

Supporting Information

Revealing photo-degradation mechanism of PM6:Y6 based high-efficiency organic solar cells

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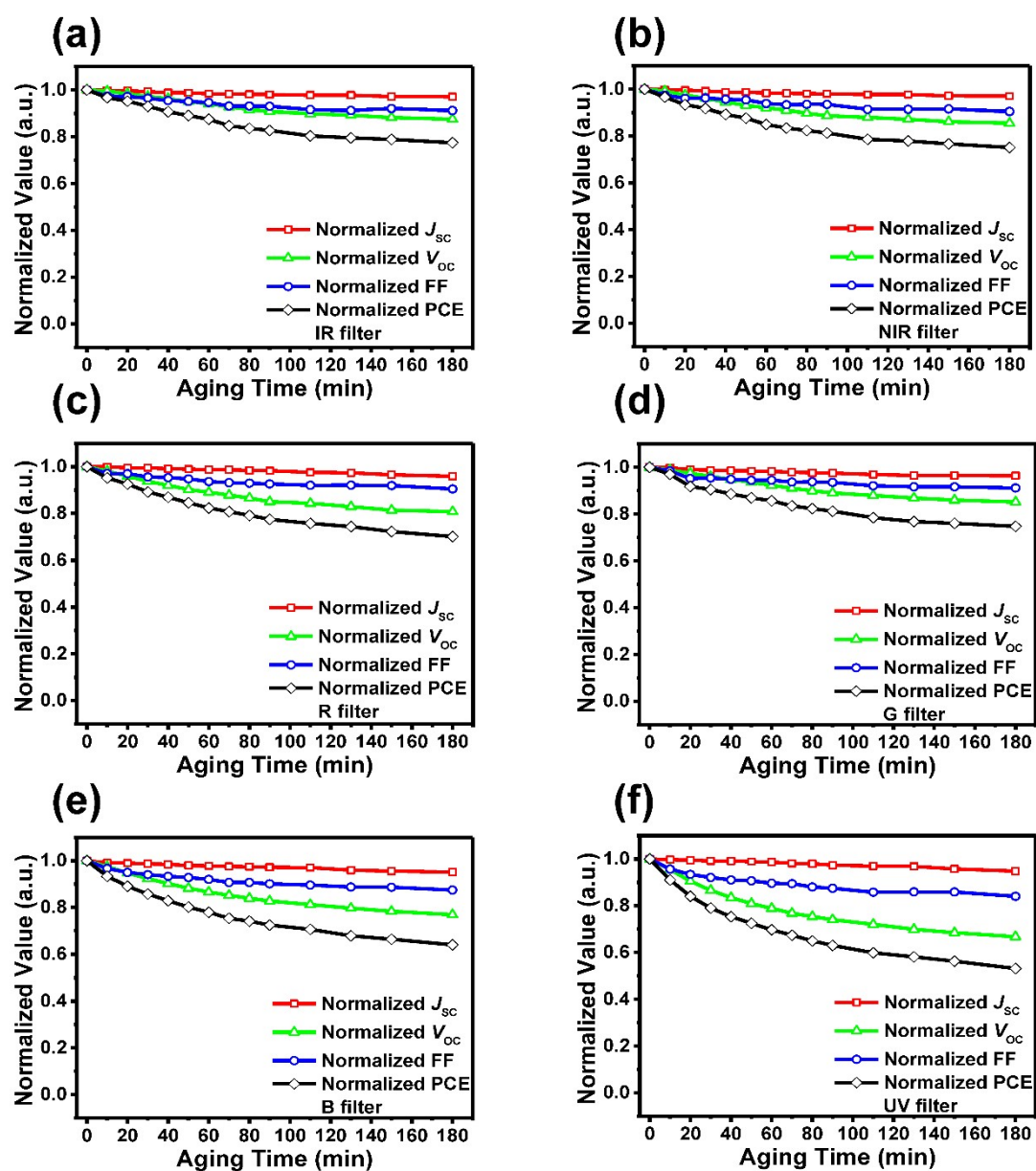


Fig. S1. Normalized photovoltaic parameters of aged devices under simulated 1-sun illumination with different filters.

Table S1 Photovoltaic parameters of aged device under illumination with IR filter.

| Aging Time (min) | J_{SC} (mA cm ⁻²) | V_{OC} (V) | FF (%) | PCE (%) |
|---------------------|---------------------------------|-------------------|------------------|------------------|
| 0 | 25.3 (100.0%) | 0.827 (100.0%) | 71.1 (100.0%) | 14.9 (100.0%) |
| 10 | 25.2 (99.8%) | 0.823 (99.5%) | 69.2 (97.4%) | 14.4 (96.7%) |
| 20 | 25.2 (99.6%) | 0.813 (98.3%) | 69.1 (97.2%) | 14.2 (95.2%) |
| 30 | 25.1 (99.2%) | 0.804 (97.2%) | 68.6 (96.5%) | 13.8 (93.0%) |
| 40 | 25.0 (98.8%) | 0.796 (96.3%) | 67.9 (95.4%) | 13.5 (90.7%) |
| 50 | 25.0 (98.7%) | 0.786 (95.0%) | 67.6 (95.0%) | 13.3 (89.1%) |
| 60 | 24.9 (98.3%) | 0.778 (94.1%) | 67.3 (94.6%) | 13.0 (87.5%) |
| 70 | 24.8 (98.2%) | 0.767 (92.7%) | 66.2 (93.1%) | 12.6 (84.8%) |
| 80 | 24.8 (98.1%) | 0.758 (91.6%) | 66.2 (93.1%) | 12.4 (83.7%) |
| 90 | 24.8 (98.0%) | 0.751 (90.8%) | 66.1 (93.0%) | 12.3 (82.8%) |
| 110 | 24.7 (97.7%) | 0.743 (89.9%) | 65.1 (91.6%) | 12.0 (80.4%) |
| 130 | 24.7 (97.7%) | 0.738 (89.3%) | 64.9 (91.2%) | 11.8 (79.6%) |
| 150 | 24.6 (97.1%) | 0.730 (88.2%) | 65.5 (92.1%) | 11.7 (78.9%) |
| 180 | 24.5 (97.1%) | 0.724 (87.6%) | 64.9 (91.2%) | 11.5 (77.5%) |

The percentage values in brackets are the remaining values relative to the fresh device.

Table S2 Photovoltaic parameters of aged device under illumination with NIR filter.

| Aging Time (min) | J_{SC} (mA cm ⁻²) | V_{OC} (V) | FF (%) | PCE (%) |
|---------------------|---------------------------------|-------------------|------------------|------------------|
| 0 | 25.1 (100.0%) | 0.836 (100.0%) | 72.3 (100.0%) | 15.2 (100.0%) |
| 10 | 25.0 (99.7%) | 0.830 (99.2%) | 70.5 (97.5%) | 14.6 (96.6%) |
| 20 | 25.0 (99.6%) | 0.815 (97.5%) | 69.5 (96.1%) | 14.1 (93.4%) |
| 30 | 24.8 (99.3%) | 0.804 (96.1%) | 69.6 (96.2%) | 13.9 (91.8%) |
| 40 | 24.5 (98.5%) | 0.790 (94.5%) | 69.2 (95.7%) | 13.4 (89.3%) |
| 50 | 24.4 (98.3%) | 0.778 (93.1%) | 69.0 (95.4%) | 13.1 (87.7%) |
| 60 | 24.3 (98.3%) | 0.769 (92.0%) | 67.9 (93.9%) | 12.7 (85.0%) |
| 70 | 24.3 (98.2%) | 0.761 (91.1%) | 67.5 (93.3%) | 12.5 (83.5%) |
| 80 | 24.2 (98.1%) | 0.751 (89.8%) | 67.6 (93.6%) | 12.3 (82.4%) |
| 90 | 24.1 (97.9%) | 0.742 (88.7%) | 67.6 (93.5%) | 12.1 (81.4%) |
| 110 | 24.0 (97.6%) | 0.736 (88.0%) | 66.1 (91.4%) | 11.7 (78.7%) |
| 130 | 23.9 (97.3%) | 0.729 (87.2%) | 66.1 (91.5%) | 11.5 (78.0%) |
| 150 | 23.7 (97.1%) | 0.721 (86.2%) | 66.2 (91.6%) | 11.3 (76.7%) |
| 180 | 23.6 (96.9%) | 0.715 (85.6%) | 65.4 (90.5%) | 11.1 (75.2%) |

The percentage values in brackets are the remaining values relative to the fresh device.

Table S3 Photovoltaic parameters of aged device under illumination with R filter.

| Aging Time (min) | J_{SC} (mA cm ⁻²) | V_{OC} (V) | FF (%) | PCE (%) |
|---------------------|---------------------------------|-------------------|------------------|------------------|
| 0 | 25.2 (100.0%) | 0.825 (100.0%) | 71.7 (100.0%) | 14.9 (100.0%) |
| 10 | 25.2 (99.9%) | 0.810 (98.1%) | 69.7 (97.1%) | 14.2 (95.2%) |
| 20 | 25.1 (99.5%) | 0.791 (95.9%) | 69.6 (97.0%) | 13.8 (92.6%) |
| 30 | 25.1 (99.5%) | 0.774 (93.8%) | 68.6 (95.6%) | 13.3 (89.2%) |
| 40 | 25.0 (99.1%) | 0.759 (92.0%) | 68.4 (95.3%) | 13.0 (87.0%) |
| 50 | 24.9 (98.9%) | 0.744 (90.2%) | 68.0 (94.8%) | 12.6 (84.6%) |
| 60 | 24.9 (98.7%) | 0.735 (89.1%) | 67.2 (93.7%) | 12.3 (82.3%) |
| 70 | 24.9 (98.7%) | 0.725 (87.9%) | 66.8 (93.2%) | 12.0 (80.8%) |
| 80 | 24.8 (98.4%) | 0.714 (86.6%) | 66.7 (92.9%) | 11.8 (79.2%) |
| 90 | 24.8 (98.3%) | 0.702 (85.1%) | 66.5 (92.6%) | 11.6 (77.5%) |
| 110 | 24.6 (97.6%) | 0.696 (84.3%) | 66.0 (92.0%) | 11.3 (75.8%) |
| 130 | 24.5 (97.4%) | 0.684 (82.9%) | 66.1 (92.1%) | 11.1 (74.4%) |
| 150 | 24.3 (96.5%) | 0.672 (81.4%) | 66.0 (91.9%) | 10.8 (72.3%) |
| 180 | 24.7 (95.9%) | 0.666 (80.8%) | 64.9 (90.5%) | 10.5 (70.1%) |

The percentage values in brackets are the remaining values relative to the fresh device.

Table S4 Photovoltaic parameters of aged device under illumination with G filter.

| Aging Time (min) | J_{SC} (mA cm ⁻²) | V_{OC} (V) | FF (%) | PCE (%) |
|---------------------|---------------------------------|-------------------|------------------|------------------|
| 0 | 25.2 (100.0%) | 0.831 (100.0%) | 71.7 (100.0%) | 15.0 (100.0%) |
| 10 | 25.1 (99.8%) | 0.821 (98.8%) | 70.5 (98.4%) | 14.5 (97.0%) |
| 20 | 24.9 (99.0%) | 0.810 (97.4%) | 68.2 (95.2%) | 13.8 (91.8%) |
| 30 | 24.8 (98.7%) | 0.798 (96.1%) | 68.4 (95.4%) | 13.6 (90.5%) |
| 40 | 24.8 (98.6%) | 0.788 (94.8%) | 68.0 (94.8%) | 13.3 (88.6%) |
| 50 | 24.8 (98.4%) | 0.778 (93.6%) | 67.7 (94.4%) | 13.0 (86.9%) |
| 60 | 24.7 (98.2%) | 0.767 (92.3%) | 67.7 (94.5%) | 12.8 (85.6%) |
| 70 | 24.6 (97.9%) | 0.756 (91.0%) | 67.2 (93.7%) | 12.5 (83.4%) |
| 80 | 24.6 (97.6%) | 0.747 (89.9%) | 67.2 (93.7%) | 12.3 (82.3%) |
| 90 | 24.5 (97.5%) | 0.740 (89.0%) | 67.0 (93.5%) | 12.2 (81.2%) |
| 110 | 24.4 (96.9%) | 0.731 (87.9%) | 66.0 (92.1%) | 11.8 (78.4%) |
| 130 | 24.3 (96.5%) | 0.722 (86.8%) | 65.7 (91.6%) | 11.5 (76.8%) |
| 150 | 24.3 (96.5%) | 0.714 (86.0%) | 65.7 (91.6%) | 11.4 (76.0%) |
| 180 | 24.2 (96.3%) | 0.707 (85.1%) | 65.3 (91.1%) | 11.2 (74.7%) |

The percentage values in brackets are the remaining values relative to the fresh device.

Table S5 Photovoltaic parameters of aged device under illumination with B filter.

| Aging Time (min) | J_{SC} (mA cm ⁻²) | V_{OC} (V) | FF (%) | PCE (%) |
|---------------------|---------------------------------|-------------------|------------------|------------------|
| 0 | 25.2 (100.0%) | 0.846 (100.0%) | 71.2 (100.0%) | 15.2 (100.0%) |
| 10 | 24.9 (99.1%) | 0.825 (97.5%) | 68.8 (96.7%) | 14.2 (93.4%) |
| 20 | 24.9 (99.0%) | 0.802 (94.8%) | 67.6 (95.0%) | 13.5 (89.1%) |
| 30 | 24.8 (98.7%) | 0.781 (92.3%) | 67.0 (94.0%) | 13.0 (85.7%) |
| 40 | 24.8 (98.5%) | 0.763 (90.2%) | 66.4 (93.3%) | 12.6 (82.9%) |
| 50 | 24.7 (98.0%) | 0.746 (88.2%) | 66.1 (92.8%) | 12.2 (80.2%) |
| 60 | 24.6 (97.8%) | 0.733 (86.6%) | 65.5 (92.0%) | 11.8 (77.9%) |
| 70 | 24.5 (97.5%) | 0.721 (85.2%) | 64.6 (90.7%) | 11.4 (75.3%) |
| 80 | 24.5 (97.4%) | 0.710 (83.9%) | 64.6 (90.7%) | 11.2 (74.1%) |
| 90 | 24.4 (97.1%) | 0.700 (82.8%) | 64.2 (90.1%) | 11.0 (72.5%) |
| 110 | 24.4 (97.1%) | 0.687 (81.2%) | 63.8 (89.6%) | 10.7 (70.6%) |
| 130 | 24.1 (95.9%) | 0.674 (79.7%) | 63.2 (88.8%) | 10.3 (67.9%) |
| 150 | 24.0 (95.6%) | 0.663 (78.3%) | 63.1 (88.7%) | 10.1 (66.4%) |
| 180 | 23.9 (95.1%) | 0.651 (76.9%) | 62.3 (87.5%) | 9.70 (64.0%) |

The percentage values in brackets are the remaining values relative to the fresh device.

Table S6 Photovoltaic parameters of aged device under illumination with UV filter.

| Aging Time (min) | J_{SC} (mA cm ⁻²) | V_{OC} (V) | FF (%) | PCE (%) |
|---------------------|---------------------------------|-------------------|------------------|------------------|
| 0 | 25.2 (100.0%) | 0.829 (100.0%) | 71.6 (100.0%) | 15.0 (100.0%) |
| 10 | 25.2 (99.7%) | 0.792 (95.5%) | 68.5 (95.7%) | 13.6 (91.0%) |
| 20 | 25.1 (99.5%) | 0.750 (90.5%) | 66.8 (93.4%) | 12.6 (84.0%) |
| 30 | 25.0 (99.1%) | 0.718 (86.6%) | 65.9 (92.1%) | 11.8 (79.0%) |
| 40 | 25.0 (99.1%) | 0.692 (83.5%) | 65.2 (91.0%) | 11.3 (75.3%) |
| 50 | 24.9 (98.9%) | 0.671 (80.9%) | 64.9 (90.6%) | 10.9 (72.5%) |
| 60 | 24.9 (98.7%) | 0.654 (78.8%) | 64.1 (89.6%) | 10.4 (69.7%) |
| 70 | 24.8 (98.1%) | 0.637 (76.8%) | 64.0 (89.4%) | 10.1 (67.4%) |
| 80 | 24.7 (98.0%) | 0.625 (75.3%) | 63.0 (88.0%) | 9.73 (65.0%) |
| 90 | 24.6 (97.4%) | 0.614 (74.0%) | 62.6 (87.4%) | 9.43 (63.0%) |
| 110 | 24.5 (97.0%) | 0.597 (72.0%) | 61.4 (85.8%) | 8.97 (59.9%) |
| 130 | 24.4 (96.8%) | 0.579 (69.9%) | 61.5 (85.9%) | 8.70 (58.1%) |
| 150 | 24.2 (95.7%) | 0.567 (68.4%) | 61.5 (85.9%) | 8.42 (56.2%) |
| 180 | 23.9 (94.8%) | 0.553 (66.7%) | 60.1 (84.0%) | 7.96 (53.1%) |

The percentage values in brackets are the remaining values relative to the fresh device.

