Electronic Supplementary Information

New insights on the organic-inorganic hybrid perovskite $CH_3NH_3PbI_3$ nanoparticles. Experimental and theoretical study of doping in Pb^{2+} sites with Sn^{2+}, Sr^{2+}, Cd^{2+} and Ca^{2+}

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Table S1. Results in weight percentage (wt.%) obtained from the elemental analysis performed using the CHNS and XRF techniques.

Sample* $MAPb_{1-x}B_xI_3$		**wt.% C**	**wt.% H**	**wt.% N**	**wt.% Pb**	**wt.% I**	**wt.% B**	**x_{real}**
$MAPbI_3$		1.95	0.97	2.27	33.56	61.25	--	0.00
B=Sn	0.05	1.95	0.98	2.28	31.87	61.86	1.06	0.05
	0.10	1.96	0.98	2.29	30.76	62.25	1.76	0.09
	0.15	1.98	0.99	2.31	29.00	62.80	2.92	0.15
B=Sr	0.05	1.96	0.98	2.28	31.93	62.08	0.77	0.05
	0.10	1.98	0.99	2.31	30.55	62.68	1.49	0.10
	0.15	1.99	0.99	2.32	29.54	63.08	2.08	0.14
B=Cd	0.05	1.95	0.98	2.28	32.03	61.79	0.98	0.05
	0.10	1.97	0.98	2.30	30.55	62.44	1.76	0.10
	0.15	1.98	0.99	2.31	29.02	62.90	2.80	0.15
B=Ca	0.05	1.97	0.98	2.29	31.97	62.38	0.41	0.06
	0.10	1.99	0.99	2.32	30.90	63.17	0.63	0.10
	0.15	2.02	1.01	2.36	29.51	64.09	1.01	0.15

*The doped samples are named according to the dopant and the nominal value of x. The real value of x is shown in the last column of the table.

Figure S1. XRD patterns of: (A) $MAPbI_3$ synthesized; (B) $MAPb_{1-x}Sn_xI_3$; (C) $MAPb_{1-x}Sr_xI_3$; (D) $MAPb_{1-x}Cd_xI_3$; (E) $MAPb_{1-x}Ca_xI_3$. Te: Tetragonal phase (I4/mcm space group); Cu: Cubic phase (Pm3m space group). x=0.05, 0.10, 015.

