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The Relation of Phase-Transition Effects and Thermal Stability of Planar Perovskite Solar Cells

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Supplementary Information

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Table S1. Statistics on solar cell performance of the PSCs using different perovskites. Average values and standard deviations were calculated for 20 cells in 3 different batches of PSCs fabricated under identical conditions.

Device	**J_{SC} / mA cm^{-2}**	**V_{OC} / V**	**FF**	**η / %**
$MA_{0.6}FA_{0.4}PbI_3$	21.15 ± 0.22	1.02 ± 0.01	0.67 ± 0.03	14.26 ± 0.32
$MAPbI_{2.6}Br_{0.4}$	19.88 ± 0.26	0.95 ± 0.02	0.72 ± 0.03	13.95 ± 0.21
$MA_{0.6}FA_{0.4}PbI_{2.8}Br_{0.2}$	20.21 ± 0.32	1.01 ± 0.01	0.71 ± 0.02	14.53 ± 0.22
$MAPbI_3$	20.51 ± 0.28	1.02 ± 0.01	0.71 ± 0.03	15.15 ± 0.28

Table S2. Fit parameters obtained from the impedance analysis. The equivalent circuit used is displayed in Figure 3a in the main article. Listed are the resistances, R_x, the time constants, τ_x, and the exponents, n_x, for the constant phase elements. The capacitances, C_x, are the effective capacitances calculated by $C_x = \tau_x / R_x$.

$MAPbI_3$ (fresh)	R_0 (Ωcm²)	R_1 (Ωcm²)	τ_1 (s)	C_1 (Fcm^{-2})	n_1	R_2 (Ωcm²)	τ_2 (s)	C_2 (Fcm^{-2})	n_2
#1 (25°C)	5.77	20.42	$1.73 \cdot 10^{-6}$	$8.46 \cdot 10^{-8}$	0.98	28.42	$9.82 \cdot 10^{-3}$	$3.45 \cdot 10^{-4}$	0.88
#2 (55°C)	5.53	15.11	$1.33 \cdot 10^{-6}$	$8.79 \cdot 10^{-8}$	0.98	12.24	$1.11 \cdot 10^{-3}$	$9.04 \cdot 10^{-5}$	0.93
#3 (70°C)	5.73	13.96	$1.20 \cdot 10^{-6}$	$8.63 \cdot 10^{-8}$	0.98	8.91	$4.19 \cdot 10^{-4}$	$4.70 \cdot 10^{-5}$	0.97
#4 (55°C)	5.40	20.68	$1.72 \cdot 10^{-6}$	$8.34 \cdot 10^{-8}$	0.98	27.39	$1.13 \cdot 10^{-3}$	$4.12 \cdot 10^{-5}$	0.89
#5 (25°C)	5.41	36.89	$2.94 \cdot 10^{-6}$	$7.97 \cdot 10^{-8}$	0.98	103.73	$1.31 \cdot 10^{-2}$	$1.27 \cdot 10^{-4}$	0.85

$MAPbI_3$ (aged)	R_0 (Ωcm²)	R_1 (Ωcm²)	τ_1 (s)	C_1 (Fcm^{-2})	n_1	R_2 (Ωcm²)	τ_1 (s)	C_2 (Fcm^{-2})	n_2
#1 (25°C)	8.41	165.35	$1.37 \cdot 10^{-5}$	$8.28 \cdot 10^{-8}$	0.96	662.12	$5.05 \cdot 10^{-2}$	$7.63 \cdot 10^{-5}$	0.89
#2 (55°C)	6.15	94.82	$7.05 \cdot 10^{-6}$	$7.43 \cdot 10^{-8}$	0.96	580.94	$1.56 \cdot 10^{-2}$	$2.68 \cdot 10^{-5}$	0.88
#3 (70°C)	5.89	79.88	$5.79 \cdot 10^{-6}$	$7.25 \cdot 10^{-8}$	0.96	582.19	$7.62 \cdot 10^{-3}$	$1.31 \cdot 10^{-5}$	0.86
#4 (55°C)	6.53	95.11	$7.01 \cdot 10^{-6}$	$7.37 \cdot 10^{-8}$	0.97	602.52	$1.49 \cdot 10^{-2}$	$2.47 \cdot 10^{-5}$	0.88
#5 (25°C)	5.73	125.34	$9.68 \cdot 10^{-6}$	$7.73 \cdot 10^{-8}$	0.96	581.30	$5.35 \cdot 10^{-2}$	$9.21 \cdot 10^{-5}$	0.91