Table S7 Photovoltaic parameters of aged device under illumination w/o filter.

| Aging Time (min) | J_{SC} (mA cm ⁻²) | V_{OC} (V) | FF (%) | PCE (%) |
|---------------------|---------------------------------|-------------------|------------------|------------------|
| 0 | 24.8 (100.0%) | 0.832 (100.0%) | 72.5 (100.0%) | 14.9 (100.0%) |
| 10 | 24.6 (99.4%) | 0.784 (94.2%) | 68.9 (95.0%) | 13.3 (89.0%) |
| 20 | 24.3 (98.3%) | 0.735 (88.3%) | 67.1 (92.5%) | 12.0 (80.3%) |
| 30 | 24.2 (98.0%) | 0.699 (84.0%) | 65.9 (90.9%) | 11.2 (74.9%) |
| 40 | 24.2 (97.9%) | 0.672 (80.8%) | 65.1 (89.8%) | 10.6 (71.0%) |
| 50 | 24.2 (97.6%) | 0.651 (78.2%) | 64.1 (88.4%) | 10.1 (67.5%) |
| 60 | 24.2 (97.6%) | 0.636 (76.4%) | 63.8 (88.1%) | 9.81 (65.7%) |
| 70 | 23.8 (96.3%) | 0.620 (74.5%) | 62.7 (86.5%) | 9.27 (62.1%) |
| 80 | 23.9 (96.6%) | 0.608 (73.1%) | 62.8 (86.6%) | 9.12 (61.1%) |
| 90 | 23.6 (95.3%) | 0.599 (72.0%) | 62.2 (85.8%) | 8.79 (58.9%) |
| 110 | 23.5 (94.8%) | 0.586 (70.4%) | 61.1 (84.2%) | 8.40 (56.3%) |
| 130 | 23.2 (93.6%) | 0.569 (68.4%) | 61.0 (84.2%) | 8.04 (53.9%) |
| 150 | 22.9 (92.5%) | 0.560 (67.3%) | 61.0 (84.1%) | 7.82 (52.4%) |
| 180 | 22.6 (91.2%) | 0.548 (65.9%) | 60.1 (82.9%) | 7.44 (49.8%) |

The percentage values in brackets are the remaining values relative to the fresh device.

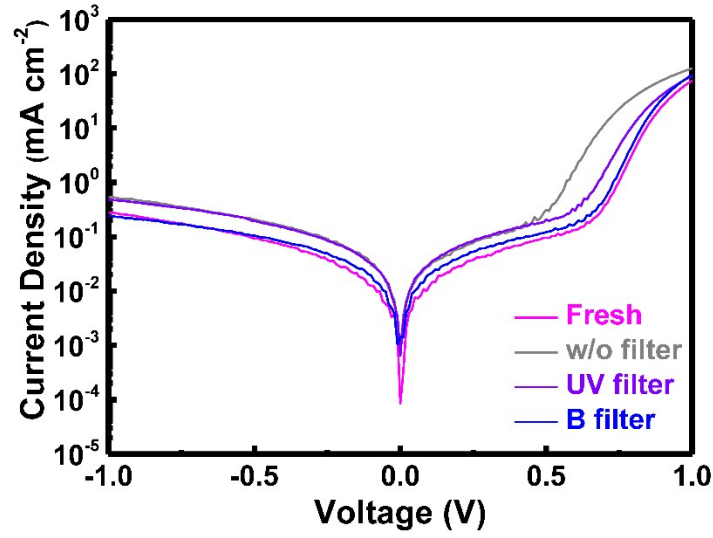


Fig. S2. Dark J - V curves of the fresh and aged devices under 1-hour illumination.

