Electronic Supplementary Information for

Electron transporting organic materials with an exceptional large scale homeotropic molecular orientation

Huan Zhao\textsuperscript{a}, Zhiqun He\textsuperscript{a}, Min Xu\textsuperscript{a}, Chunjun Liang\textsuperscript{a}, Sandeep Kumar\textsuperscript{b}

\textsuperscript{a} Key Laboratory of Luminescence and Optical Information, Ministry of Education, Institute of Optoelectronic Technology, Beijing Jiaotong University, Beijing 100044, PR China;

\textsuperscript{b} Raman Research Institute, C.V. Raman Avenue, Bangalore 560 080, India
1. Homeotropic alignment of AQ6 on different substrates

Homeotropic alignments of hexa(hexyloxy)anthraquinone (AQ6) specimen have been carried out on a variety of substrates ranging from ITO coated glass, glass slides (or cover slips) and quartz surfaces. Figure S1 shows additional alignment images of AQ6 films on glass cover slips and on quartz substrates. It can be seen that the materials have been homeotropically aligned and the birefringence was disappeared with cross-polarised optical microscope (Figure S1(a) and (c)). Figure S1(b) and (d) demonstrated the images when the crossed polarisers were pulled out in order to see the film surfaces.

![Figure S1](image)

Figure S1. Optical microscopy images taken from AQ6 specimens at room temperature, which were previously aligned homeotropically on a glass cover slip (a) and (b) as well as on a quartz (c) and (d). [(a) and (c) with cross-polarizers; (b) and (d) without cross-polarizers. Scale bars represent 100 μm].

2. Homeotropic alignment of AQ6 at different thickness

Homeotropic alignments of hexa(hexyloxy)anthraquinone (AQ6) specimen having a variety of film thickness were also investigated with thicknesses ranging from ~350 nm to ~4 μm, which are the two extremes at thicker or thinner ends. Figure S2 shows the alignment of the film thicknesses of 350 nm and 4 μm on ITO substrates prepared with a cooling rate of 5 °C/min. It can be seen that within a 350 nm thick film, a uniformly homeotropic alignment was formed on a large scale, but the film became discontinued and formed many de-wetting zones [Figure S2 (a) and (b)]. If the film thickness was
over 4 μm, many highly birefringent defect regions began to show up and the film appeared to be less uniform [Figure S2 (c) and (d)]. However, within the range of ~350 nm to ~4 μm, the homeotropic alignments are generally uniform.

Figure S2. Optical microscopy images of AQ6 specimens cooled at 5 °C/min from the isotropic state with different thickness: 350 nm for (a) and (b), or 4 μm for (c) and (d) on thick glass slides at room temperature. [(a) and (c) without cross-polarizers; (b) and (d) with cross-polarizers condition. Scale bars represent 100 μm].

3. Calculation of electron carrier mobility from the J-V measurement

Electron carrier mobility was carried out according to the equation S1 (equation 2 in the manuscript)

\[ J_{SCLC} = \frac{9}{8} \varepsilon_0 \varepsilon_r \mu_0 \exp(0.891 \gamma \sqrt{\frac{V}{L}}) \left( \frac{V^2}{L} \right) \Theta \]  

(S1)

where \( J \) is the current density, \( V \) is the applied voltage, \( \varepsilon_0 \) is the vacuum permittivity, \( \varepsilon_r \) is the dielectric constant of the material, \( L \) is the film thickness, \( \mu \) is the charge carrier mobility and \( \Theta \) is a factor less than unity which takes account of possible effects, such traps and contacts. If defines electric field, \( F = \frac{V}{L} \), then the above formula can be re-written into,

\[ J = \frac{9}{8} \varepsilon_0 \varepsilon_r \mu_0 \Theta \exp(0.891 \gamma \sqrt{F}) \left( \frac{F^2}{L} \right) \]  

(S2)
i.e., \[ \frac{J}{F^2} = \frac{9}{8} \frac{e \varepsilon_0 \varepsilon_0 \Theta}{L} \exp(0.891 \gamma \sqrt{F}) \] or \[ \ln \left( \frac{J}{F^2} \right) = \ln \left( \frac{9}{8} \frac{e \varepsilon_0 \varepsilon_0 \Theta}{L} \right) + 0.891 \gamma \sqrt{F} \] (S3)

In order to calculate the mobility, a diagram of \( \ln \left( \frac{J}{F^2} \right) \) versus \( \sqrt{F} \) can be plotted. It is then able to obtain a slop of 0.891\( \gamma \) and an intercept of \( \ln \left( \frac{9}{8} \frac{e \varepsilon_0 \varepsilon_0 \Theta}{L} \right) \) (when \( \ln \left( \frac{J}{F^2} \right) \to 0 \)). The \( \mu_0 \) can be evaluated from the intercept and the \( \mu \) is then obtained from Poole-Frenkel expression, \[ \mu = \mu_0 \exp(0.891 \gamma \sqrt{F}) \]. In current work, a plot of \( \ln \left( \frac{J}{F^2} \right) \) versus \( \sqrt{F} \) of current-voltage measurement from the AQ6 electron-only devices before and after homeotropic alignment is shown in Figure S3. The equation is fulfilled in the high field range where space charge limited current was dominated. If non-ohmic contact is not considered (\( \Theta = 1 \)) and we assumes \( \varepsilon_r \sim 3 \) for AQ6, the mobility can then be obtained.

![Figure S3. A \( \ln (J/F^2) \) vs \( \sqrt{F} \) plot of current-voltage measurement of AQ6 electron-only devices before and after homeotropic alignment.](image)

References: