Supporting Information

Organic-inorganic hybrid perovskites ABI_3 (A = CH_3NH_3, NH_2CHNH_2; B = Sn, Pb) as potential thermoelectric materials: A density functional evaluation

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Table S1. Atomic positions of $(MA)PbI_3$

atom	x	y	z
Pb	0.492821	0.513813	0.474085
C	0.000857	0.002167	0.899801
N	0.004811	0.986031	0.135257
I	0.49793	0.017346	0.439128
I	0.992556	0.506915	0.444901
I	0.492249	0.51508	0.967781
H	0.019755	0.168599	0.854664
H	0.131397	0.907481	0.835962
H	0.848926	0.941239	0.842441
H	0.14683	0.040081	0.198811
H	0.882931	0.070896	0.204886
H	0.988716	0.83003	0.187442

Table S2. Atomic positions of $(MA)SnI_3$

atom	x	y	z
Sn	0.997367	0.008319	0.911056
C	0.50034	0.520452	0.329258
N	0.502098	0.472681	0.563454
I	0.496732	0.993083	0.880919
I	0.997605	0.511189	0.87725
I	0.997356	0.021399	0.393866
H	0.515407	0.693992	0.306589
H	0.636028	0.437724	0.254348
H	0.348876	0.46312	0.261031
H	0.642867	0.524355	0.636786
H	0.374402	0.544374	0.642577
H	0.490923	0.30931	0.595953

Table S3. Atomic positions of $(FA)PbI_3$

atom	x	y	z
Pb	0.6657	0.3343	0.8401
Pb	0.0004	0.9997	0.5053
Pb	0.3334	0.6666	0.1683
C	0.3338	0.6660	0.6240
C	0.6556	0.3443	0.3563
C	0.0110	0.9891	0.9931
N	0.4239	0.8338	0.6333
N	0.1660	0.5759	0.6333
N	0.5663	0.1760	0.3562
N	0.8240	0.4337	0.3564
N	0.8428	0.8991	0.9867
N	0.1009	0.1572	0.9867
I	0.1490	0.8510	0.3021
I	0.1685	0.3355	0.3400
I	0.6646	0.8313	0.3402
I	0.8429	0.1570	0.6875
I	0.8155	0.6662	0.6700
I	0.3330	0.1847	0.6712
I	0.5264	0.4737	0.0517
I	0.4866	0.9851	0.9881
I	0.0151	0.5135	0.9881
H	0.4030	0.5967	0.6070
H	0.5853	0.4145	0.3569
H	0.0906	0.6296	0.6506
H	0.1030	0.4447	0.6282
H	0.3702	0.9091	0.6505
H	0.5551	0.8967	0.6280
H	0.6219	0.1000	0.3529
H	0.4350	0.1129	0.3519
H	0.9000	0.3783	0.3531
H	0.8870	0.5650	0.3525
H	0.7669	0.9539	0.9782
H	0.7798	0.7682	0.9955
H	0.0808	0.9192	0.0040
H	0.0461	0.2332	0.9781
H	0.2318	0.2203	0.9954

Table S4. Atomic position of (FA)SnI_3

atom	x	y	z
Sn	0.5000	0.0000	0.4561
Sn	0.5000	0.5000	0.9561
C	0.0000	0.0000	0.0048
C	0.0000	0.5000	0.5048
N	0.8170	0.0000	0.9369
N	0.8170	0.5000	0.4369
N	0.1830	0.0000	0.9369
N	0.1830	0.5000	0.4369
I	0.5000	0.2674	0.7065
I	0.5000	0.7674	0.2065
I	0.5000	0.7326	0.7065
I	0.5000	0.2326	0.2065
I	0.0000	0.0000	0.4939
I	0.0000	0.5000	0.9939
H	0.8019	0.0000	0.8228
H	0.8019	0.5000	0.3228
H	0.1981	0.0000	0.8228
H	0.1981	0.5000	0.3228
H	0.6838	0.0000	0.0014
H	0.6838	0.5000	0.5014
H	0.3162	0.0000	0.0014
H	0.3162	0.5000	0.5014
H	0.0000	0.0000	0.1277
H	0.0000	0.5000	0.6277

