Supplementary Document of Perovskites for Solar Thermoelectric Applications: a First Principle Study of $CH_3NH_3AI_3$ (A=Pb and Sn)

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Table SI: Ab initio optimized lattice constants a, b and c (Å) (see Fig. 1a) of the pseudo-cubic $MAPbI_3$ with MA along the <100>, <110> and <111> directions, and those of pseudo-cubic $MASnI_3$ with MA along the <100> direction. The term AVE represents the average value over three lattice constants. The displacement of the metal Pb ion of $MAPbI_3$ in each of the three cases is shown in Fig. S1.

Lattice Constant	$MAPbI_3$			$MASnI_3$
	MA100	MA110	MA111	MA100
a	6.4504	6.4271	6.4113	6.3535
b	6.3810	6.4470	6.4192	6.3384
c	6.4601	6.3373	6.4132	6.3641
AVE.	6.4305	6.4038	6.4145	6.3520

Table SII: Calculated longitudinal ($m^*_{||}$), transverse ($m^*_{\perp}$), conductivity (m^*_I), band (m^*_b), and density of state effective mass (m^*) of electrons (e^-) and holes (h^+) at two splitted conduction edges (LUMO1 and LUMO2) and two splitted valence band edges (HOMO1 and HOMO2) at the R point in the Brillouin Zone (see Fig. 2a and 3a). All effective masses are in units of the electron mass (m_e). The term AVE represents the averaged value over the two splitted bands. All results were obtained with DFT-PBE calcuations. The effective mass m^* was obtained by summing over two bands and it is indicated by the bold figures.

	$MAPbI_3$	(e^-)		$MAPbI_3$	(h^+)		$MASnI_3$	(e^-)		$MASnI_3$	(h^+)	
	LUMO1	LUMO2	AVE.	HOMO1	HOMO2	AVE.	LUMO1	LUMO2	AVE.	HOMO1	HOMO2	AVE.
$m^*_{||}$	0.2527	0.1282	0.1905	0.3435	0.3366	0.3398	0.2825	0.3021	0.2923	0.1872	0.1711	0.1792
$m^*_{\perp}$	0.0853	0.0750	0.0802	0.1012	0.0855	0.0934	0.0935	0.0868	0.0902	0.0887	0.0857	0.0872
m^*_I	0.1095	0.0870	0.0983	0.1323	0.1138	0.1231	0.1203	0.1138	0.1171	0.1076	0.1028	0.1052
m^*_b	0.1227	0.0897	0.1062	0.1521	0.1350	0.1436	0.1352	0.1315	0.1334	0.1138	0.1079	0.1109
m^*	0.1227	0.0897	**0.2124**	0.1521	0.1350	**0.2871**	0.1352	0.1315	**0.2668**	0.1138	0.1079	**0.2217**

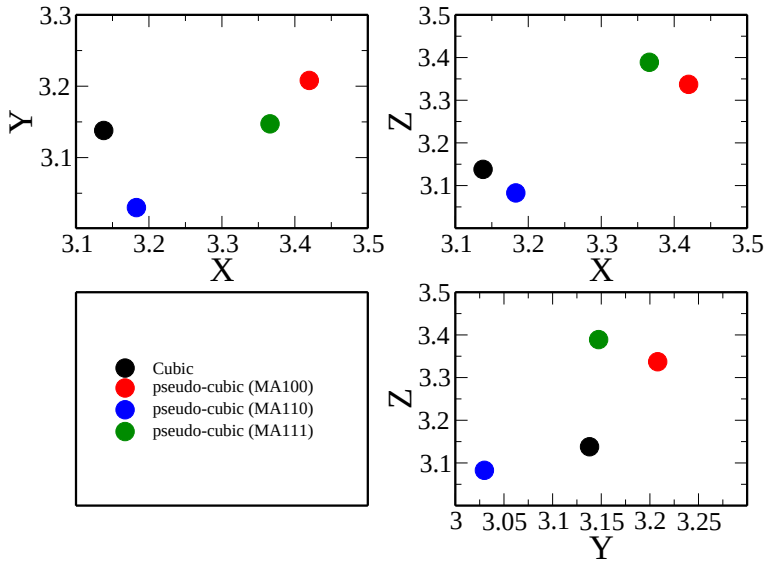

Figure S1: Positions of Pb atoms in $MAPbI_3$ samples for the perfect cubic structure (black), pseudo-cubic with MA along <100> (red), pseudo-cubic with MA along <110> (blue) and pseudo-cubic with MA along <111> (green) direction, respectively.

