Supporting Information

On Pyrene-Fullerene Interaction and its Effect on the Behaviour of Photovoltaic Blends

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Digital filtering of LEPR data

The filtering procedure of the *normalized* decay data $\{(y_k,t_k)\}_k$ is a combination of simple exponential (ES) and smooth transition exponential smoothing (STES),[S1] to avoid excessive data distortion at short acquisition times when the decay is fastest and few data points are available. The smoothing aims to reduce the noise at long acquisition time, improving the detail in the estimation of the deep traps DOS features. To illustrate the procedure, let f_k be the k-th filtered point from the original data $\{y_j\}_j$; both ES and STES are based on the relation:

$$f_k = f_{k-1} + \beta\cdot\Delta_k, \qquad 0< \beta<1 \tag{S1}$$

where $|\Delta_k| = |y_k - f_{k-1}|$ may be interpreted as a "distance" between original and filtered data. The choice of the parameter β is peculiar of the ES and STES methods.

In ES we choose $\beta = 1- \exp[-(T/\tau_{ES})]$; this value is defined (once and for all) from the constant delay between successive data points (*dwell time*) $T = t_k - t_{k-1}$ and the user defined *time constant* τ_{ES} (usual values range between 0.01 and 0.2).

In STES the value of β is dependent on $|\Delta_k|$, thus adaptively changing as the smoothing proceeds. The adaptive algorithm $\beta_k = \beta(|\Delta_k|)$ is chosen to be "active" only within a (user defined) range of distances $(|\Delta_{min}|, |\Delta_{max}|)$ so that β varies in an interval $\delta\beta = \beta_{max} - \beta_{min} < 1$; figure S1 illustrates the concept. Note that the actual functional form $\beta = \beta(|\Delta_k|)$ is not necessarily linear. For our purposes, we modify equation (S1) to:

$$f_k = f_{k-1} + 2\cdot\beta_k\cdot\Delta_k \tag{S2}$$

and choose:

$$\beta_k = \beta_0 + (1-\varepsilon_k)\cdot\delta\beta, \qquad \text{(S3)}$$

$$\varepsilon_k = \{1+\exp[(|\Delta_k| - \Delta_c)/\tau_{STES}]\}^{-1}, \qquad \text{(S4)}$$

where $\Delta_c = (|\Delta_{max}| - |\Delta_{min}|)/2$ and the user-defined time constant τ_{STES} is introduced; the functional form $\beta = \beta(|\Delta_k|)$ is illustrated in figure S1. We apply STES to the initial part of the decay only, up to a few seconds, and choose the filtering parameters to provide a smooth transition to ES. An example of application is shown in Figure S2: the results obtained by filtering the initial part of the decay with the two methods (ES, STES) are evidently different, in favour of STES.

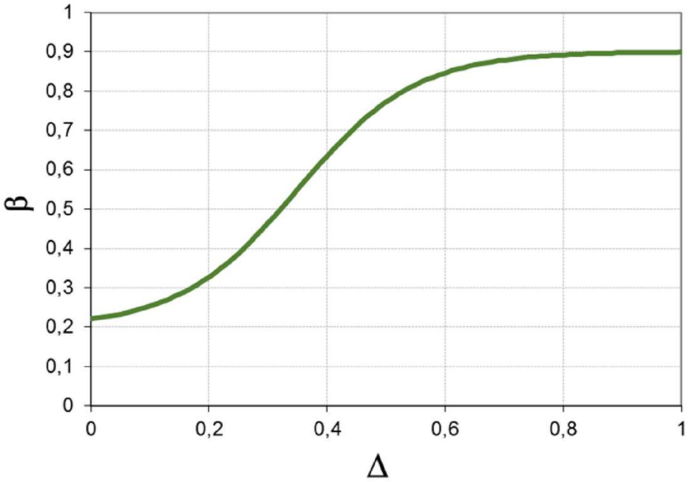
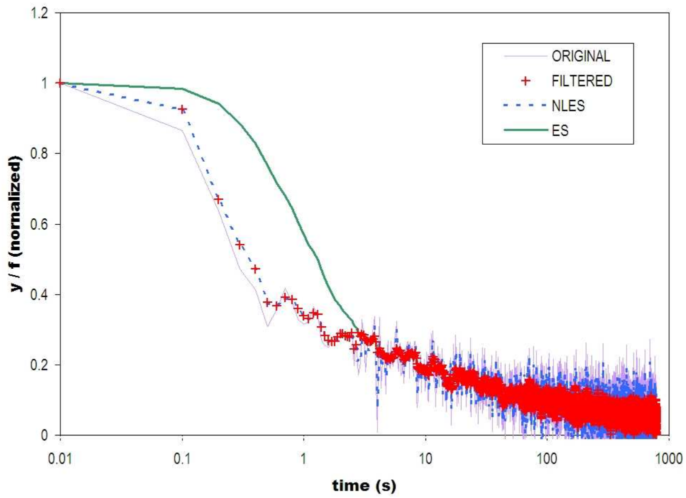


