Supporting Information

Interplay between long range crystal order and short range molecular interactions tunes carrier mobility in liquid crystal dyes

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Powder XRD pattern of FPPTB

The unit cell of FPPTB was determined from XRD studies on single FPPTB crystals, as described in the main text. The powder XRD pattern of FPPTB was calculated from the unit cell parameters using the freeware *Mercury*.

Figure S1 shows normalized simulated (red line) and experimental (black line) XRD patterns. The most prominent peaks are labelled. There is good agreement between the simulated and experimental XRD patterns.

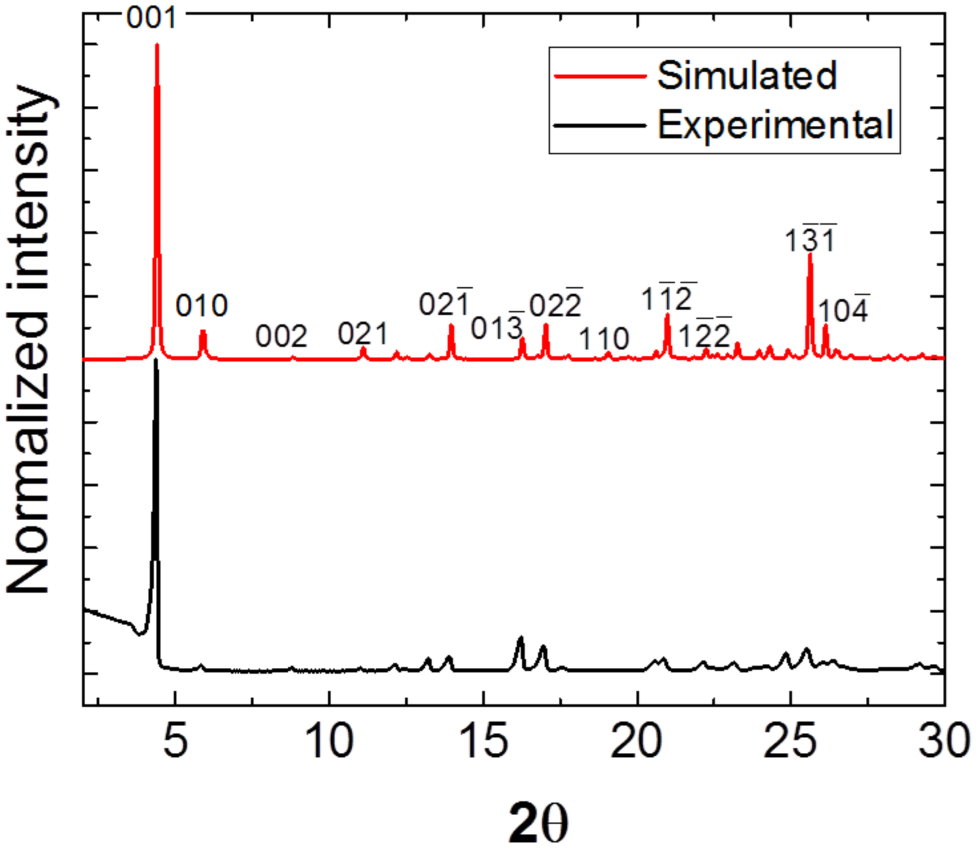

Figure S1: Simulated (red line, top) and experimental (black line, bottom) powder XRD pattern of FPPTB.

Electrical characteristics of FPPTB diodes

Extraction of device resistances from impedance data

The device resistances can be extracted from the Nyquist plot of the impedance data in a straight forward manner. An example is shown in **Figure S2** for FPPTB diodes prepared with FPPTB annealed at 250 ^{o}C. The total device resistance **R** is given by the maximum value of Z' (the real component of Z, i.e. the resistance). Series resistances $\mathbf{R_s}$ will shift the spectra towards higher values of Z' on the real axis. This is illustrated with a dotted line (not part of the measured data, but as a guide for the eye).