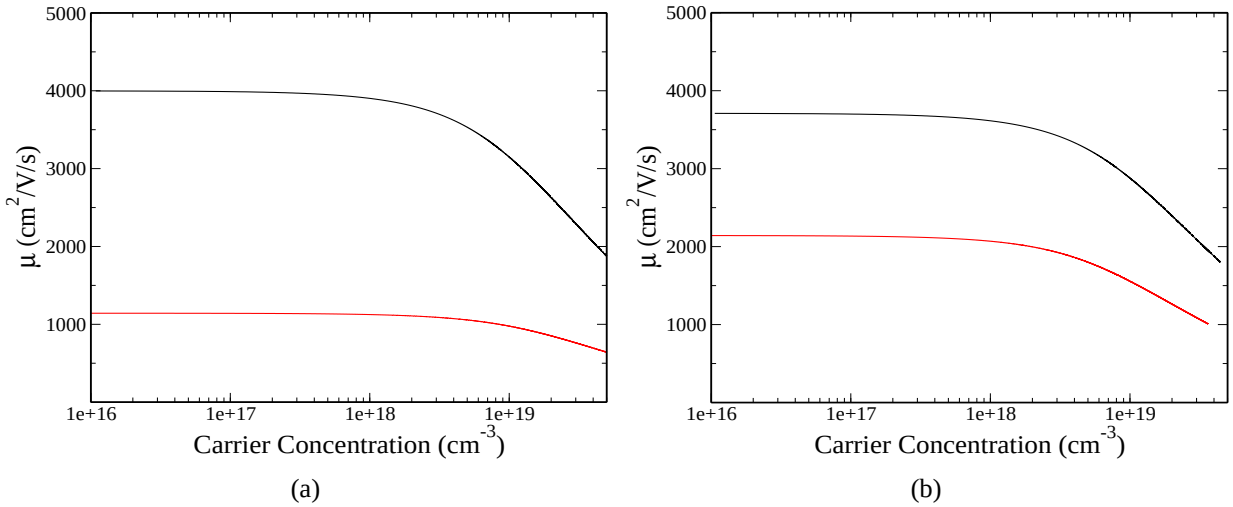

Figure S2: Calculated electron (black) and hole (red) mobilities (μ) as a function of carrier concentration at 400 K in pseudo-cubic $CH_3NH_3PbI_3$ (a) and at 300 K in pseudo-cubic $CH_3NH_3SnI_3$ (b), by using the Kane model with G_0W_0 band gaps and DFT-PBE effective masses.

