

Supporting Information (SI) for master's thesis: Film formation of mixed halide perovskites for PSCs

Author: Lina Ekstedt

May 2021

SI:1. Batch overview with all fabricated samples

Table S1: OB1 – sample overview

Sample number	Mix I [%]	Antisolvent type and drip time	Data on sample
1	0	No AS	Yes
9	0	Failed	Yes
14	0	Toluene 15s	Yes
17	0	Toluene 5s	Yes
18	0	Failed	Yes
2	30	Toluene 10s	Yes
5	30	Toluene 30s	Yes
15	30	No AS	Yes
8	60	Toluene 30s	Yes
16	60	Toluene 55s	Yes
20	60	No AS	Yes
21	60	Toluene 10s	Yes
4	70	No AS	Yes
6	70	Ethyl Acetate 55s	Yes
12	70	Ethyl Acetate 10s	Yes
49	70	Toluene 30s	Yes
51	70	Ethyl Acetate 30s	Yes
3	100	Ethyl Acetate 30s	Yes
50	100	No AS	Yes

Table S2: OB2 – sample overview

Sample number	Mix I [%]	Antisolvent type and drip time	Data on sample
4	0	Toluene 15s	No
5	0	No AS	No
6	100	Ethyl Acetate 30s	Yes
7	100	No AS	Yes
8	70	Ethyl Acetate 10s	Yes
9	70	No AS	Yes
10	60	Toluene 10s	Yes
11	60	No AS	Yes
12	30	Toluene 30s	Yes
13	30	No AS	Yes
14	0	Toluene 5s	Yes
15	0	No AS	Yes

Table S3: SCB1 – sample overview

Sample number	Mix I [%]	Antisolvent type and drip time	Data on sample
1	100	Ethyl Acetate 10s	No
2	100	Ethyl Acetate 10s	Yes
3	100	Ethyl Acetate 15s	No
4	100	Ethyl Acetate 30s	Yes
5	70	Ethyl Acetate 10s	Yes
6	70	Ethyl Acetate 10s	Yes
7	70	Ethyl Acetate 30s	Yes
8	70	Ethyl Acetate 55s	Yes
9	60	Toluene 10s	Yes
10	60	Toluene 10s	Yes
11	60	Toluene 30s	Yes
12	60	Toluene 30s	Yes
13	30	Toluene 10s	Yes
14	30	Toluene 10s	Yes
15	30	Toluene 30s	Yes
16	30	Toluene 30s	Yes
17	0	Toluene 5s	Yes
18	0	Toluene 5s	Yes
19	0	Toluene 10s	Yes
20	0	Toluene 15s	Yes

Table S4: SCB2 – sample overview

Sample number	Mix I [%]	Antisolvent type and drip time	Data on sample
1	0	Toluene 5s	Yes
2	0	Toluene 5s	Yes
3	0	Toluene 15s	Yes
4	30	Toluene 10s	Yes
5	30	Toluene 10s	Yes
6	30	Toluene 30s	No
7	60	Toluene 10s	No
8	60	Toluene 10s	Yes
12	60	Toluene 30s	Yes
10	70	Ethyl Acetate 10s	No
11	70	Ethyl Acetate 10s	Yes
9	70	Ethyl Acetate 30s	Yes
13	100	Ethyl Acetate 20s	Yes
14	100	Ethyl Acetate 30s	Yes
16	100	Ethyl Acetate 30s	Yes

Table S5: SCB3 – sample overview

Sample number	Mix I [%]	IM	Antisolvent type and drip time	Data on sample
1	0	-	Toluene 10s	No
2	0	-	Toluene 10s	Yes
3	30	-	Toluene 30s	Yes
4	30	-	Toluene 30s	Yes
5	60	-	Toluene 30s	Yes
6	60	-	Toluene 30s	Yes
7	80	-	Ethyl Acetate 30s	Yes
8	80	-	Ethyl Acetate 30s	Yes
9	100	-	Ethyl Acetate 30s	Yes
10	100	-	Ethyl Acetate 30s	Yes
11	0	KNO ₃	Toluene 10s	Yes
12	0	KNO ₃	Toluene 10s	Yes
13	30	KNO ₃	Toluene 30s	Yes
14	30	KNO₃	Toluene 30s	No
15	60	KNO ₃	Toluene 30s	Yes
16	60	KNO ₃	Toluene 30s	Yes
17	60	KNO ₃	Toluene 30s	Yes
18	80	KNO ₃	Ethyl Acetate 30s	Yes
19	80	KNO ₃	Ethyl Acetate 30s	Yes
20	100	KNO ₃	Ethyl Acetate 30s	Yes
31	100	KNO ₃	Ethyl Acetate 30s	Yes
32	100	KNO ₃	Ethyl Acetate + Toluene 30s	Yes

Table S6: SCB4 – sample overview

Sample number	Mix I [%]	IM	Antisolvent type and drip time	Data on sample
1	0	NaCl	Toluene 10s	Yes
2	0	NaCl	Toluene 10s	Yes
3	30	NaCl	Toluene 30s	Yes
4	30	NaCl	Toluene 30s	Yes
5	60	NaCl	Toluene 30s	Yes
6	60	NaCl	Toluene 30s	Yes
7	80	NaCl	Ethyl Acetate 30s	Yes
8	80	NaCl	Ethyl Acetate 30s	Yes
9	100	NaCl	Ethyl Acetate 30s	Yes
10	100	NaCl	Ethyl Acetate 30s	Yes
21	0	KCl	Toluene 10s	Yes
22	0	KCl	Toluene 10s	Yes
23	30	KCl	Toluene 30s	Yes
24	30	KCl	Toluene 30s	Yes
25	60	KCl	Toluene 30s	Yes
26	60	KCl	Toluene 30s	Yes
27	80	KCl	Ethyl Acetate 30s	Yes
28	80	KCl	Ethyl Acetate 30s	Yes
29	100	KCl	Ethyl Acetate 30s	Yes
30	100	KCl	Ethyl Acetate 30s	Yes

SI:2. SEM images of film surface

In the following section further SEM images from the AS treatment study are included, showing firstly different AS conditions and secondly, films with and without AS treatment when spin coated on a SnO₂ layer, i.e. the same underlying surface as it is spin coated on when fabricating solar cells.

