*Additional Supporting Information:*

# Molecular Oligothiophene-Fullerene Dyad Reaching Over 5% Efficiency in Single Material Organic Solar Cells

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# 1. Current density-voltage characterization (before the stability test)

**Table S1.** Performance parameters: power conversion efficiency, *PCE*; open-circuit voltage, $V_{oc}$; short-circuit current density, $J_{sc}$; fill factor, *FF*. The bandgap energy, $E_g$, is taken from the external quantum efficiency, *EQE*, as described by Almora et al.[1] (see **Figure S2**).

| $E_g$ [eV] | *PCE* [%] | $V_{oc}$ [mV] | $J_{sc}$ [mA cm$^{-2}$] | *FF* [%] | Statistic type of report | *PCE* after 24 h [%] |
|---|---|---|---|---|---|---|
| 1.62 | 5.1 | 820 | 13.0 | 48 | Average over 10 cells | 5.0 |

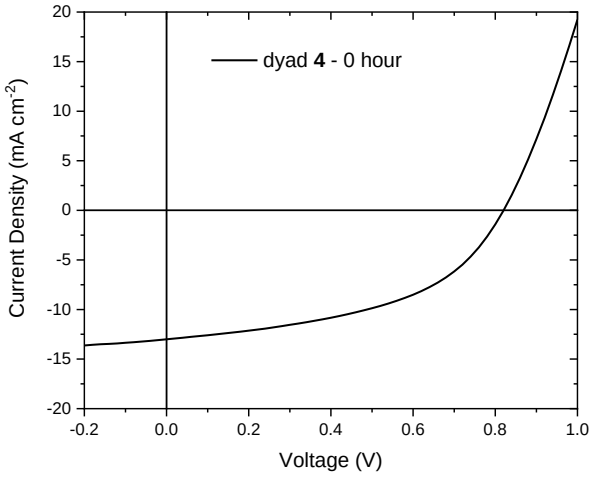
**Table S2.** Device materials: absorber material; electron transport material, ETM; Hole transport material, HTM, bottom electrode, top electrode

| Absorber | ETM | HTM | Bottom electrode | Top Electrode | DOI link of article including the original recipe (if it is a reproduction) |
|---|---|---|---|---|---|
| dyad 4 | ZnO (N10) | MoOx | ITO | Ag | No |

**Table S3.** Current density-voltage (*J-V*) measurement conditions. The designated area is as defined by Green et al.[2].

| **Parameter** | **Value/description** |
|---|---|
| Incident light intensity [mW cm$^{-2}$] | 100 |
| Incident spectrum | White LED |
| Mask aperture area [cm²] | 0.104 |
| Total device active area [cm²] | 0.104 |
| Designated Area [cm²] | 0.104 |

| | |
|---|---|
| Initial J-V measurement graph/data list | **Figure S1** top |
| Maximum power point (MPP) tracking data during 5 minutes | No |
| *J-V* measurement data file link/graph after 24h: | **Figure S1** bottom |
| *J-V* Solar simulator (type, standard, brand, model) | Home-made white LED based |
| Atmosphere composition | $N_2$ |
| Temperature [°C] | 30 |
| Use of black matte background | No |



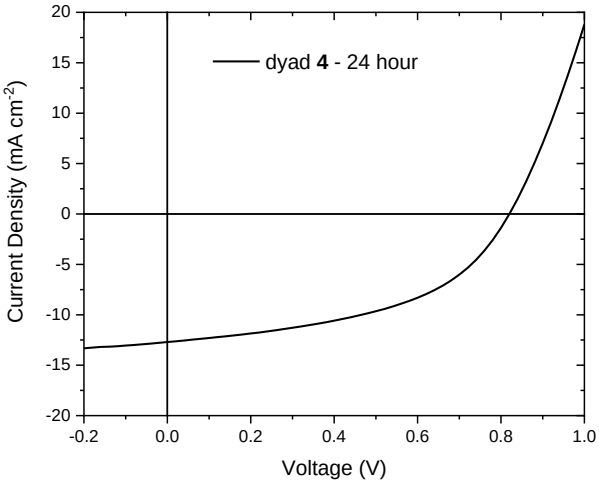



**Figure S1.** Current density-voltage measurement. The top and bottom graphs correspond to just after fabrication and 24 hours later, respectively.

