Supporting Information

Bandgap bowing in a zero-dimensional hybrid halide perovskite derivative: spin-orbit coupling versus lattice strain†

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Table S1 Unit cell parameters of $MA_3(Sb_{1-x}Bi_x)_2I_9$ ($0 \leq x \leq 1$) obtained from XRD patterns fitted using Pawley refinement.

Bi-content (*x*) in $MA_3(Sb_{1-x}Bi_x)_2I_9$	**Lattice parameters**		**Unit cell volume (Å)^3**
	***a* = *b* (Å)**	***c* (Å)**	
0.0	8.611(2)	21.458(2)	1378.8(4)
0.1	8.548(1)	21.530(2)	1362.4(4)
0.2	8.559(2)	21.529(3)	1365.9(6)
0.3	8.549(1)	21.547(1)	1363.8(3)
0.4	8.562(2)	21.578(2)	1370.1(5)
0.5	8.545(2)	21.597(2)	1365.9(5)
0.6	8.546(3)	21.620(1)	1368.0(4)
0.7	8.547(2)	21.635(2)	1371.8(7)
0.8	8.573(2)	21.670(2)	1379.4(6)
0.9	8.568(1)	21.704(1)	1383.1(3)
1.0	8.605(2)	21.737(1)	1394.0(4)

Table S2 Band energies and transport gap of $MA_3(Sb_{1-x}Bi_x)_2I_9$ ($0 \leq x \leq 1$) composites obtained from STS measurements and DOS spectra.

Bi-content (*x*) in $MA_3(Sb_{1-x}Bi_x)_2I_9$	**CB-edge (eV)**	**VB-edge (eV)**	**Transport gap (eV)**
0.0	-1.37	1.23	2.60
0.1	-1.27	1.21	2.48
0.2	-1.18	1.19	2.37
0.3	-1.14	1.16	2.30
0.4	-1.11	1.15	2.26
0.5	-1.09	1.13	2.22
0.6	-1.23	1.19	2.42
0.7	-1.28	1.23	2.51
0.8	-1.30	1.24	2.54
0.9	-1.33	1.24	2.57
1.0	-1.34	1.25	2.59

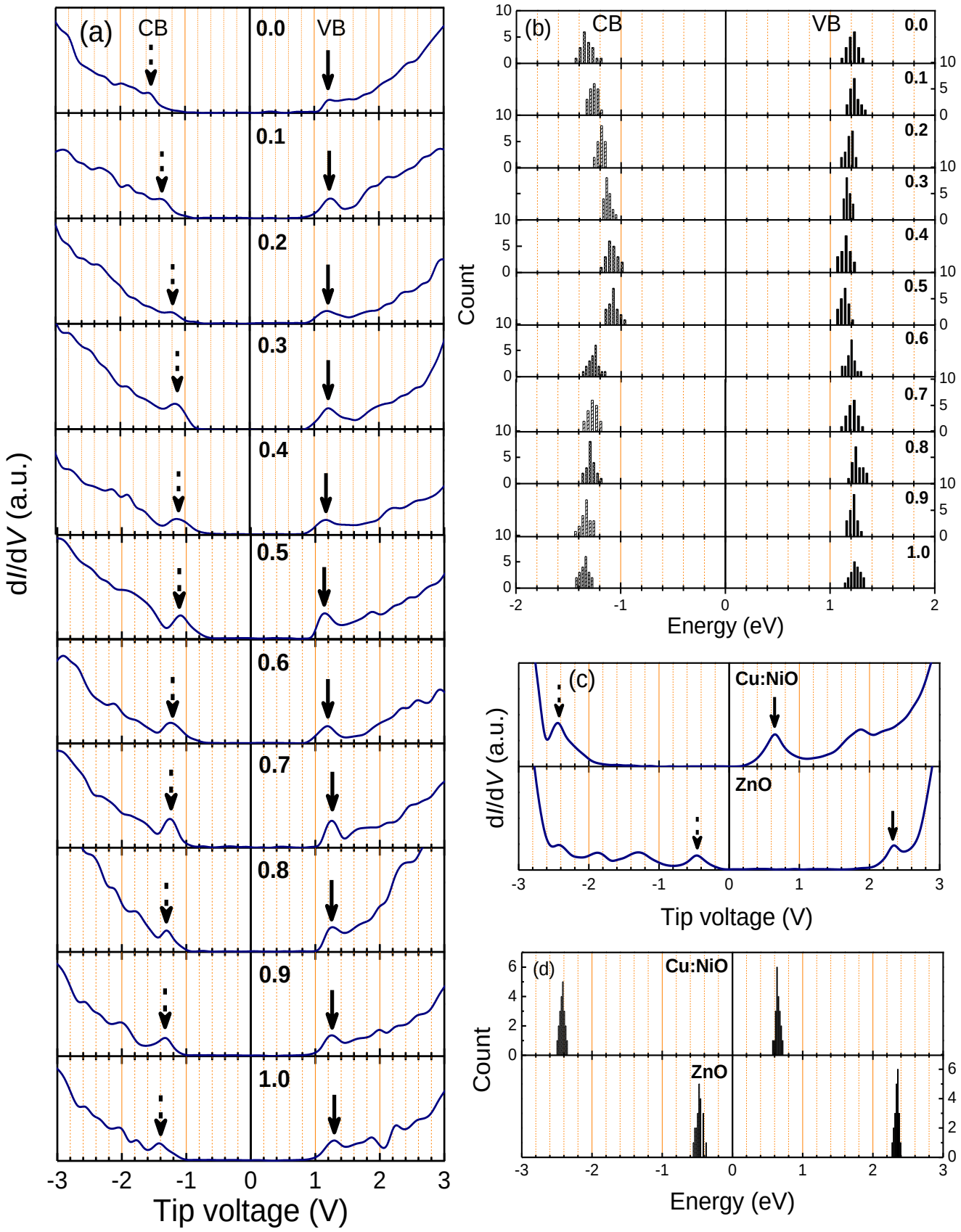

Fig. S1 (a) d*I*/d*V* versus tip voltage plots of $MA_3(Sb_{1-x}Bi_x)_2I_9$ thin-films with different bismuth-content (*x*) as stated in the legends, and (b) respective histogram of CB and VB edges, (c) and (d) present d*I*/d*V* versus tip voltage plots and histogram of CB and VB edges of Cu:NiO and ZnO carrier selective contacts, respectively.

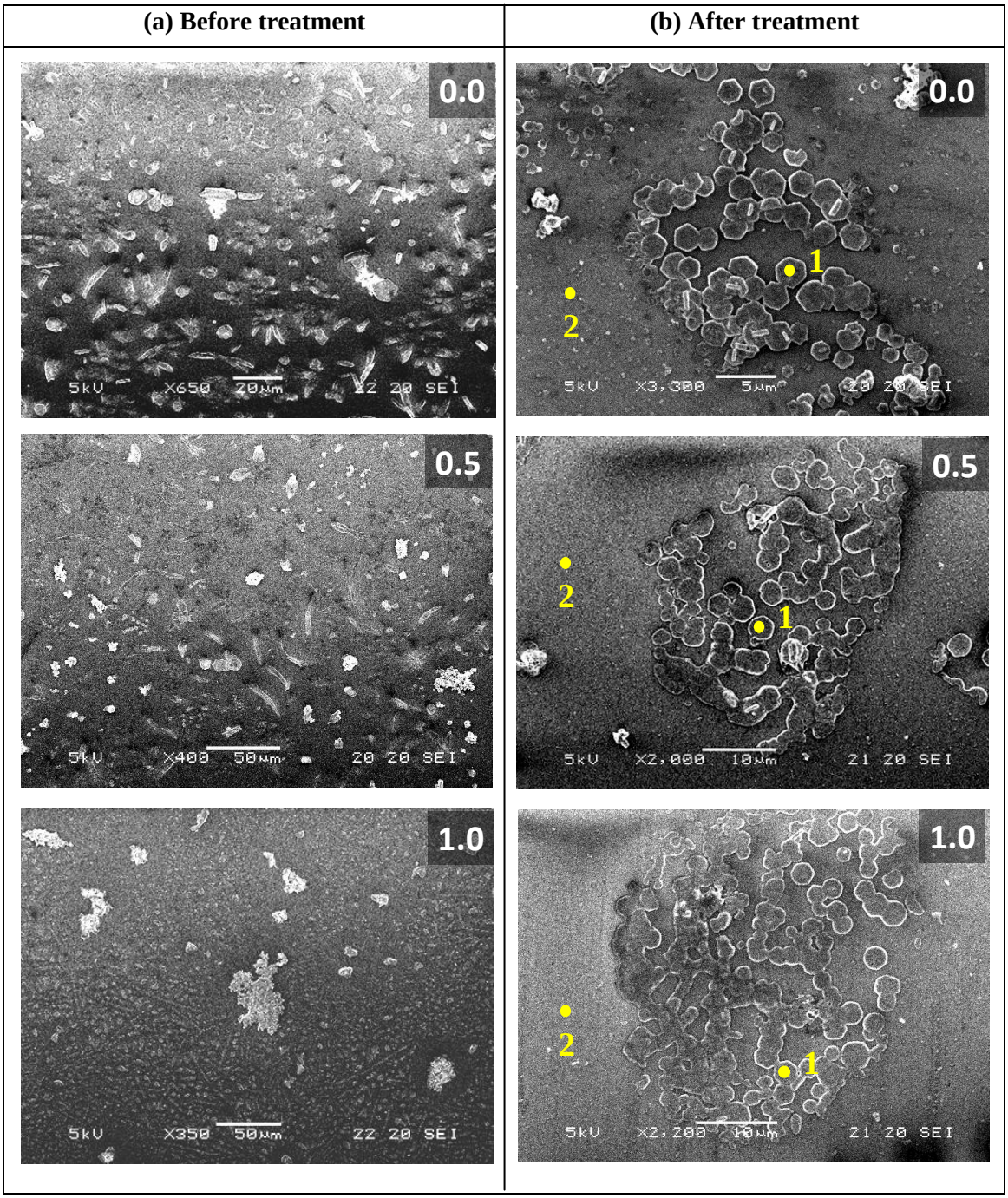

Fig. S2 SEM images of $MA_3(Sb_{1-x}Bi_x)_2I_9$ films having bismuth-content (x) as specified in the legends (a) before and (b) after chlorobenzene treatment. The points of EDX measurement have been marked with yellow dots and numbers.

Table S3 Distribution (atomic %) of individual elements observed on particular spots of $MA_3(Sb_{1-x}Bi_x)_2I_9$ thin-films having specified bismuth-content (x).

Bi-content (x) in $MA_3(Sb_{1-x}Bi_x)_2I_9$	Position	Elements			Ratio	
		Sb L	Bi M	I L	Sb/Bi	I/(Bi+Sb)
0.0	Point 1: Hexagon	0.0	22.2	77.8	–	3.6
	Point 2: Film	0.0	6.3	93.7	–	14.3
0.5	Point 1: Hexagon	10.4	11.5	78.1	0.9	3.6
	Point 2: Film	3.5	5.4	91.1	0.6	10.0
1.0	Point 1: Hexagon	21.5	0.0	78.5	–	3.7
	Point 2: Film	13.9	0.0	86.1	–	6.2

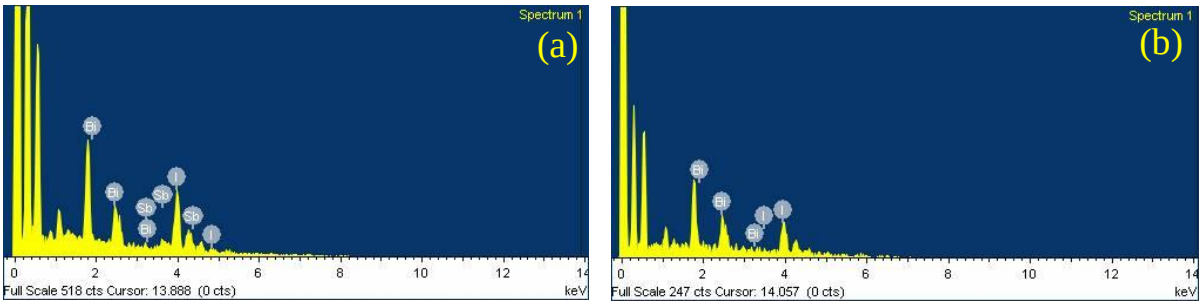

Fig. S3 EDX spectra of $MA_3(Sb_{0.5}Bi_{0.5})_2I_9$ thin-films taken on the (a) Point 1: hexagon and (b) Point 2: film, respectively.

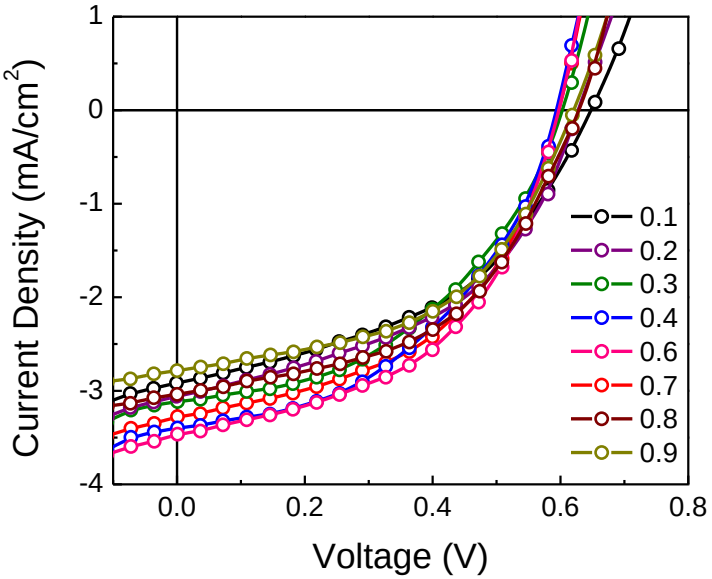

Fig. S4 Current-voltage characteristics of $MA_3(Sb_{1-x}Bi_x)_2I_9$ with bismuth-contents (x) as specified in the legends (under 1 sun illumination).