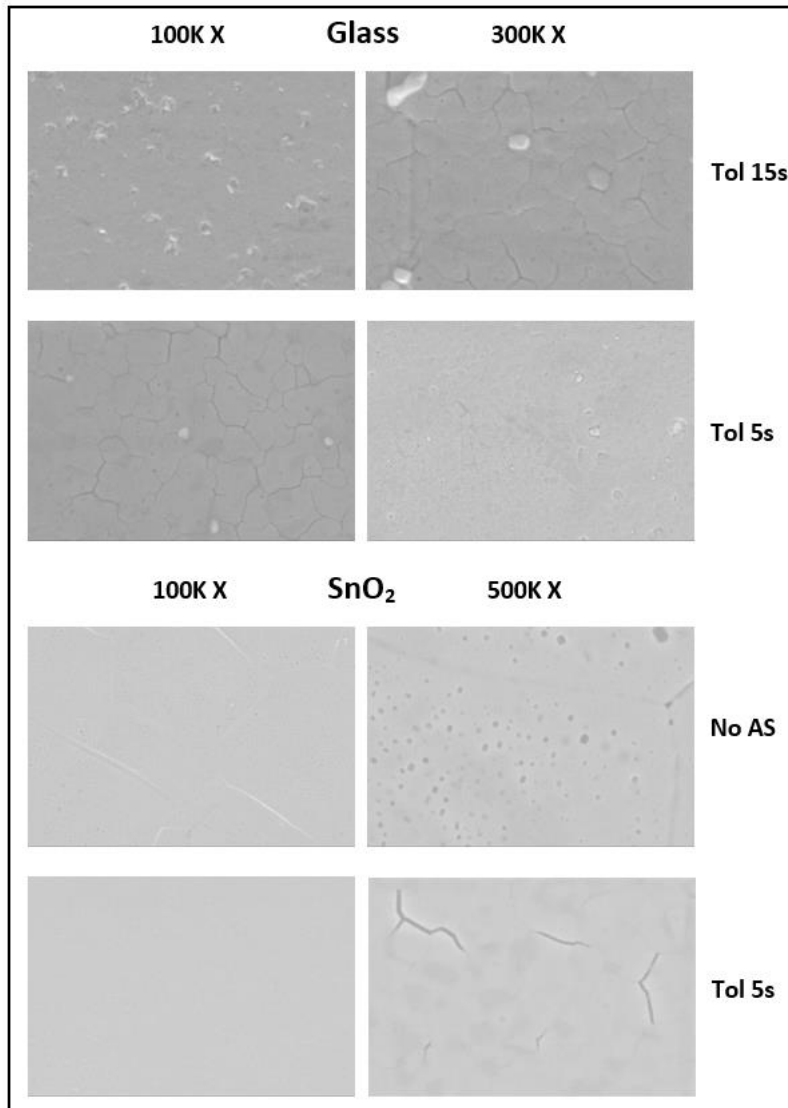


Figure S1: SEM images for samples with $X_{sol} = 0$.

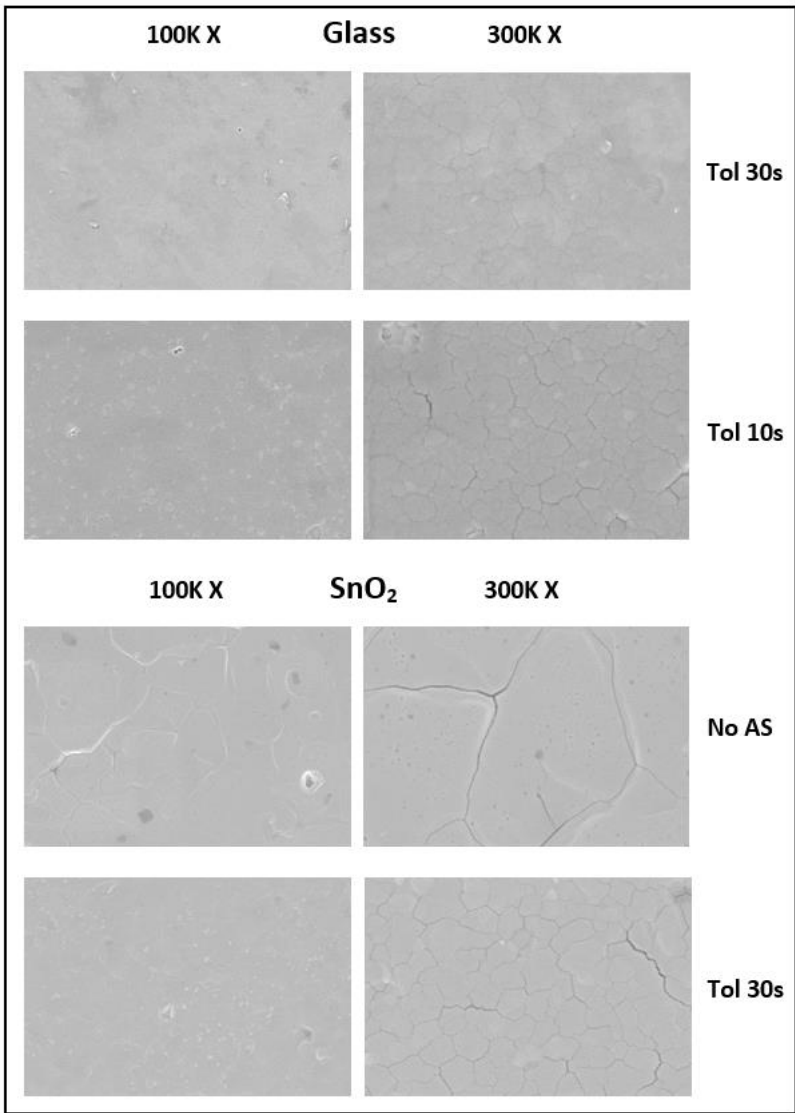


Figure S2: SEM images for samples with $X_{sol} = 0.3$.