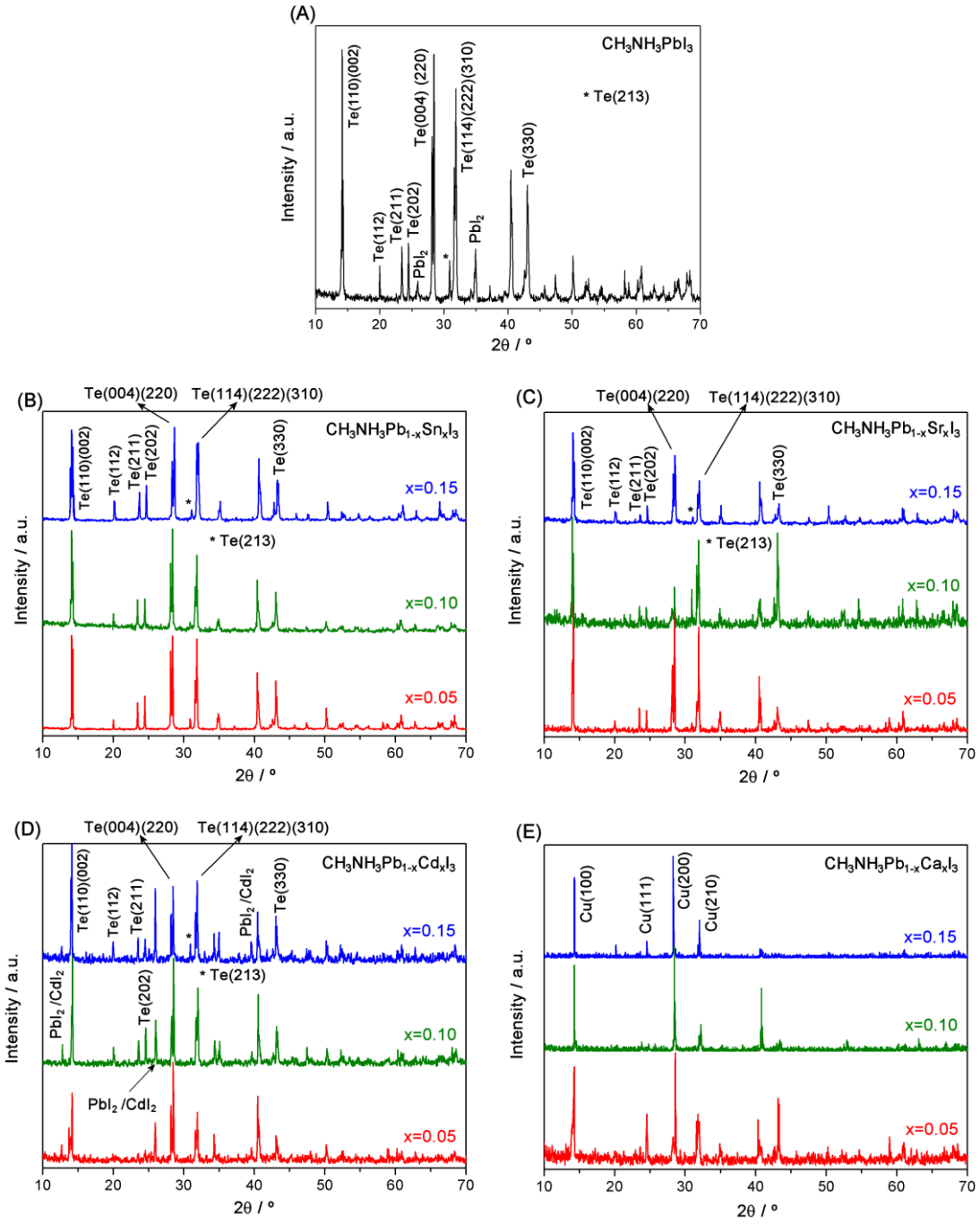

Figure S2. XRD patterns of commercials (A) PbI_2; and (B) CdI_2 used as reagents.

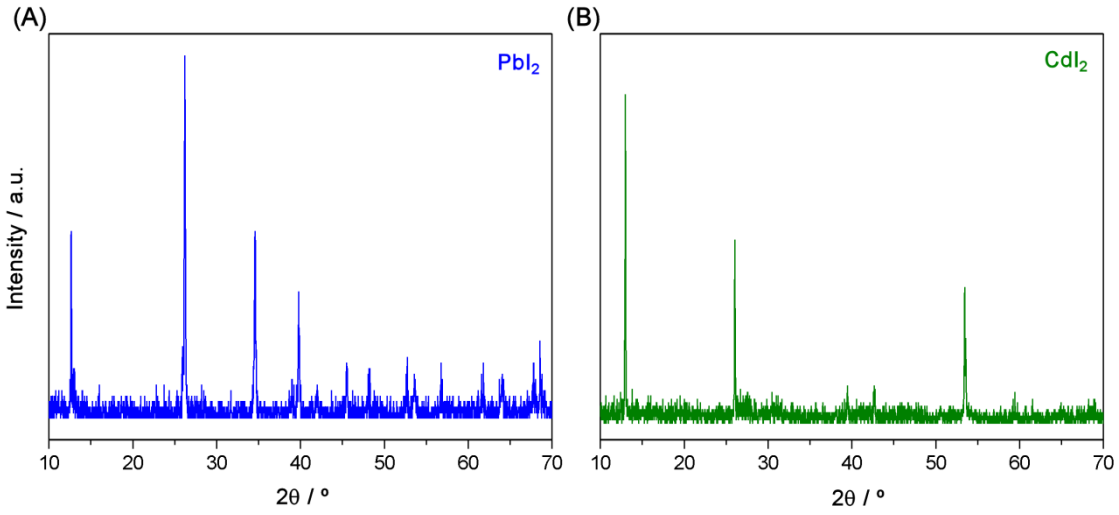

Figure S3. XRD patterns of $MAPb_{0.5}Sn_{0.5}I_3$. Te: Tetragonal phase (I4/mcm space group).

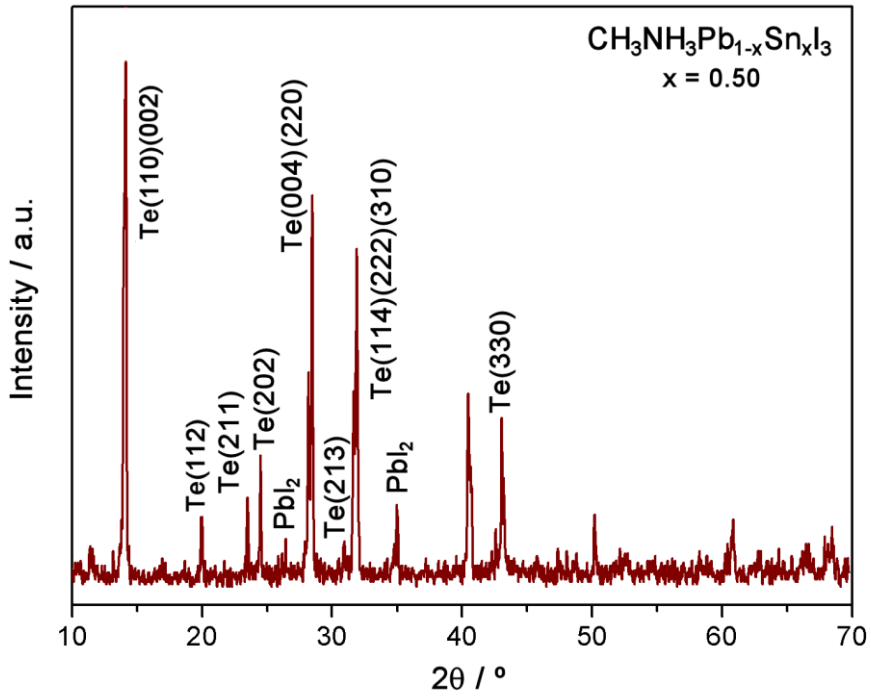

Figure S4. UV-Vis spectra, in mode reflectance diffuse, of: (A) $MAPbI_3$; (B) $MAPb_{1-x}Sn_xI_3$; (C) $MAPb_{1-x}Sr_xI_3$; (D) $MAPb_{1-x}Cd_xI_3$; (E) $MAPb_{1-x}Ca_xI_3$. x=0.05, 0.10, 015.

