SUPPLEMENTARY INFORMATION

Engineering of a kinetically driven phase of phenoxazine by surface crystallisation

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Content

The Supplementary Information contains additional experimental results of drop casted thin-films from tetrahydrofuran solutions at high concentrations (Figure S1). This information complements the results depicted in Figure 2.

The grazing incidence X-ray diffraction pattern of a spin coated film is presented together with its calculated structure factors (Figure S2), more diffraction peaks of phenoxazine are visible than in Figure 4.

The result of the theoretical work in terms of molecular conformation is shown for the Molecular Dynamics calculations and for Density Functional Theory calculations (Figure S3). The structure factors of individual Bragg peaks obtained from GIXD experiments and calculated from Molecular Dynamics and DFT are shown in Figure S4.

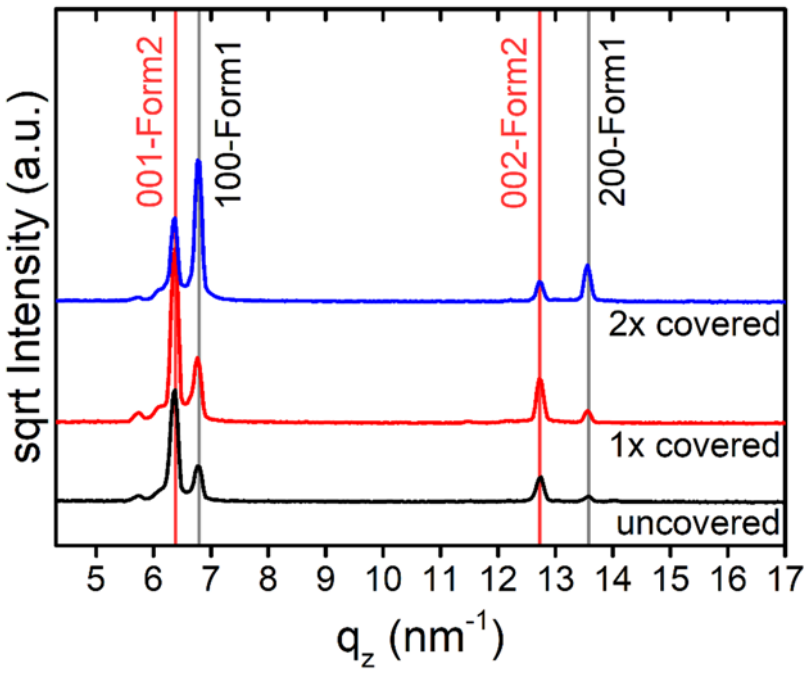

Figure S1: Specular XRD on phenoxazine crystallized on a silicon oxide surface. The deposition was prepared via drop casting from a 50 g/l tetrahydrofuran solution and different evaporation velocities, which were reached by covering the samples with no, one and two petri dishes. The curves are shifted for clarity.

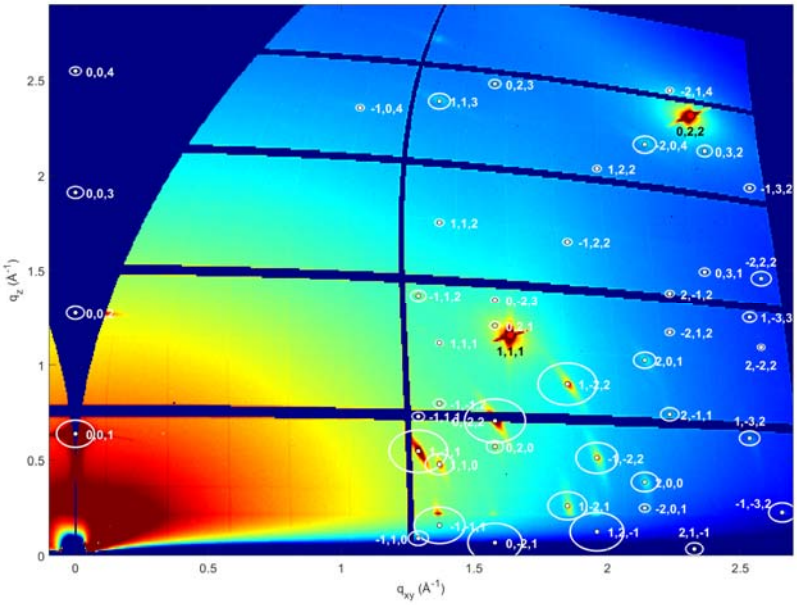

Figure S2: GIXD reciprocal space map obtained for a spin coated thin film from phenoxazine / tetrahydrofuran solution of 10 g/l. The white circles indicate the calculated diffraction peaks of Form 2; the area of the white rings correspond to the square of the absolute value of the structure factors.

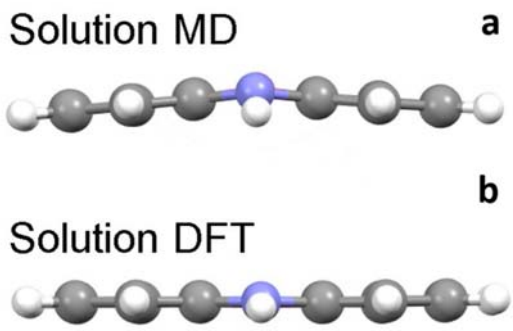

Figure S3: Bending of the phenoxazine molecule as resulted from (a) the molecular dynamics (MD) simulation or (b) the density functional theory (DFT) calculation.

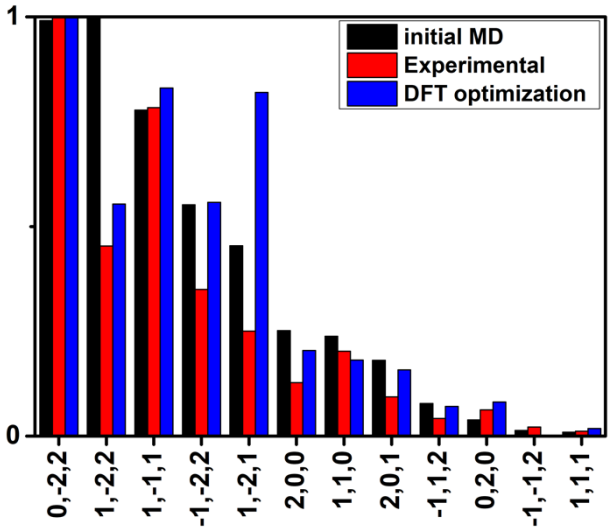

Figure S4: Comparison among the measured (red), the molecular dynamics (MD) simulated (black) and the density functional theory (DFT) optimized (blue) structure factors. The structure factors are normalized to the highest intensity.