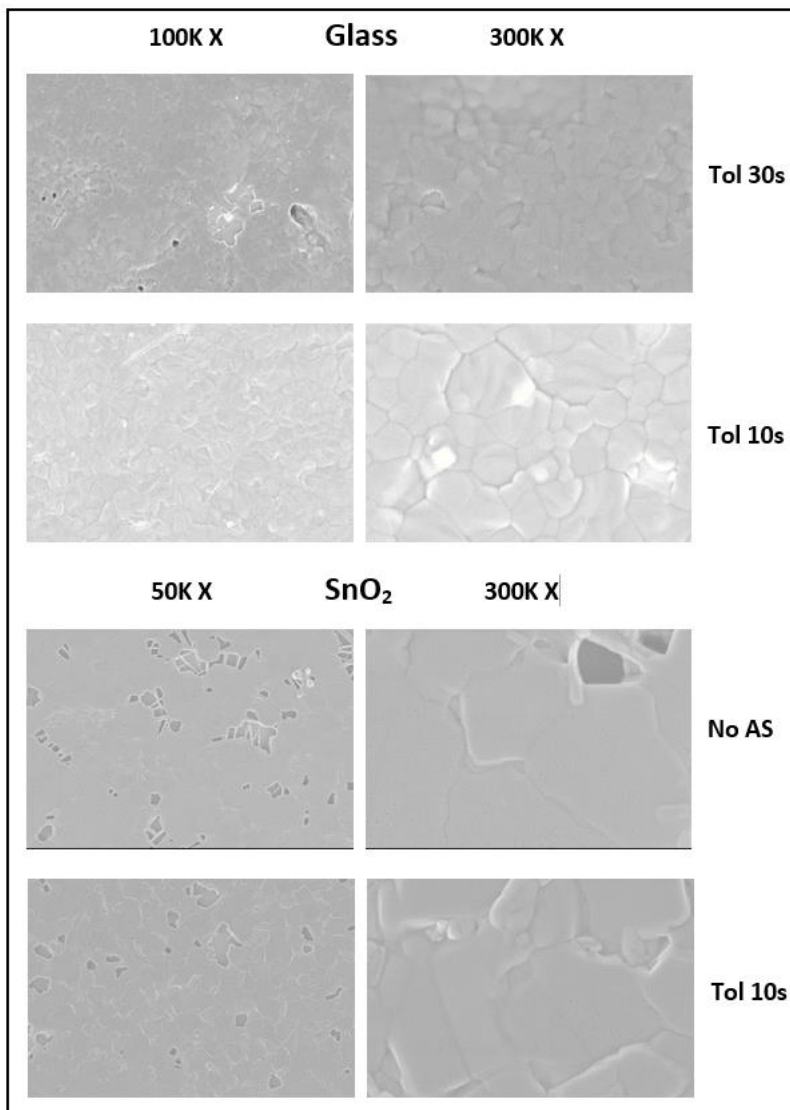


Figure S3: SEM images for samples with $X_{sol} = 0.6$.

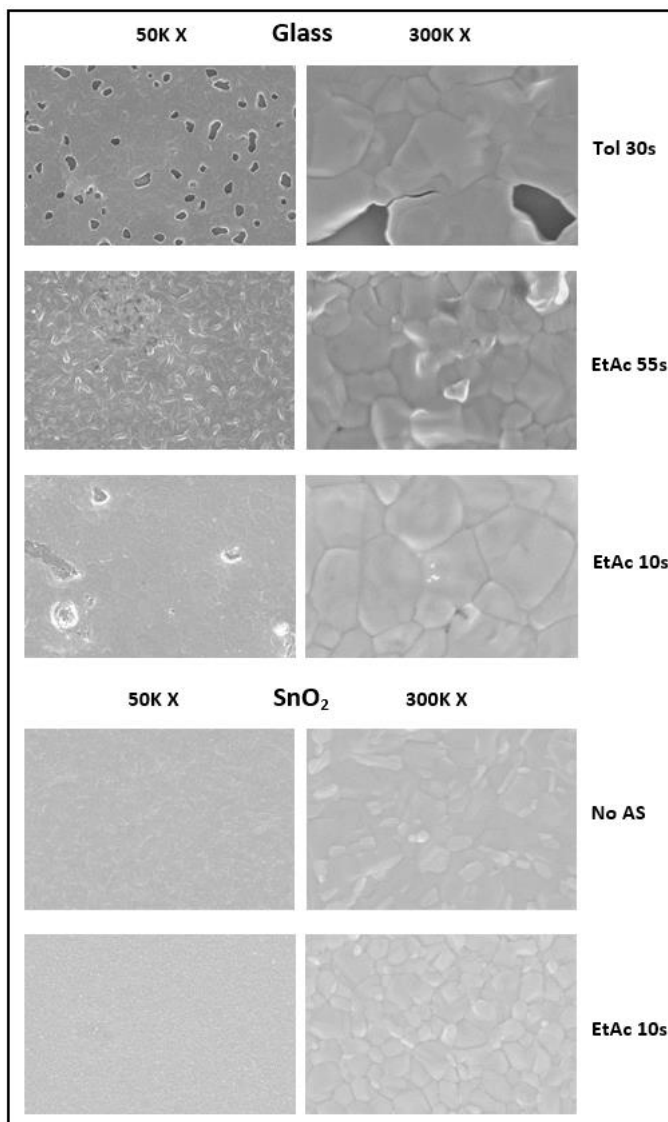


Figure S4: SEM images for samples with $X_{sol} = 0.7$.

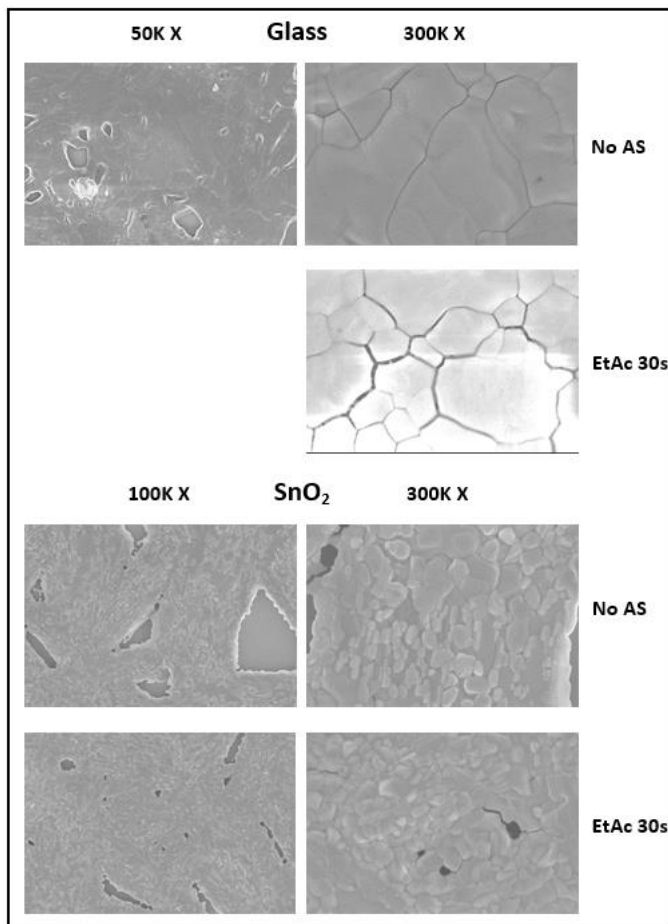


Figure S5: SEM images for samples with $X_{\text{sol}} = 1$.

SI:3. Film formation – additional plots.

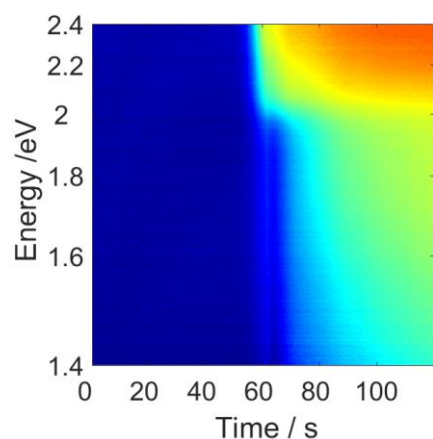


Figure S6: $X_{\text{sol}} = 0.6$: Heat map with extended time range.

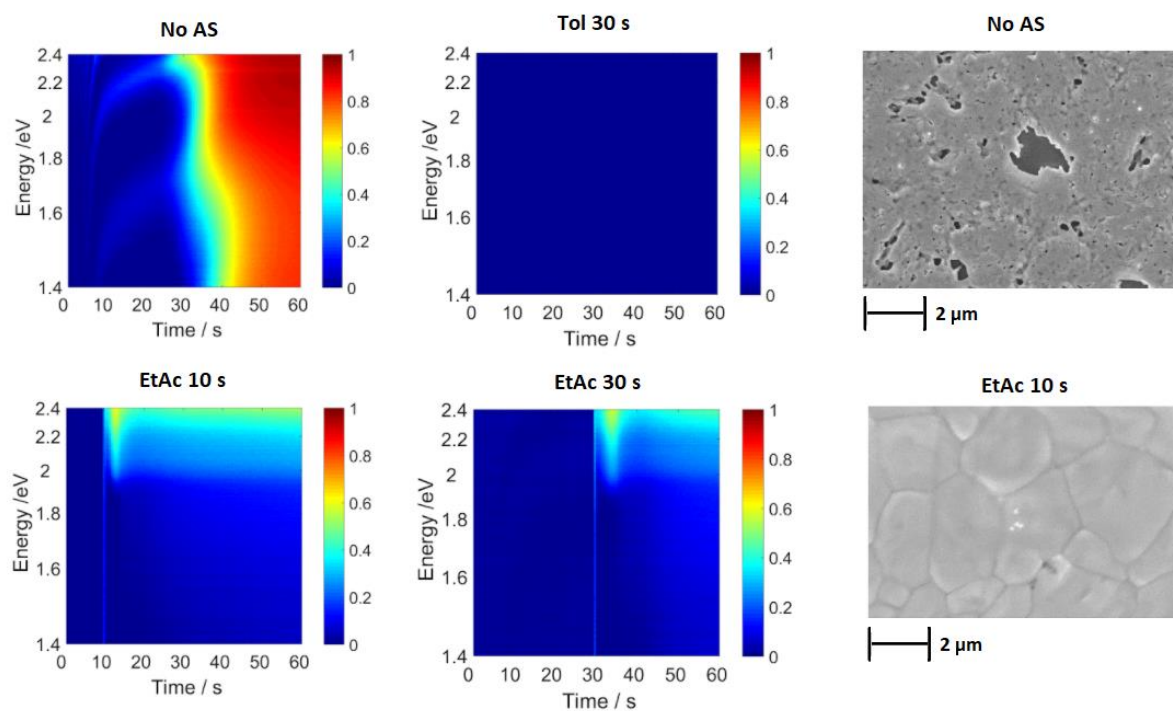


Figure S7: $X_{\text{sol}} = 0.7$: The no AS in-situ tracking failed as can be seen from the wavy behavior in the heat map. With toluene as AS there was no crystallization within the 60 s time window. EtAc induced crystallization of a non-perovskite phase for both 10 and 30 s drip time. The SEM images to the right show that the sample without AS has much lower quality compared to the sample treated with EtAc.

SI:4. Choosing which solar cells to include

In order to reduce the noise in the dataset of the solar cells in the project, each solar cell was assessed individually based on its produced JV-curve. If the JV-behavior of a solar cell differed too much from the characteristic JV-curve of a solar cell, and hence the resulting parameters were assessed as not reliable to use for any analysis or conclusions, the data from that SC was removed from the plotted datasets presented. A SC was discarded from the dataset presented if:

- it did not produce any photocurrent.
- either the short circuit current or the open circuit voltage was very close to or even exceeding the theoretical upper limit for a solar cell with the expected bandgap.
- the shape of the curve was linear, i.e. it behaved like a resistor rather than a solar cell.
- the noise of the curve, either in the form of wave-like behavior or abrupt irregularities had a magnitude close to the absolute value of the current density.

Examples of JV-curves of SCs that were disregarded can be seen in Fig. S8. The left scan shows a very wavy behavior, the middle scan shows abrupt irregularities, and the right scan shows a resistor like behavior.

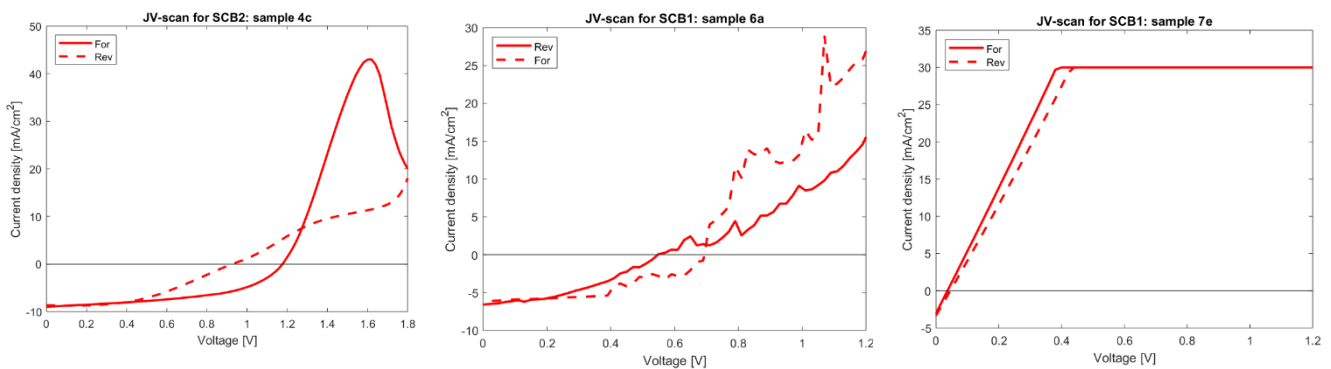


Figure S8: Examples of JV-scans that differ too much from the characteristic SC JV-curve to be included in the presented datasets.

SI:5. AS timing on device level

In the plots including all devices, the dashed line represents the theoretical upper limit for the J_{SC} and V_{OC} respectively for the perovskite with that particular ionic composition, based on the bandgap of the material. As can be seen, several samples include devices which have J_{SC} or V_{OC} values above the theoretical maximum. The error bars represent standard deviation, which means that there are devices with values deviating more than the range of the error bar.

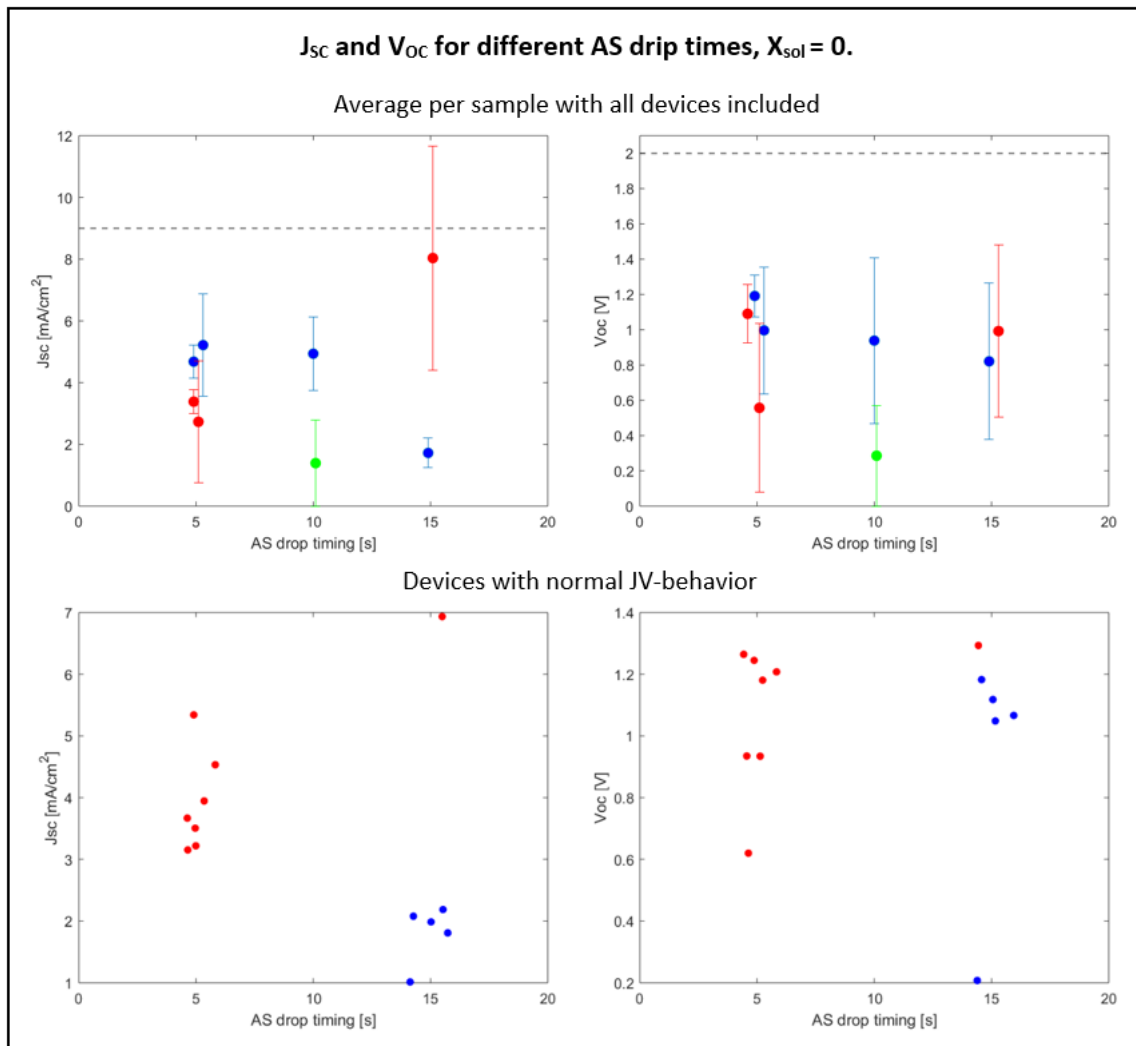


Figure S9: J_{SC} and V_{OC} plots for devices with $X_{sol} = 0$.

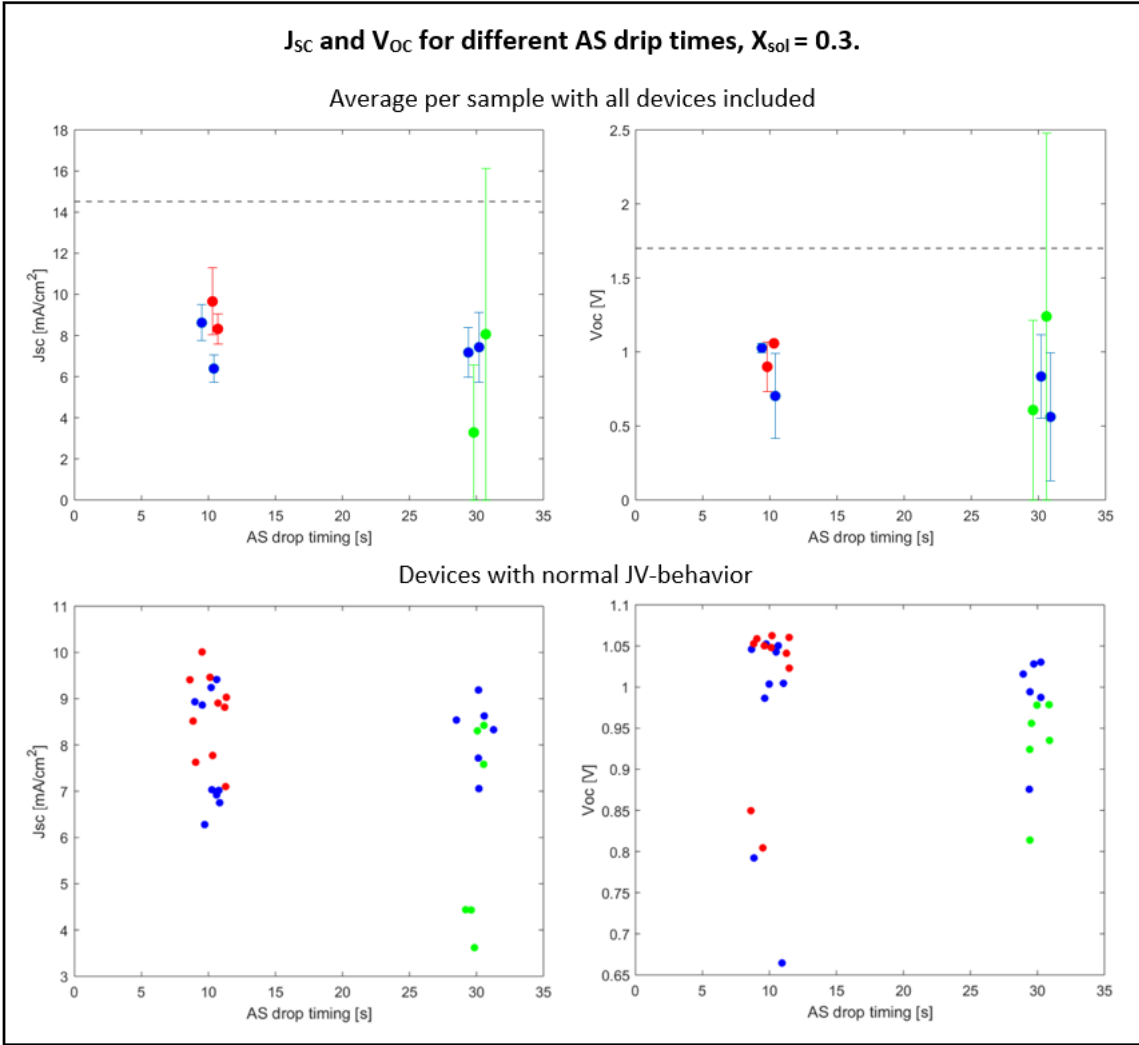


Figure S10: J_{SC} and V_{OC} plots for devices with $X_{sol} = 0.3$.