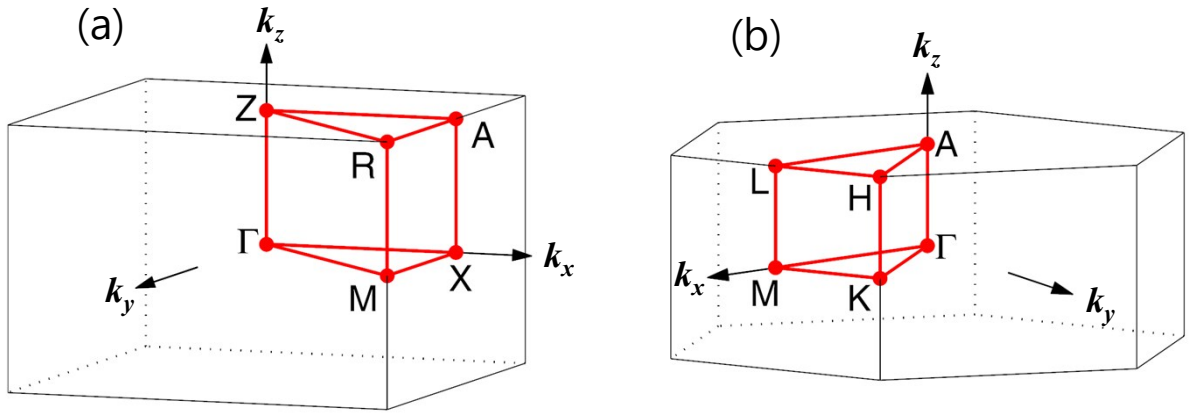

Figure S1. The first Brillouin zone for (a) $(MA)PbI_3$, $(MA)SnI_3$, and $(FA)SnI_3$, and (b) $(FA)PbI_3$.

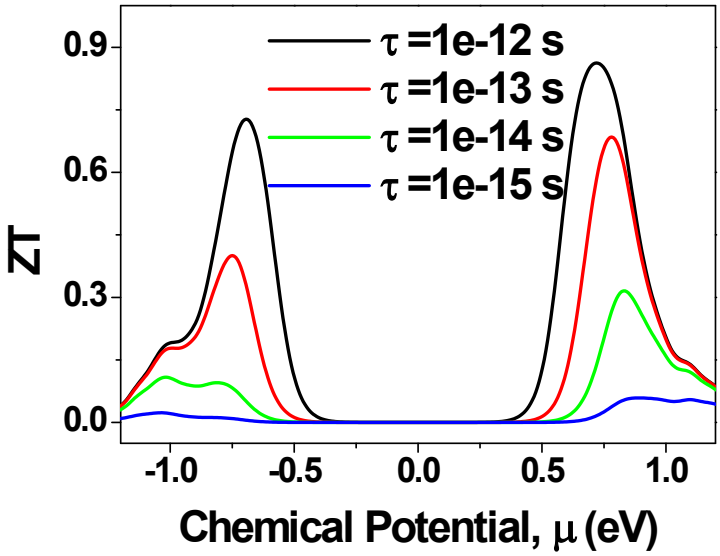

Figure S2. The calculated ZT values of $(MA)PbI_3$ system at various relaxation times τ.

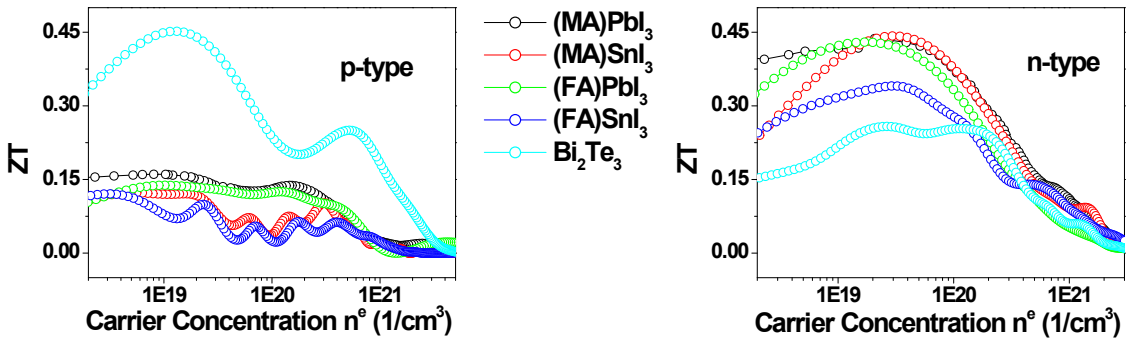

Figure S3. The calculated ZT values of ABI_3 systems as a function of the carrier concentration at 400 K.