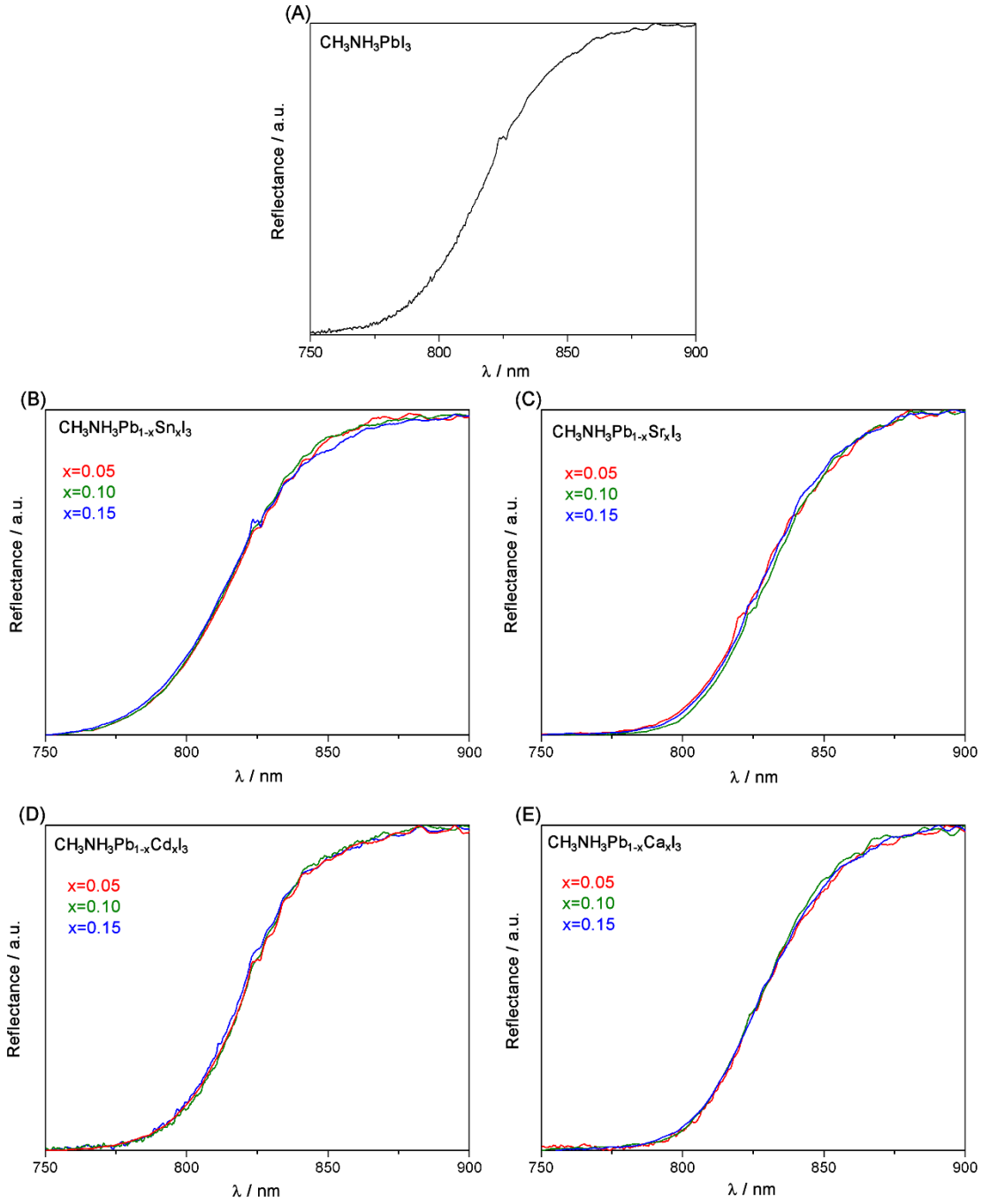

Figure S5. UV-Vis spectra, in mode reflectance diffuse, of $MAPbI_3$ and $MAPb_{0.5}Sn_{0.5}I_3$ samples.

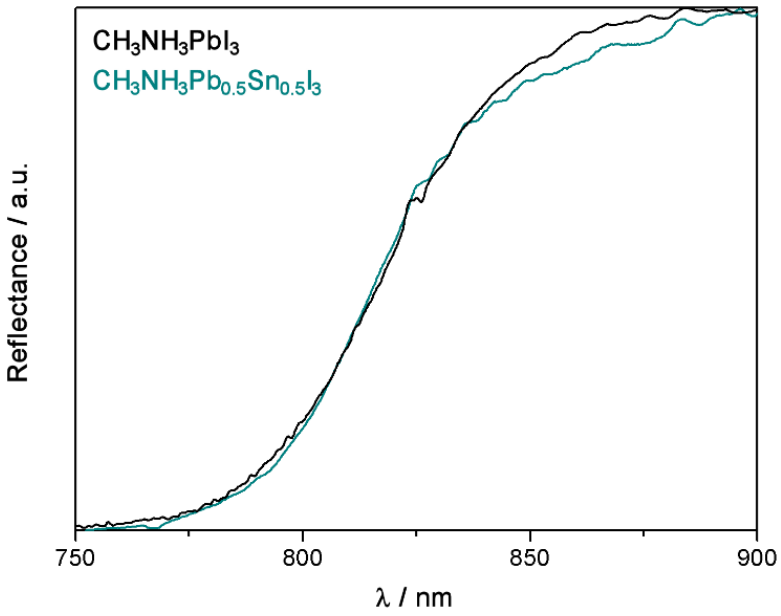

Figure S6. XPS spectra for $MAPbI_3$; and $MAPb_{1-x}B_xI_3$ (B: Sn, Sr, Cd, Ca) with x=0.10.