Figure S1. Functional form of the adaptive value $\beta = \beta(|\Delta_k|)$ used in the calculations. In this example, $|\Delta_{max}| = 0.9$, $|\Delta_{min}| = 0.2$, τ_{STES}=0.1.



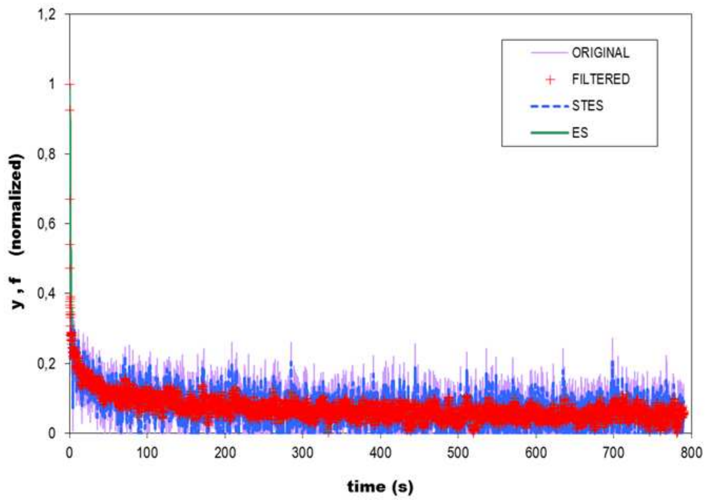


Figure S2. Digital filtering of a LESR decay using STES in the initial part (up to 2.8 s) and ES for the remaining part of the decay. The time axis is in log scale (top) and linear scale (bottom). STES filtering allows a moderate data smoothing with no significant deviation from the original data, while ES (useful for smoothing the long-time decay) substantially deviates from the initial points.