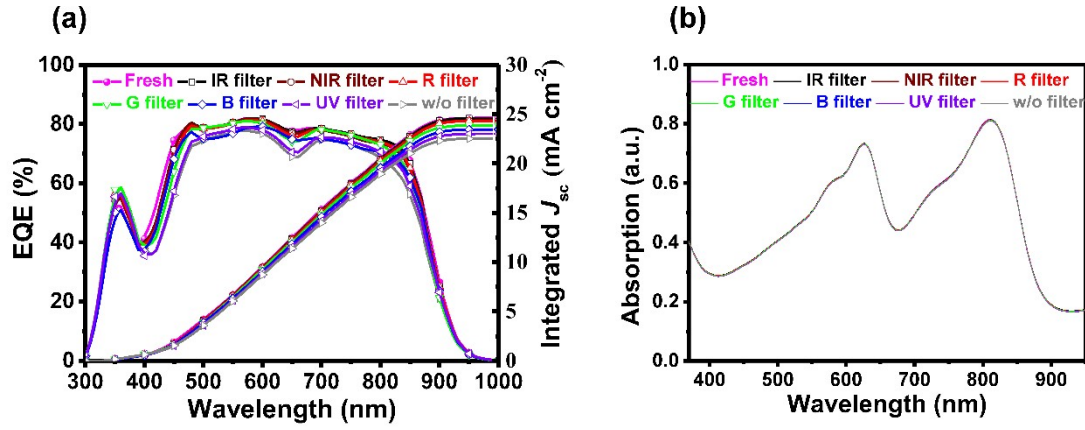


Fig. S3. (a) EQE curves and (b) UV absorption spectra of the fresh and aged devices under 1-hour illumination.

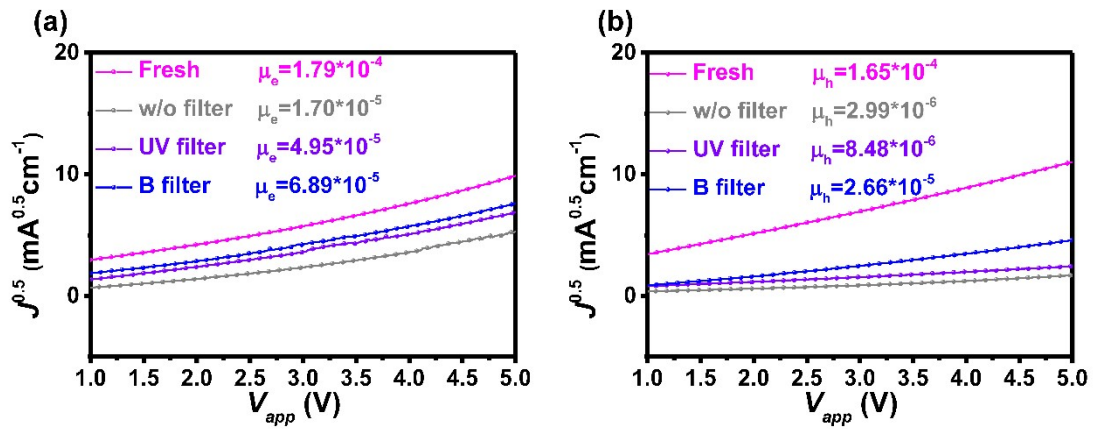


Fig. S4. J - V characteristics of (a) electron-only and (b) hole-only of the fresh and aged devices under 1-hour illumination.

Table S8 The μ_e/μ_h mobilities of blend films under 1-hour illumination.

| condition | μ_e ($\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$) | μ_h ($\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$) | μ_e/μ_h |
|------------|----------------------------------------------------------|----------------------------------------------------------|---------------|
| fresh | 1.79×10^{-5} | 1.65×10^{-5} | 1.08 |
| w/o filter | 1.70×10^{-6} | 2.99×10^{-7} | 5.69 |
| B | 6.89×10^{-6} | 2.66×10^{-6} | 2.59 |
| UV | 4.95×10^{-6} | 8.84×10^{-7} | 5.60 |

Table S9 Photovoltaic parameters of PM6:BTP-ec9 and PM6:BTP-BO-4Cl based devices.

| Acceptor | condition | J_{SC} (mA cm^{-2}) | J_{SC}^{EQE} (mA cm^{-2}) | V_{OC} (V) | FF (%) | PCE (%) |
|----------------|------------------|-------------------------------------|-------------------------------------------|-----------------|-----------|----------------------|
| BTP-ec9 | fresh | 25.7 | 24.4 | 0.849 | 78.5 | 17.1 (16.7±0.244) |
| | w/o filter-1h | 25.3 | 24.1 | 0.779 | 72.8 | 14.3 (14.2±0.432) |
| | w/o filter-3h | 25.1 | 23.8 | 0.724 | 69.9 | 12.7 (12.6±0.534) |
| BTP-BO- 4Cl | fresh | 26.3 | 25.1 | 0.847 | 74.7 | 16.7 (16.3±0.201) |
| | w/o filter-1h | 26.0 | 24.8 | 0.768 | 68.6 | 13.7 (13.5±0.384) |
| | w/o filter-3h | 26.0 | 24.7 | 0.701 | 63.9 | 11.6 (11.5±0.546) |