$MA_{0.6}FA_{0.4}PbI_{2.8}Br_{0.2}$ (fresh)	R_0 (Ωcm²)	R_1 (Ωcm²)	τ_1 (s)	C_1 (Fcm^{-2})	n_1	R_2 (Ωcm²)	τ_1 (s)	C_2 (Fcm^{-2})	n_2
#1 (25°C)	5.57	17.81	$1.55 \cdot 10^{-6}$	$8.70 \cdot 10^{-8}$	0.98	108.03	$9.51 \cdot 10^{-2}$	$8.80 \cdot 10^{-4}$	0.87
#2 (55°C)	5.69	19.35	$1.56 \cdot 10^{-6}$	$8.08 \cdot 10^{-8}$	0.99	120.65	$2.30 \cdot 10^{-2}$	$1.90 \cdot 10^{-4}$	0.88
#3 (70°C)	5.64	17.71	$1.40 \cdot 10^{-6}$	$7.90 \cdot 10^{-8}$	0.98	92.74	$9.79 \cdot 10^{-3}$	$1.06 \cdot 10^{-4}$	0.88
#4 (55°C)	5.77	21.10	$1.59 \cdot 10^{-6}$	$7.52 \cdot 10^{-8}$	0.98	163.99	$2.94 \cdot 10^{-2}$	$1.79 \cdot 10^{-4}$	0.84
#5 (25°C)	5.62	22.03	$1.67 \cdot 10^{-6}$	$7.58 \cdot 10^{-8}$	0.97	276.10	$2.54 \cdot 10^{-1}$	$9.22 \cdot 10^{-4}$	0.77

$MA_{0.6}FA_{0.4}PbI_{2.8}Br_{0.2}$ (aged)	R_0 (Ωcm²)	R_1 (Ωcm²)	τ_1 (s)	C_1 (Fcm^{-2})	n_1	R_2 (Ωcm²)	τ_1 (s)	C_2 (Fcm^{-2})	n_2
#1 (25°C)	5.11	24.81	$1.49 \cdot 10^{-6}$	$6.02 \cdot 10^{-8}$	0.98	85.08	$3.48 \cdot 10^{-2}$	$4.10 \cdot 10^{-4}$	0.87
#2 (55°C)	5.12	28.32	$1.67 \cdot 10^{-6}$	$5.91 \cdot 10^{-8}$	0.98	71.29	$7.94 \cdot 10^{-3}$	$1.11 \cdot 10^{-4}$	0.92
#3 (70°C)	5.13	25.90	$1.54 \cdot 10^{-6}$	$5.95 \cdot 10^{-8}$	0.97	47.16	$3.71 \cdot 10^{-3}$	$7.86 \cdot 10^{-5}$	0.98
#4 (55°C)	5.09	21.96	$1.30 \cdot 10^{-6}$	$5.94 \cdot 10^{-8}$	0.98	42.06	$6.13 \cdot 10^{-3}$	$1.46 \cdot 10^{-4}$	0.93
#5 (25°C)	5.04	18.62	$1.11 \cdot 10^{-6}$	$5.98 \cdot 10^{-8}$	0.97	44.72	$2.40 \cdot 10^{-2}$	$5.38 \cdot 10^{-4}$	0.86