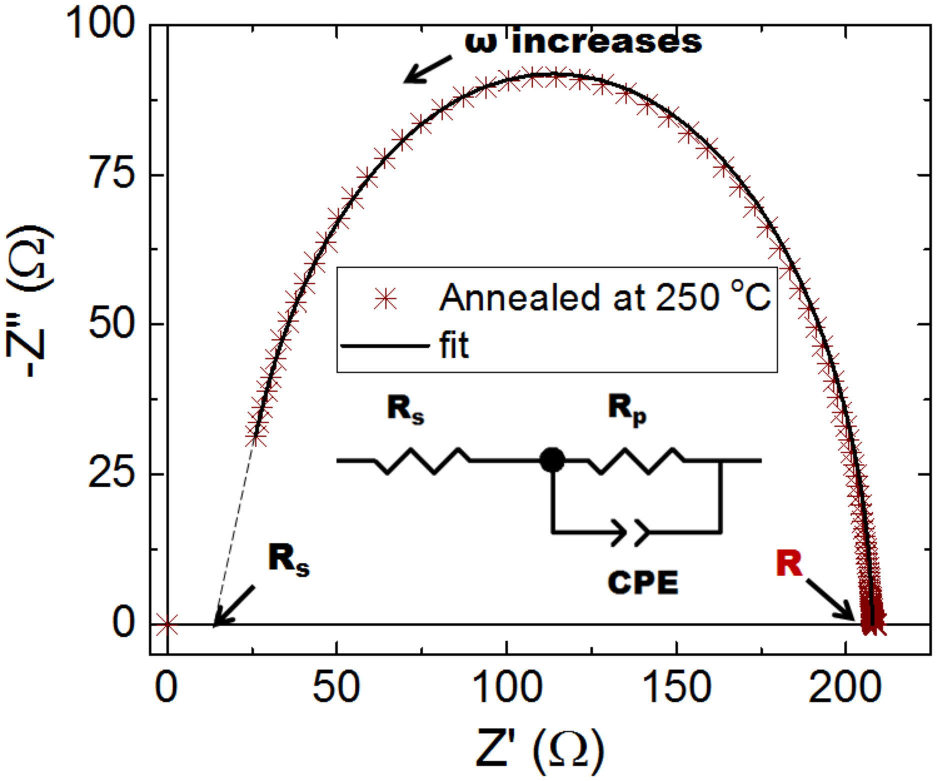

Figure S2: Nyquist plot (-Z" versus Z') of impedance data taken over a frequency range between 1 MHz and 10 Hz**)** for a diode prepared with FPPTB annealed film at 250 ^{o}C. The solid line shows the simulation using the equivalent circuit described in the main text. The dashed line is intended as a guide for the eye to demonstrate the shift of the frequency dependent data along the real axis. The series resistance $\mathbf{R_s}$ and total device resistance **R** are labelled.

The total device resistance **R** is a combination of the resistance contributions from $\mathbf{R_s}$ and $\mathbf{R_p}$-**CPE**. The values of the FPPTB film resistance, $\mathbf{R_p}$, were extracted from the data using the equivalent circuit model in **Figure 8** and **Figure S2**.

Relation of R_p to conductivity and mobility

The values of $\mathbf{R_p}$ from the circuit model are plotted together in **Figure S3** with the values of conductance **G** (**G = 1/$\mathbf{R_p}$**) versus annealing temperature.

