Supporting_Information

Anisotropic growth of organic semiconductor based on mechanical contrast of pre-patterned monolayer

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1. Molecular structure of perylene.

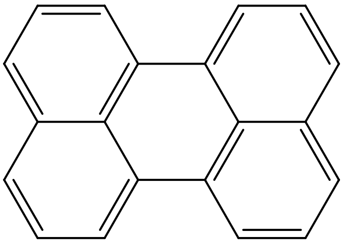

Fig. S1. Molecular structure of perylene.

2. Isotropic diffusion of perylene film on pure condensed and pure expanded DPPC monolayer.

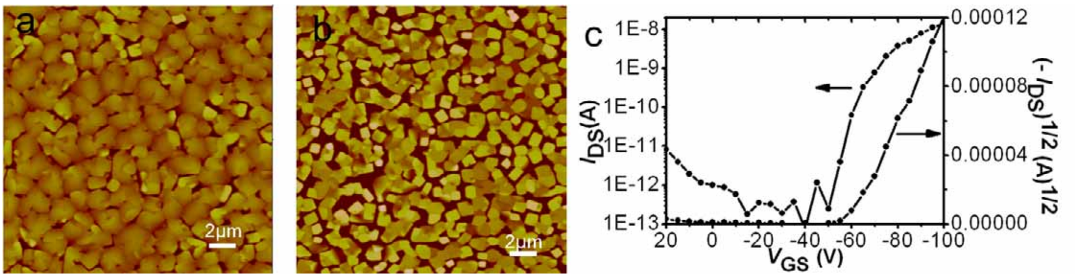

Fig. S2. AFM images of 130 nm perylene film on pure LE and LC phase of DPPC monolayer: (a) LE phase; (b) LC phase. (c) Transfer characteristics of drain current versus gate voltage on LE phase, the mobility in the saturation regime is $2.74\times10^{-5} cm^2\ V^{-1}\ s^{-1}$*, while there is almost no conductivity on the LC phase monolayer. The pure condensed DPPC monolayer is prepared at the conditions of 30 mN/m, 2 mm/min, and room temperature in subphase. The pure expanded DPPC monolayer is prepared at the conditions of 2 mN/m, 60 mm/min, and 29 ℃ in subphase.*

3. Molecular dynamics (MD) simulations on the diffusion of perylene on DPPC films.

The MD simulations were conducted in GROMACS 4.0.3[1] with the GROMOS96 53A6 force field (FF).[2] A silicon oxide slab (9.6 nm × 9.8 nm × 1.4 nm, α-Quartz) with the (1,0,-1) Miller plane as surface saturated by silanol groups was used as solid substrate. FF parameters were taken from the literature.[3] A thin layer of water (about 3000 molecules, SPC[4] model) with an equilibrated DPPC film (obtained by previous simulations of a monolayer on water compressed to the desired molecular area, DPPC FF parameter taken from literature[5]) is placed on top of the silicon substrate and equilibrated once more. The molecular area for LC phase simulation is 0.58 nm^2, for LE phase 0.77 nm^2. Phases were determined by order parameter of the DPPC chains. The topology for the perylene was obtained from the Dundee PRODRG 2.5 Server.[6] The simulations were conducted with constant volume and temperature (Berendsen thermostat[7] at 300 K) and the number of particles is not changing during simulation (NVT ensemble). Particle-mesh Ewald[8] is used for long range coulomb interactions and a cut off of 1.4 nm was applied for the short range interactions. Van der Waals settings included a shift function switching from 0.9 nm to a cut off of 1.2 nm. The bonds to hydrogen atoms were constraint using the LINCS algorithm.[9] A timestep of 1 fs was used. Four simulations with different start positions of the perylene molecule were performed for each phase. Snapshots of a typical simulation are shown in Fig. S3.

