

Supplementary Information

Comparison of drop-cast and spin-coated PCBM

The PCBM deposition from solution was performed both via spin-coating in a N₂ glove box and via drop casting in an Ar environment in the glass cell. For both depositions, the same solution was used. The resulting spectra show perfect agreement concerning line shape and binding energy position for the core level spectra (Fig S1 a, b) and the valence region spectra (Fig S1 c, d). Additionally, the ionization potential is 6.1 eV independent of the deposition technique and environment.

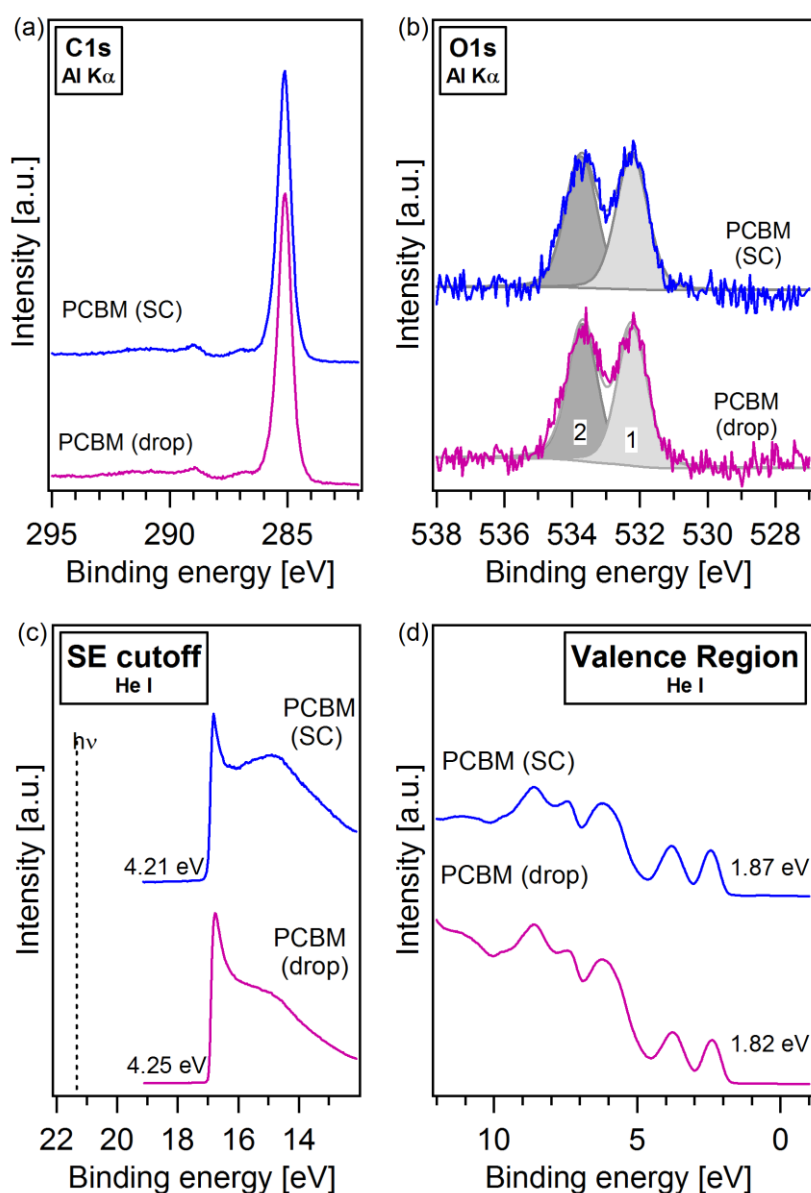


Figure S1: Comparison of PCBM spectra obtained for thin films deposited via drop casting in a glass cell in Ar atmosphere (bottom) and via spin coating in a N₂ glove box (top).

Calculation of the difference spectra for Si2p, C1s, and O1s

In a first step a difference spectrum of the Si2p emission measured in the crucible residue spectrum and the original substrate emission was calculated in such a way to eliminate the Si2p contribution. The intensity scaling factor as well as the observed shift in binding energy were then taken to subtract the oxygen contribution originating from the SiO₂ from the crucible residue signal. This approach is based on the assumption that all substrate peaks are damped in intensity and possibly shifted in energy by the same amount