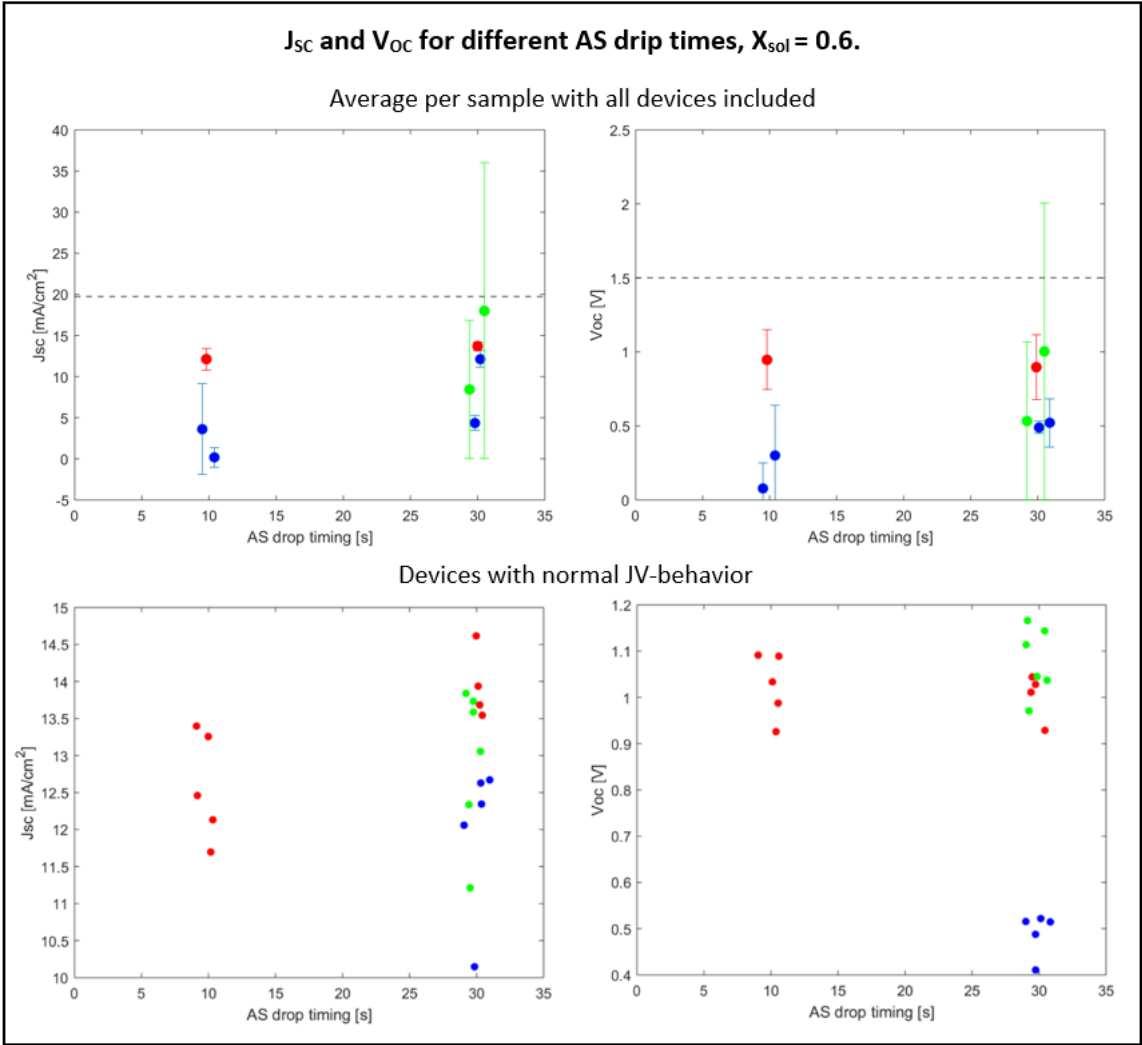


Figure S11: J_{SC} and V_{OC} plots for devices with $X_{sol} = 0.6$.

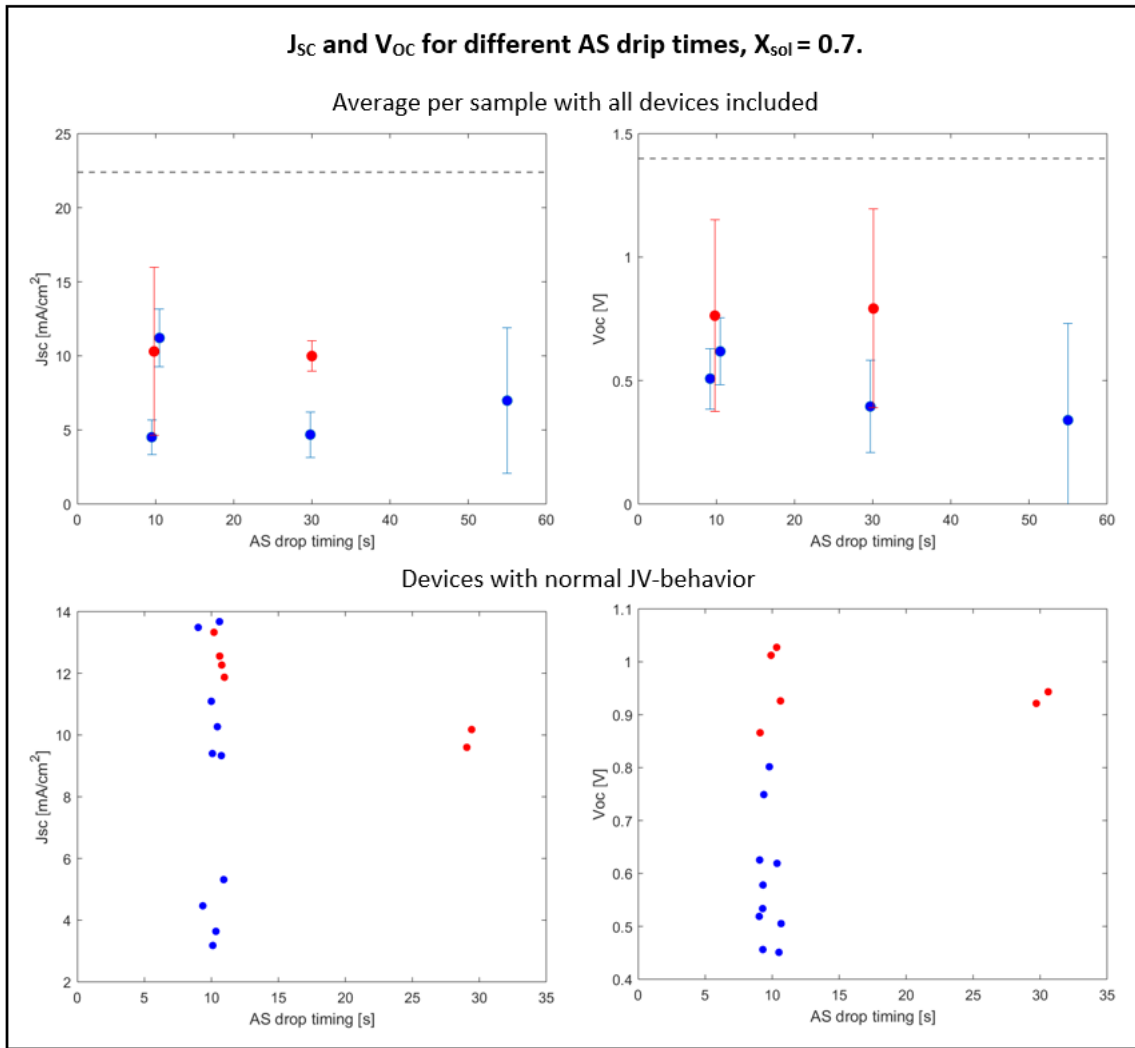


Figure S12: J_{SC} and V_{OC} plots for devices with $X_{sol} = 0.7$.