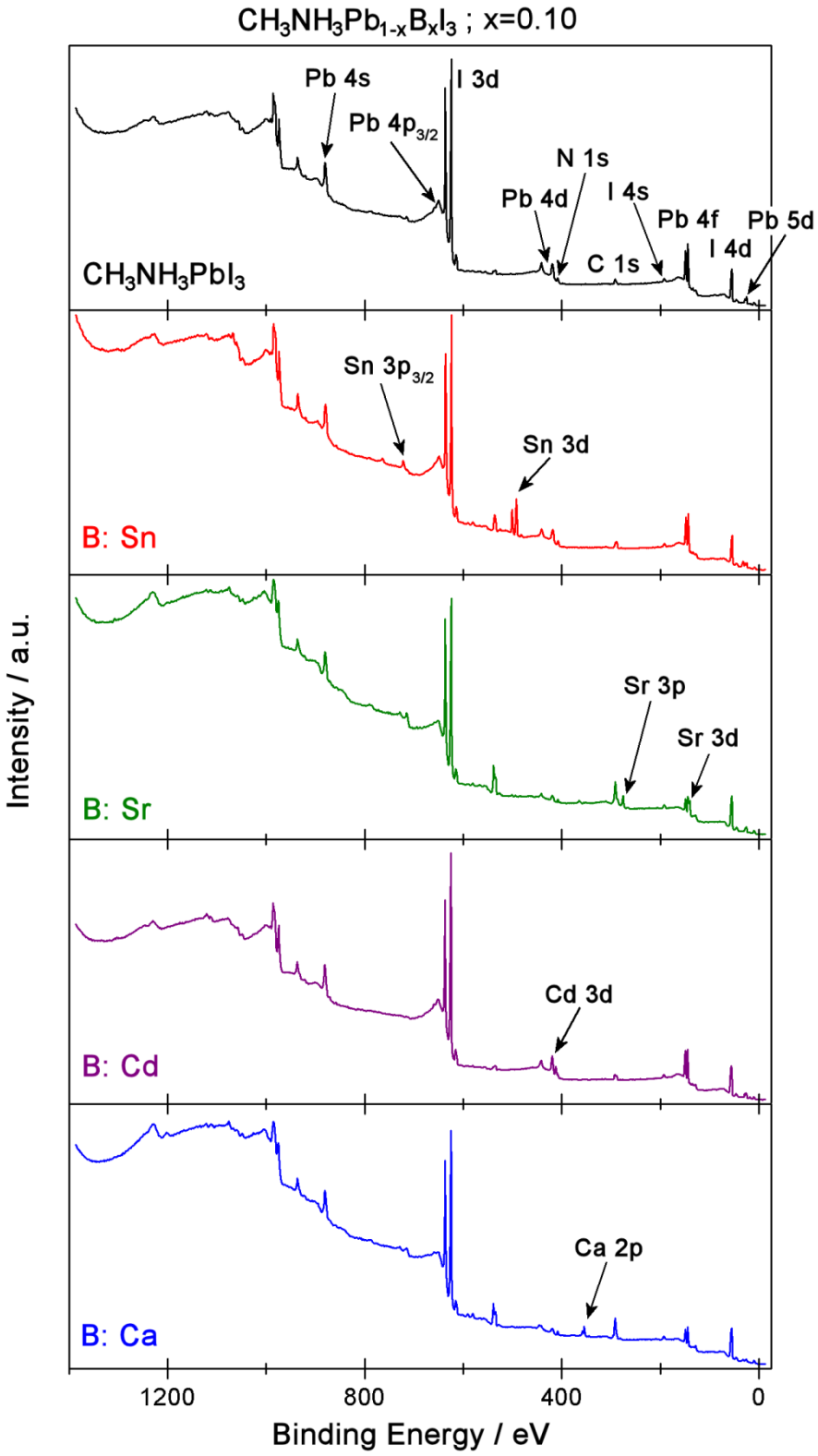

Figure S7. UV-Vis spectra, in mode reflectance diffuse, of commercial PbI_2 used as a reagent.