## 2. External quantum efficiency (EQE)

**Table S4.** External quantum efficiency, EQE, measurement conditions.

| Parameter | Value/description |
|---|---|
| EQE data/graph | **Figure S2** |
| Background illumination intensity [mW/cm²] | 0 |
| EQE measurement instrument (model and brand | Enli Technology (from Taiwan) |
| Atmosphere composition | Air |
| Temperature [°C] | 30 |
| Use of black matte background | No |

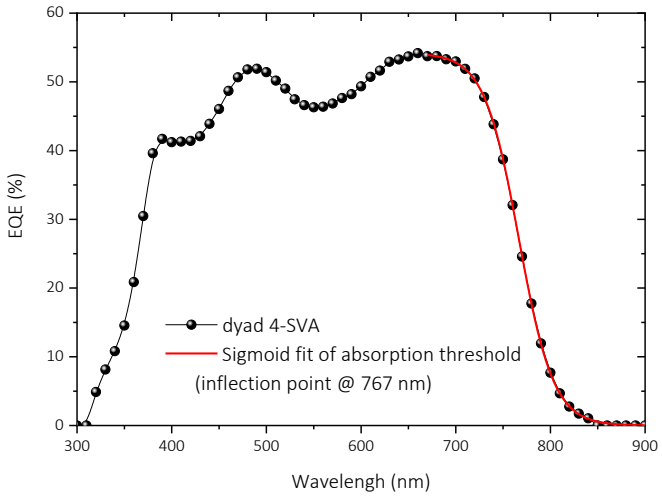



**Figure S2.** External quantum efficiency measurement and sigmoid fit of the absorption threshold, for the calculation of the bandgap energy, following the method by Almora et al.[1].

## 3. Operational stability test

**Table S5.** Degradation test measurement results and conditions. The stability test energy yields at 200 and 1000 hours are as defined by Almora et al.[3]

| Parameter | Value/description | Comment |
|---|---|---|
| In-situ stability test data/graph | **Figure S3** | |
| Stability test PCE after 200 h [%] | 4.89 | |
| Stability test PCE after 1000h [%] | 4.91 | Extrapolated |
| Stability test integrated energy output after 200h [Wh/cm²] | 1.08 | |
| Stability test integrated energy output after 1000h [Wh/cm²] | 4.91 | Extrapolated |
| Incident light intensity [mW/cm²] | 100 | |
| Incident illumination spectrum | White LED | |
| UV filter | No | |
| UV filter description | No | |
| Temperature [°C] | 30 | |
| Encapsulation | No | |
| Atmosphere composition | $N_2$ | |
| Relative humidity [%] | 0 | |
| Degradation condition | Open circuit | |
| Stability test degradation instrument info | Home-made chamber | |
| Use of black matte background | No | |

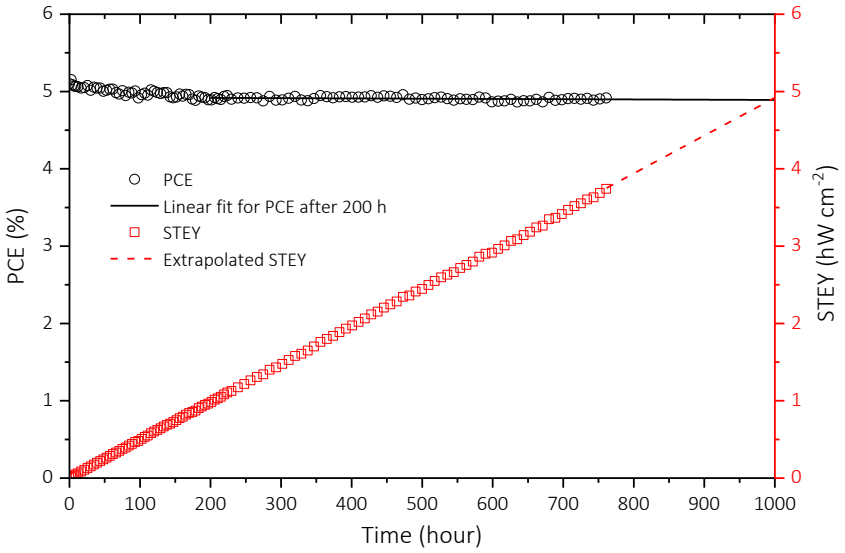



**Figure S3.** Stability test maximum power point tracking and energy yield, STEY, as defined by Almora et al.[3].

# References

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[2] M.A. Green, K. Emery, Y. Hishikawa, W. Warta and E.D. Dunlop, Solar Cell Efficiency Tables (Version 39), *Prog. Photovoltaics* **2012**, *20*, 12-20. https://doi.org/10.1002/pip.2163

[3] O. Almora, D. Baran, G.C. Bazan, C. Berger, C.I. Cabrera, K.R. Catchpole, S. Erten-Ela, F. Guo, J. Hauch, A.W.Y. Ho-Baillie, T.J. Jacobsson, R.A.J. Janssen, T. Kirchartz, Y. Li, M.A. Loi, R.R. Lunt, X. Mathew, M.D. McGehee, J. Min, D.B. Mitzi, M.K. Nazeeruddin, J. Nelson, A.F. Nogueira, U.W. Paetzold, N.-G. Park, B.P. Rand, U. Rau, H.J. Snaith, E. Unger, L. Vaillant-Roca, H.-L. Yip and C.J. Brabec, Device Performance of Emerging Photovoltaic Materials (Version 1), *Adv. Energy Mater.* **2021**, *11*, 2002774. https://doi.org/10.1002/aenm.202002774