 1382	1102 1117 1379 1385
C-C stretch					1014	1063		
Symmetric C-H stretch (CH_3)	3043	3032 3033	3038 3039	3045 3046	2998	3000 3001		
Symmetric C-H stretch (CH_2)					3050	3047 3048		
C-H stretch (CH)							3190	3162 3185
Asymmetric C-H stretch (CH_3)	3168 3168	3147 3147 3163 3163	3153 3153 3167 3168	3159 3160 3174 3175	3090 3107 3128	3093 3094 3124 3125 3127 3129		
Asymmetric C-H stretch (CH_2)								
Symmetric N-H stretch (NH_3)	3321	3194 3194	3200 3201	3198 3202	3316	3170 3174		
Asymmetric N-H stretch (NH_3)	3427 3432	3253 3254 3357 3358	3259 3260 3351 3351	3254 3259 3338 3347	3429 3433	3232 3237 3348 3350		
Symmetric N-H stretch (NH_2)							3491 3505	3362 3398 3400 3426
Asymmetric N-H stretch (NH_2)							3624 3625	3495 3534 3536 3547