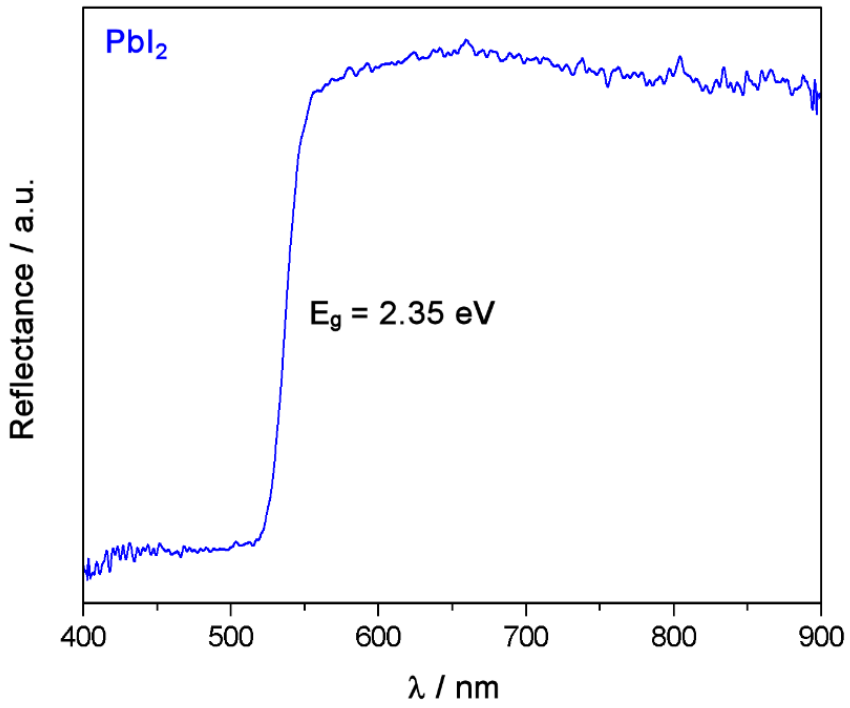

Figure S8. Detail of the ELF for the simulated structures from Figure 10 of the manuscript.

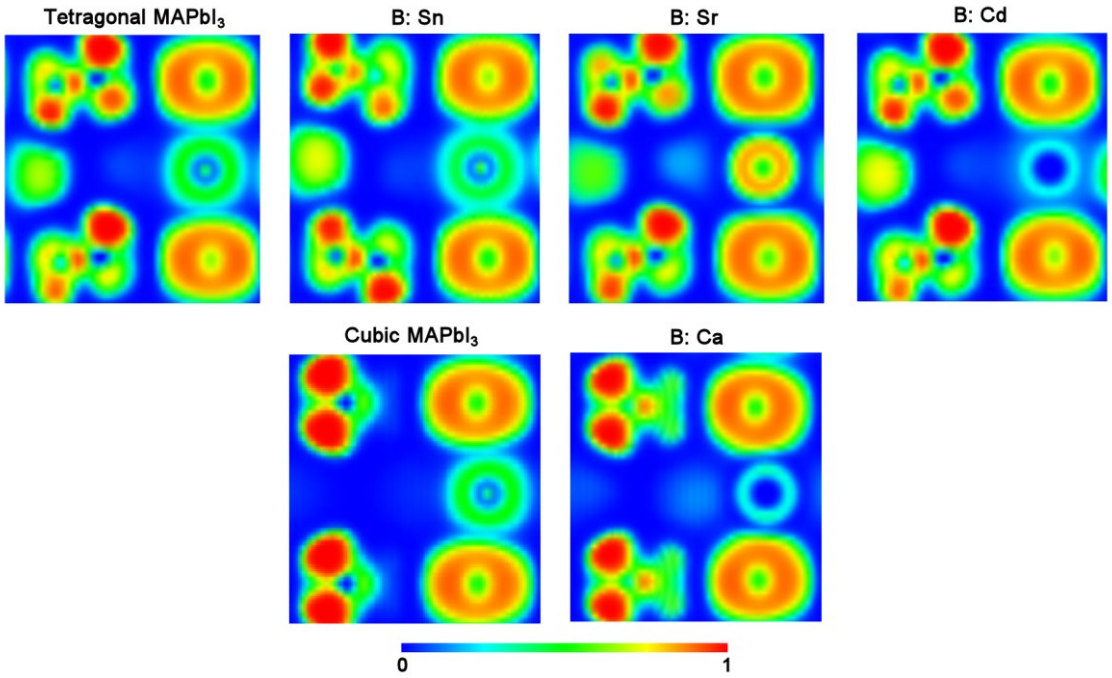

Figure S9. Starting configurations of the MA groups in the structure.