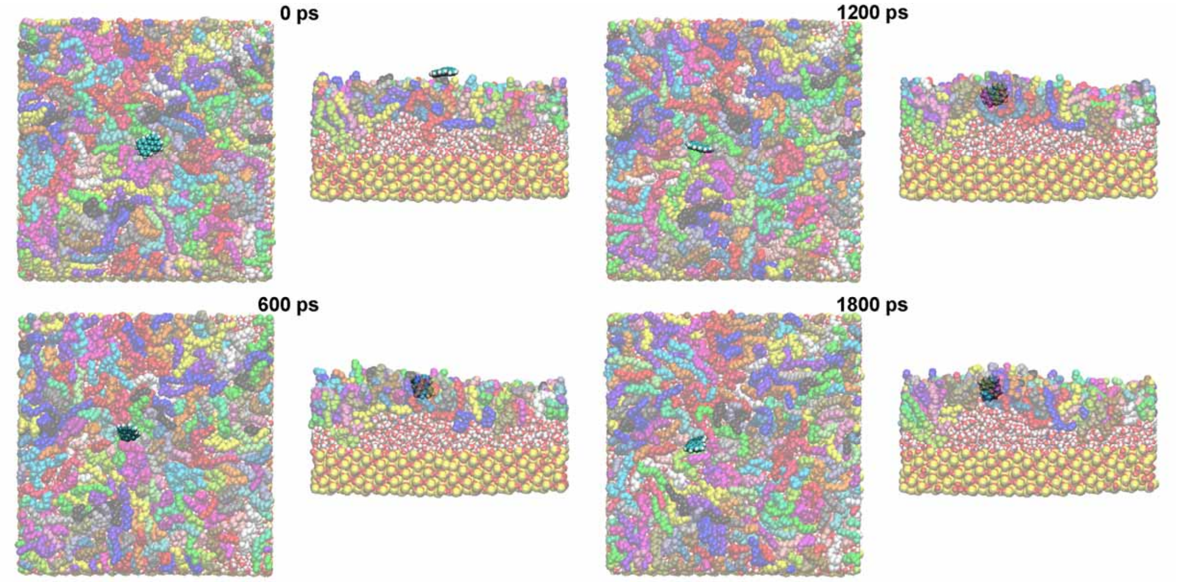

Fig. S3. Snapshots of a typical simulation of a perylene molecule diffusing on a LE-phase substrate at different times into the simulation (top and side view).

The mean square displacement (MSD) in the x-y-plane was calculated by the program g_msd of the GROMACS suite and averaged over the four simulations for each substrate (Fig. S4).

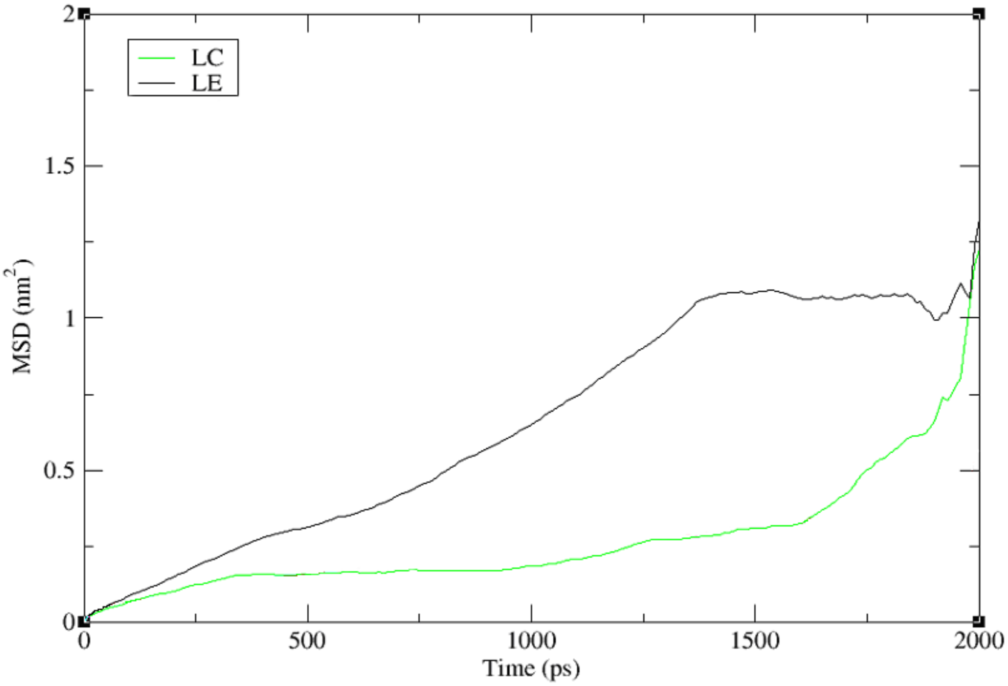

Fig. S4. MSD of perylene on LC and LE phases.

The diffusion constants of perylene on the different substrate phases were obtained by a linear fit to the MSD between 500 and 1500 ps (to avoid etch artifacts). The diffusion constants were found to be $(1.60 \pm 0.06)\ 10^{-6}\ \mathrm{cm^2/s}$ for LC phase and $(8.64 \pm 0.09)\ 10^{-6}\ \mathrm{cm^2/s}$ for the LE phase. The molecular mechanism behind the distinct difference in diffusion and the selective deposition on the different phases as revealed by the MD simulation arise from the immersion of the molecule into the hydro carbon chains and the variation of the film plasticity in the different phases. A detailed account of the findings by MD simulations for this and other systems of DPPC template guided deposition of organic molecules is in preparation for publication.

4. Discussion about the anisotropic mobility in the perylene film induced by DPPC stripes.

In polycrystalline materials, charge-carriers transport is most likely dominated by grain boundaries, which can trap and scatter the mobile charge carriers, thereby increasing the overall film resistance.[10] The effective mobility can be obtained from the grain boundary trapping model using the following formula.[11]

$$\mu_{eff} = \frac{\mu_G}{1 + (L_{GB}/L_G)(\mu_G/\mu_{GB})}$$

Here, μ_G is the effective mobility of the grains, L_{GB} is the average length of the grain boundaries, L_G is the average length of the grains, and μ_{GB} is the effective mobility of the grain boundaries. As shown in Fig. 3, the long grains along the stripes show fewer grain boundaries than that in the vertical direction.

This implies that the values of L_{GB} and L_G are quite different in the devices with parallel and vertical configurations, resulting in anisotropic behavior of the field effect mobility.

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