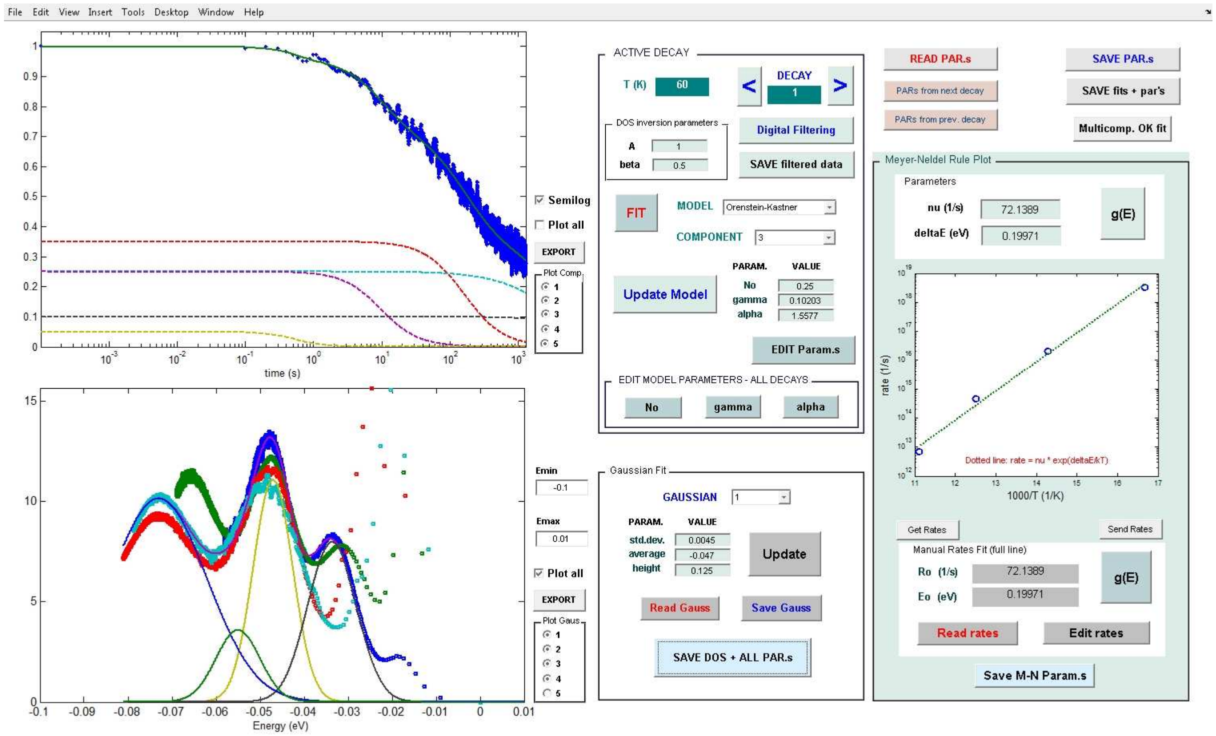


Figure S3. A screenshot of the GUI designed for data processing under MATLAB®. Left side: plots of a fitted decay and complete DOS reconstruction; right side: Meyer-Neldel Rule applied for DOS alignment (for details, see Ref.15 of the main text).

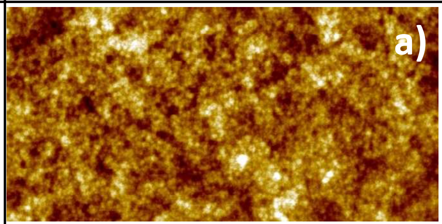
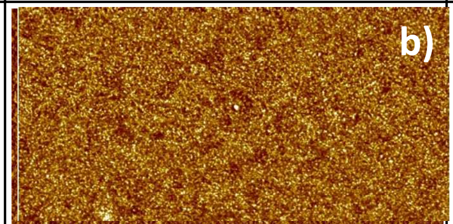
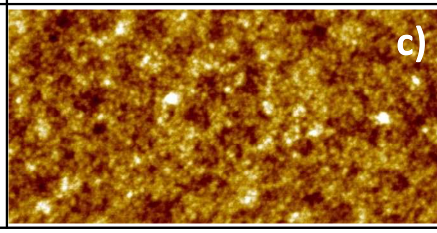
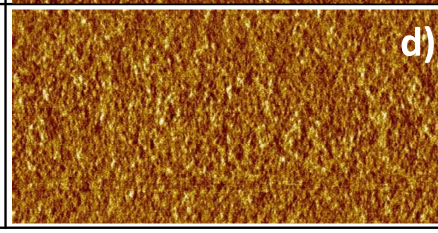
Blend	Height	Phase	R_q (nm)
PTB7:PyBB:C_{60} 1:2 w/w			0.83
PTB7:PyBB:C_{60} 1:3 w/w			0.89

Figure S4. AFM images (2 μm x 1 μm) of PTB7:PyBB:C_{60} blends, deposited onto ITO/PEDOT:PSS substrates in different PTB7:C_{60} weight ratios: a) and b) 1:2 w/w; c) and d) 1:3 w/w. PyBB:C_{60} 1:1 mol/mol in both cases.