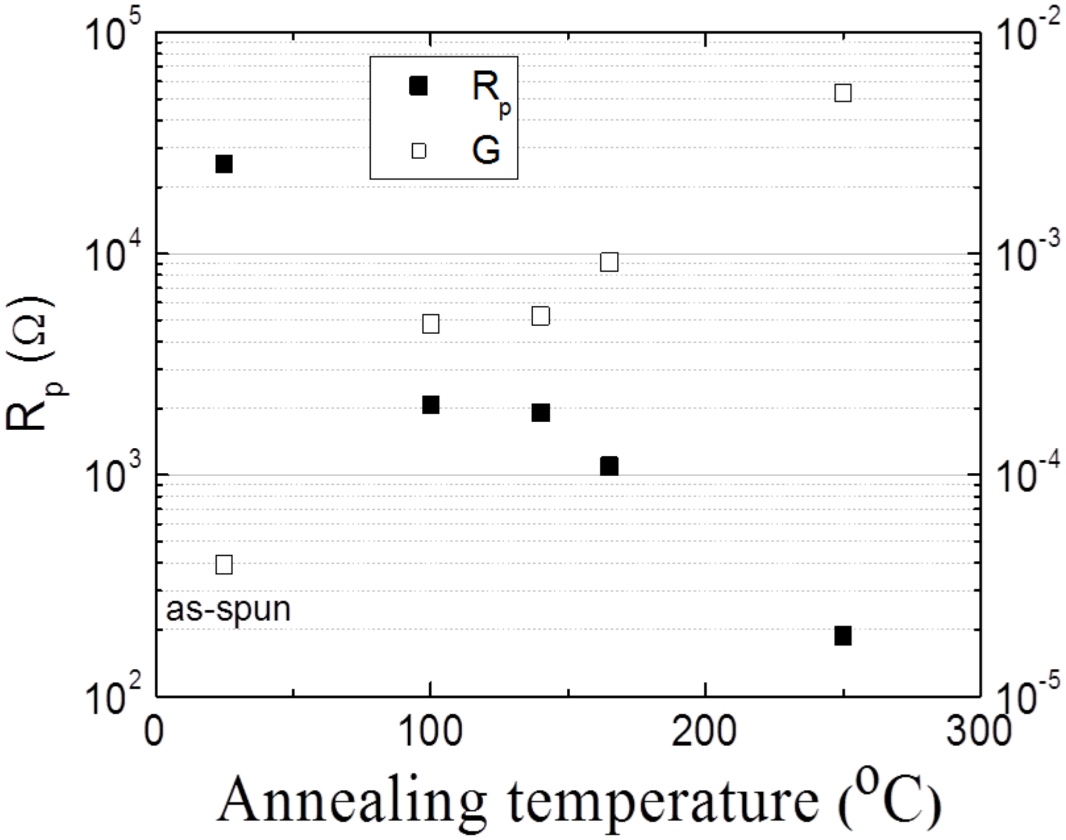

Figure S3: Resistance $\mathbf{R_p}$ and Conductance **G** versus annealing temperature.

The conductance **G** is related to carrier mobility **μ** according to

$$\frac{G}{A} = \sigma = nq\mu$$

Where **A** is the active area of the diode, **σ** is the conductivity**,** **n** is the carrier density and **q** is elementary charge. Note that we consider only hole transport in this discussion.

Assuming that the density of holes **n** is the same for all diodes at the same applied voltage

$$nq = constant$$

$$G \propto \mu$$

This means that changes in FPPTB resistance/conductivity are consistent with changes in carrier mobility. The conductance values extracted from the model are compared to the mobility values extracted from the **–Im Z** versus frequency spectra (**Figure 9**). Indeed we observe that conductance **G** and hole mobility **μ** follow the same trend with annealing temperature, **Figure S4**. Both values increase over two orders of magnitude from measurements taken on as spun films to measurements taken on FPPTB films annealed at 250 °C.

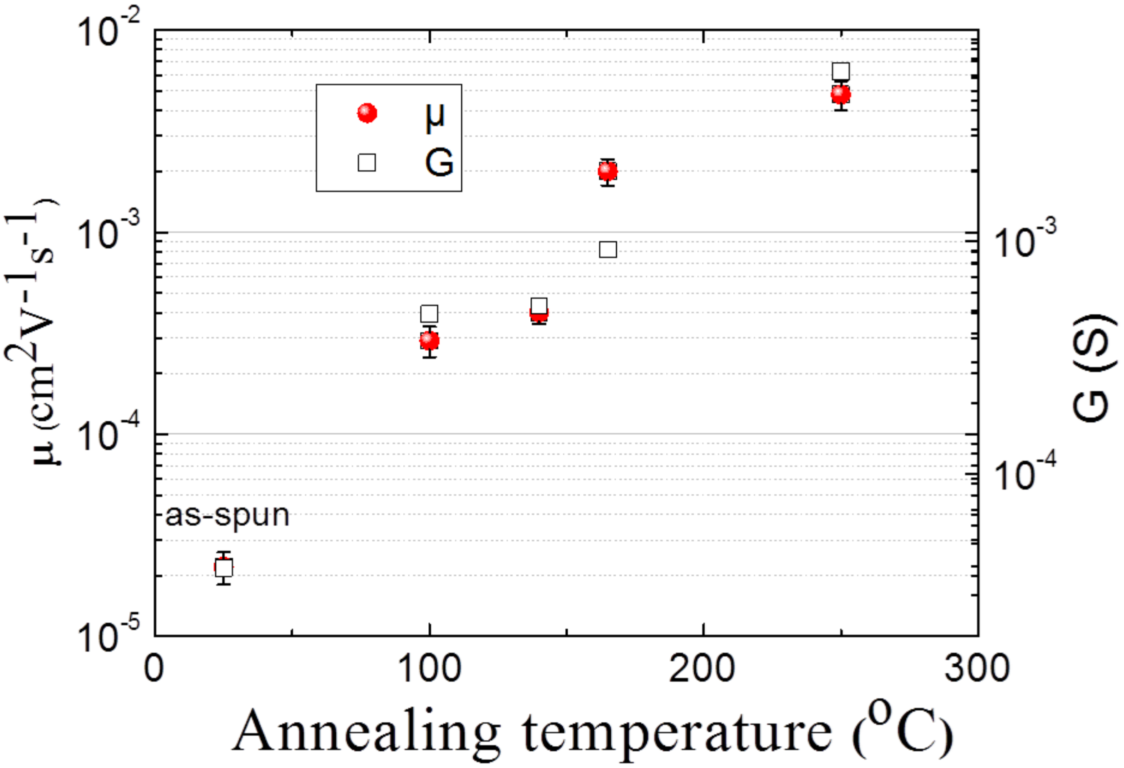

Figure S4: Hole mobility **μ** and Conductance **G** versus annealing temperature.