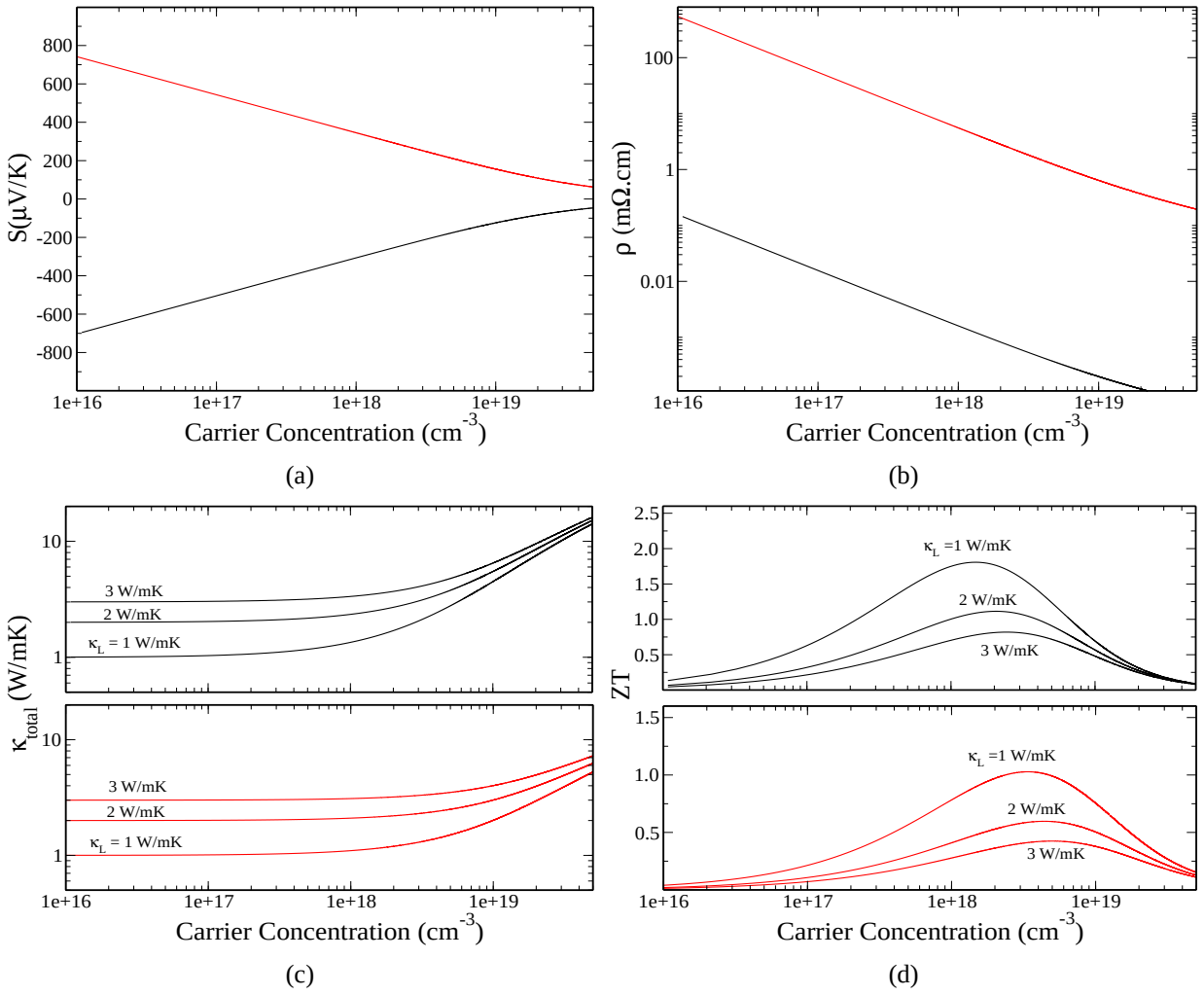

Figure S3: (a) Seebeck coefficients (S), (b) electrical resistivities (ρ), (c) total thermal conductivities (κ_{total}), and (d) the predicted values of the material figure of meritz (ZT) as a function of carrier concentration with κ_L =1, 2 and 3 W/mK, at 400 K for n-type (black) and p-type (red) doped, pseudo-cubic $CH_3NH_3PbI_3$, obtained from the Kane model with G_0W_0 band gaps and DFT-PBE effective masses. At the carrier concentration for which ZT is maximum, κ_e varies between 0.45 and 0.75 W/mK for n-type, and between 0.30 and 0.43 W/mK for p-type.