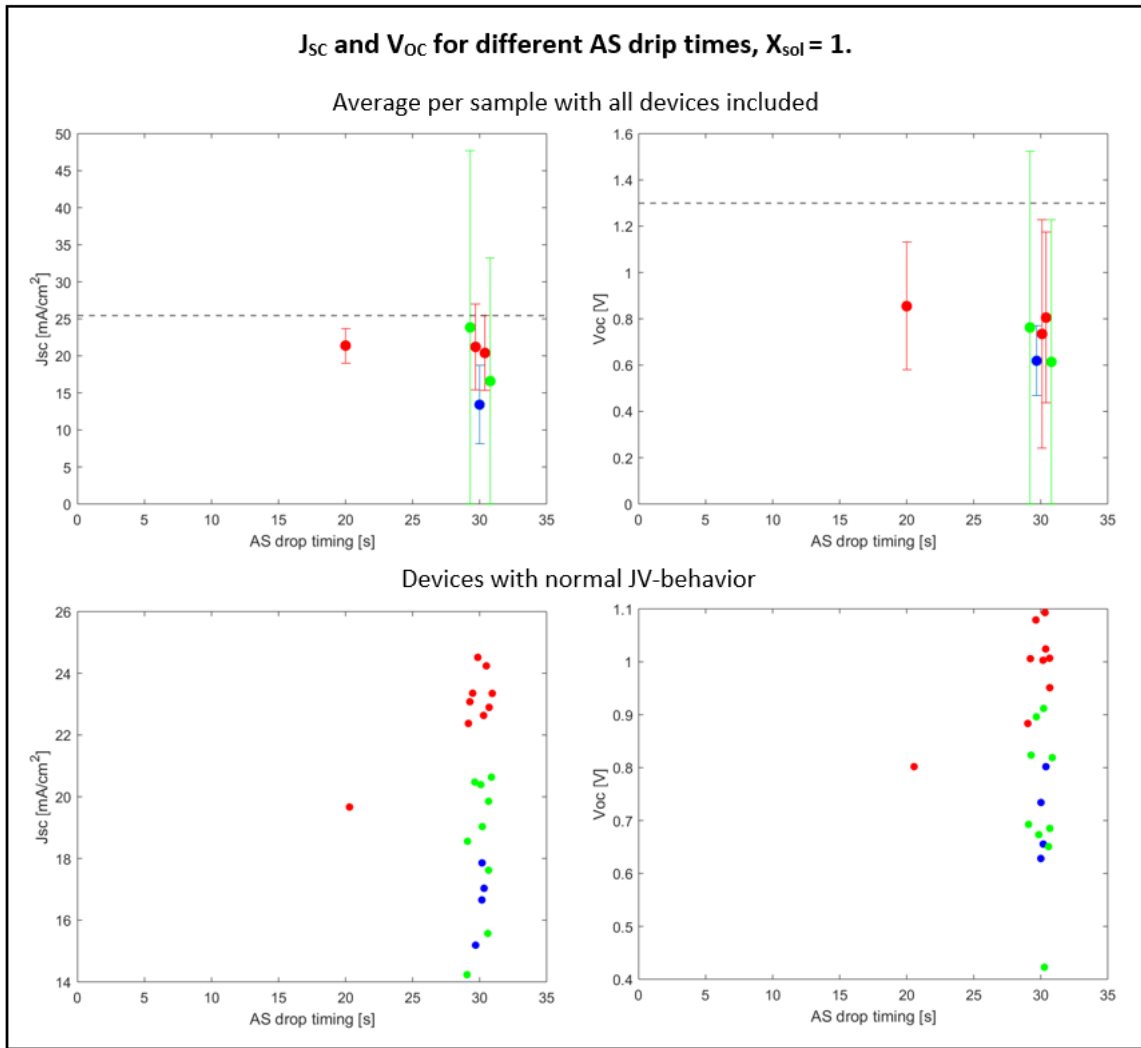


Figure S13: J_{SC} and V_{OC} plots for devices with X_{Sol} = 1.

SI:6. Estimated hole fraction of film area

Plot of estimated hole fraction of film area with the two images with different magnifying levels differentiated. For each type (same IM and halide mix), the two images with different magnifying level represent the same sample.

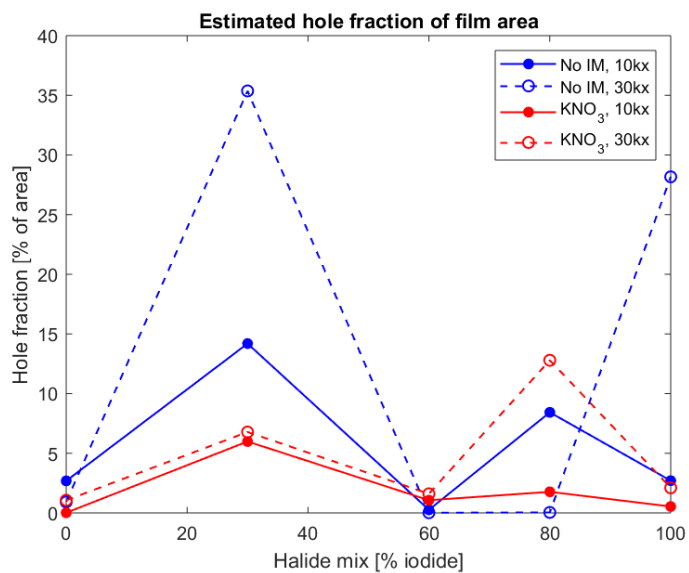


Figure S14: Estimated hole fraction of film area at contact interface.