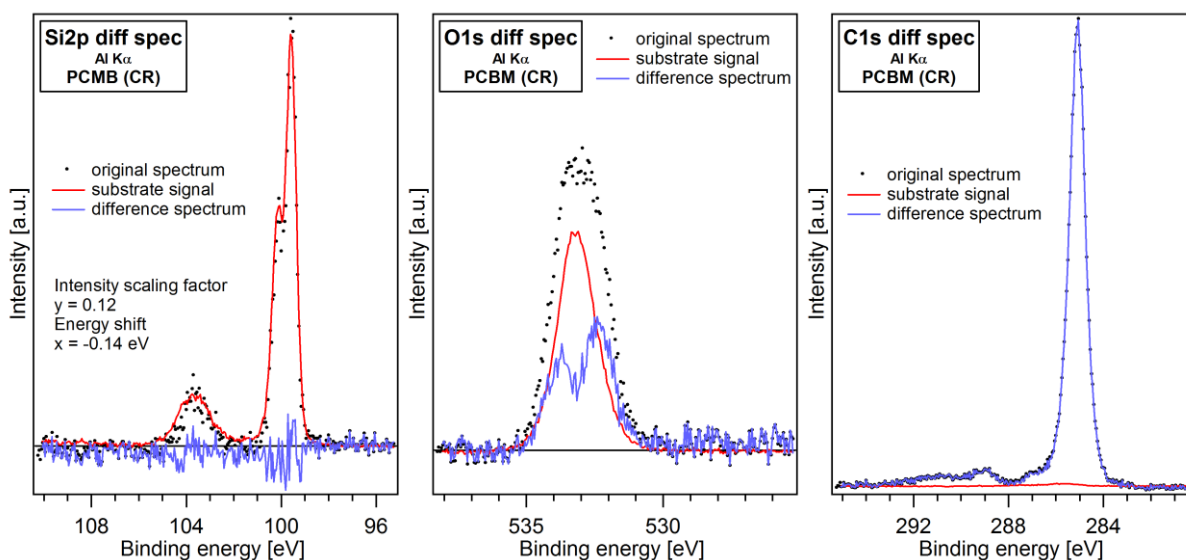


Figure S2: Calculation of difference spectra for the crucible residue spectra to eliminate the substrate signal. At first the Si2p difference spectrum was calculated in such a way that the intensity of the Si2p peak was (almost) 0. The intensity scaling factor of $y = 0.12$ and the energy shift $x = -0.14$ eV were then taken to subtract the substrate peak contributions from the crucible residue data for the O1s emission as well as the C1s emission.

Mass spectrometric analysis

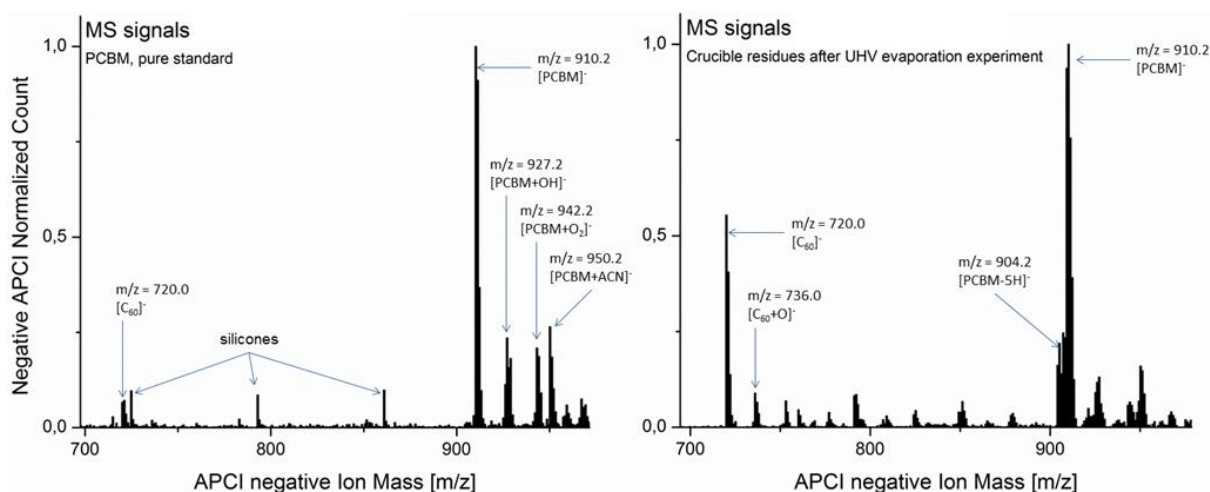


Figure S3: Accumulation of all detected ion masses between retention time = 3 and 11 min. PCBM standard (left) and crucible residues (right).

Thermal treatment of PCBM

Table S1: Overview of results for different temperature treatments of PCBM prior to solar cell fabrication.

Sample / Retention Time	PCBM	SP 1	SP 2	C ₆₀
	4.8 min	5.7 min	8.0 min	9.6 min
310 °C – 60 min	83.1 %	7.6 %	0.1 %	0.7 %
315 °C – 60 min	77.6 %	9.7 %	1.2 %	1.2 %
320 °C – 60 min	66.7 %	11.2 %	2.8 %	5.9 %
Evaporated sample	77.3 %	6.2 %	0.9 %	6.5 %