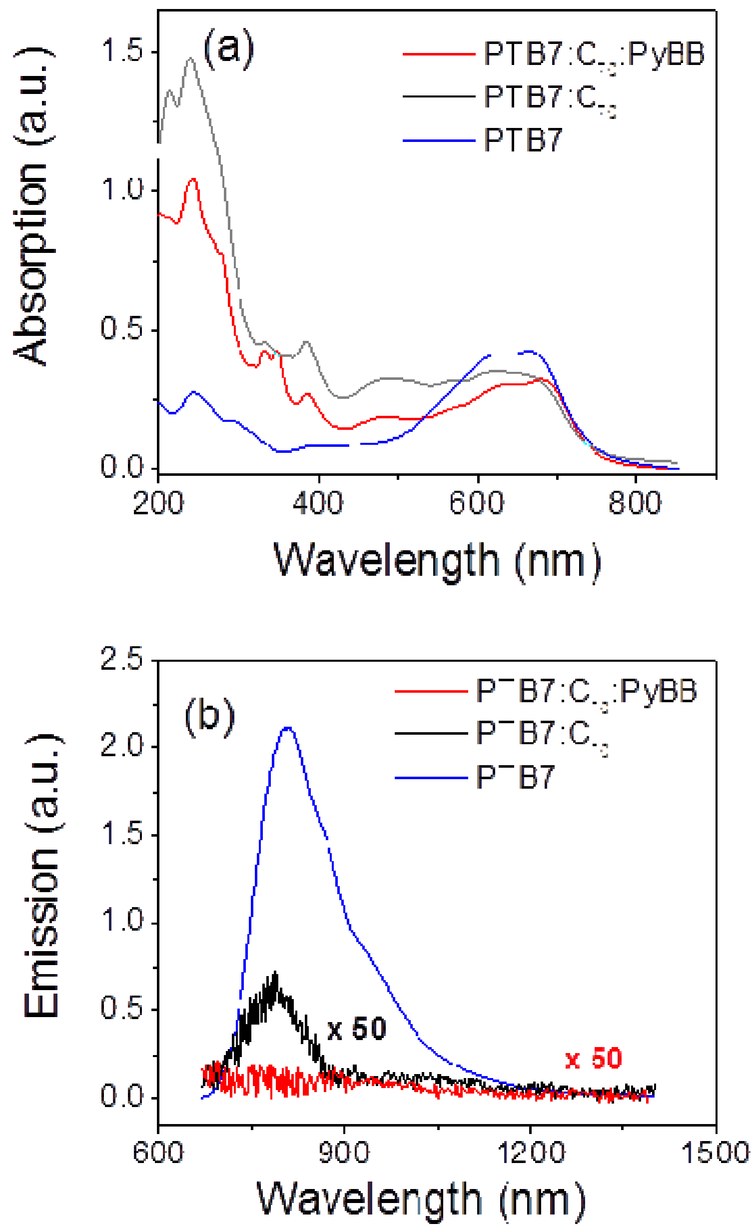


Figure S5. Absorption (a) and emission (b) of PTB7:C_{70}:PyBB (red), PTB7:C_{70} (black), and PTB7 (blue) films. The blends were prepared in 1:1 PTB7:C_{70} weight ratio. PyBB:C_{70} 1:1 mol/mol. Excitation wavelength 620 nm.

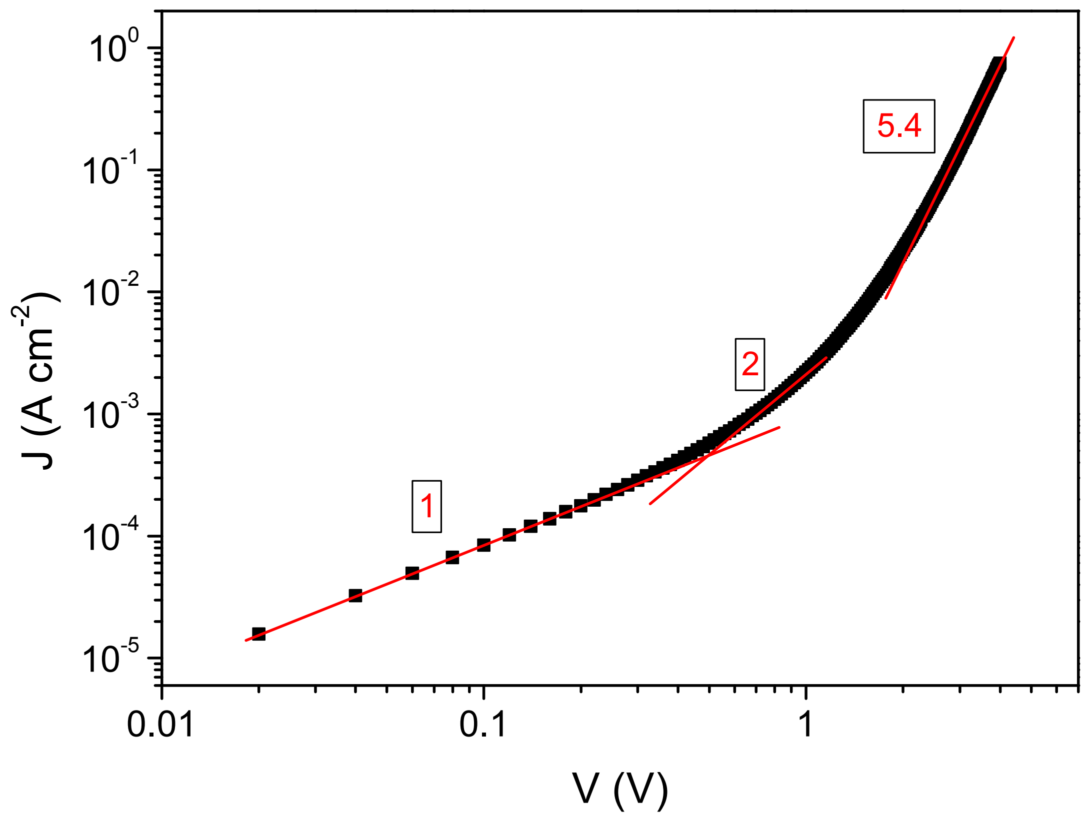


Figure S6. Current-voltage curve of an electron-only PTB7:PyBB:C_{60} device, prepared with a PTB7:C_{60} weight ratio of 1:3 and a PyBB:C_{60} molar ratio of 1:1. The lines indicate the linear fits to the experimental data. The slopes are indicated in the figure.

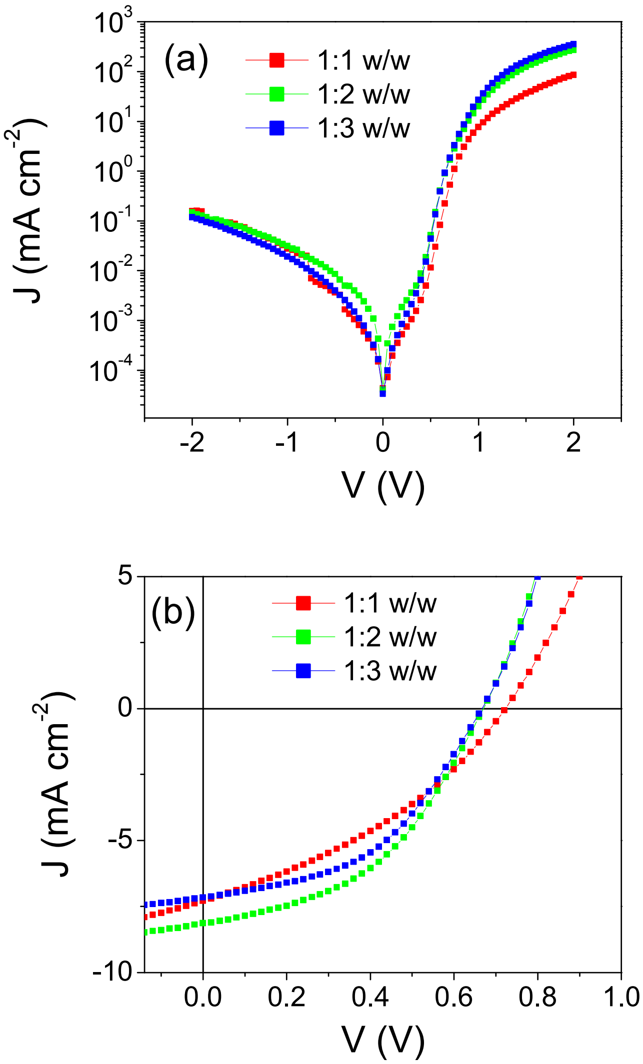


Figure S7. *J-V* characteristics in the dark (a) and under 100 mW cm^{-2} AM1.5G irradiation (b) for PTB7:PyBB:C_{70} solar cells, prepared with different PTB7:C_{70} weight ratios (shown in the figure) and with 1:1 molar ratio for PyBB:C_{70}.

REFERENCES

S1. Taylor, J.W. Smooth Transition Exponential Smoothing. *Journal of Forecasting* **2004**, *23*, 385-394.