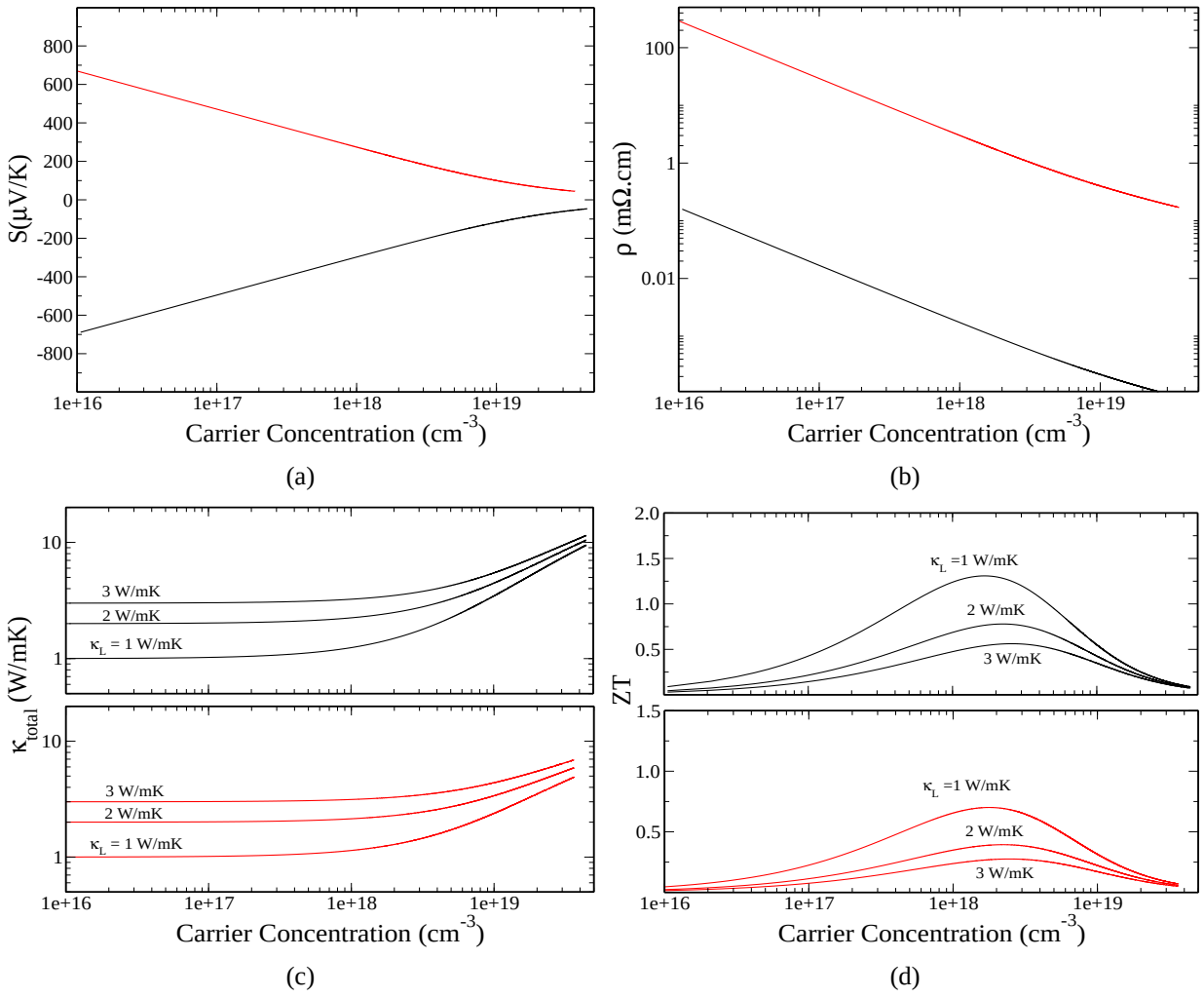

Figure S4: (a) Seebeck coefficients (S), (b) electrical resistivities (ρ), (c) total thermal conductivities (κ_{total}), and (d) the predicted values of the material figure of meritz (ZT) as a function of carrier concentration with κ_L =1, 2 and 3 W/mK, at 300 K for n-type (black) and p-type (red) doped, pseudo-cubic $CH_3NH_3SnI_3$, obtained from the Kane model with G_0W_0 band gaps and DFT-PBE effective masses. At the carrier concentration for which ZT is maximum, κ_e varies between 0.38 and 0.62 W/mK for n-type, and between 0.24 and 0.31 W/mK for p-type.