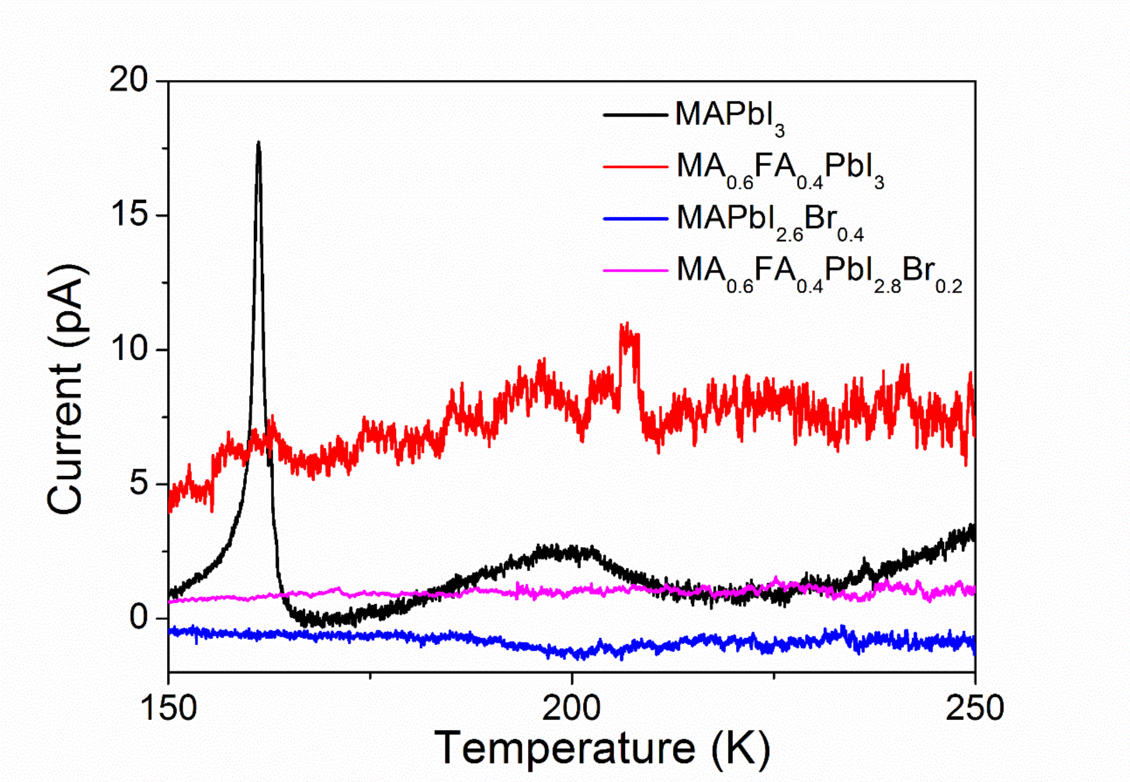

Figure S1. TSC curves in the low-temperature region for PSCs aged after 500 h at 85 °C.

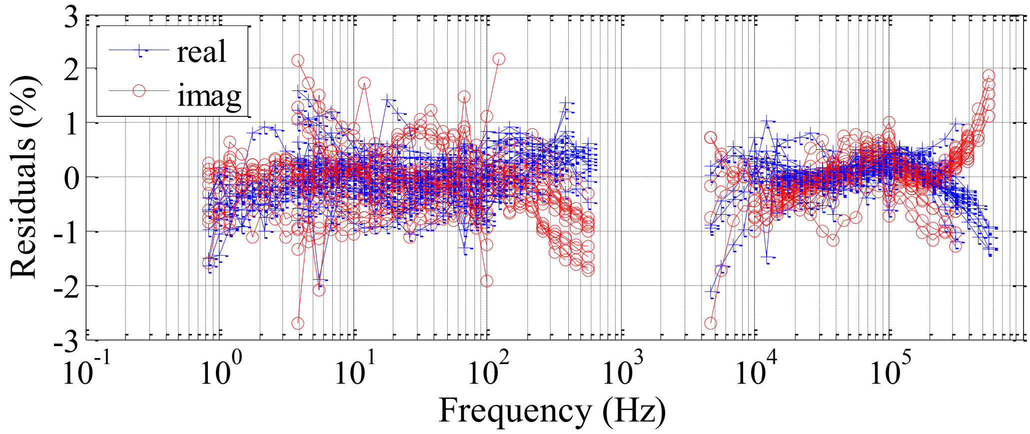

Figure S2. Residuals for the impedance fits. In this figure, all residuals for the fits that lead to the parameters in Table S2 are overlaid in one diagram. Note that the fit was performed in two stages because also the impedance spectra were recorded in two steps in order to be able to use optimized settings for the measurement at high and low frequencies.

All residuals are below 3% with the majority being below 1%, which proves the accuracy of the results presented in this study.