Electronic Supplementary Material (ESI) for Materials Horizons.

Supplementary information

Comparison of Organic and Inorganic Layers for Structural Templating of Pentacene Thin Films

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Note 1

The AFM images of 20 nm CuI films grown on silicon, quartz and glass are presented in Figure S1. No significant differences in topography is observed which indicates CuI to be substrate independent.

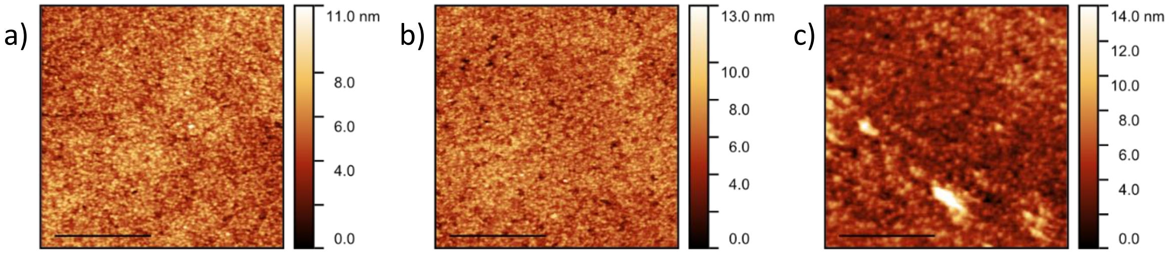

Figure S1: AFM images of 20 nm CuI films grown on **a)** silicon, **b)** quartz and **c)** glass. All scale bars are set to 2 µm.

Note 2

As mentioned in the main text, the 200°C CuI templated pentacene film is compared to literature pentacene powder patterns presented in Figure S2. Among all the literature patterns, no viable direct match with the 200°C CuI templated pentacene film pattern is found. However, the 2θ positions of the additional peaks of the 200°C CuI templated pentacene film are similar to those of the experimental powder pattern. Although none of the literature patterns provide a good comparison with the experimental pattern, the powder pattern (CCDC 665900)[1] is deemed to be the most valid fit to the best of our knowledge. This is due to similarities in the peak shape and intensity and successful comparisons with previous work[2]. A clear 2θ shift of approximately 1° to higher 2θ positions is observed between the experimental powder pattern and CCDC 665900 powder pattern, attributed to a possible variation in the lattice parameters. The structural properties of the various literature powder patterns presented here have been regularly redetermined suggesting the high possibility of the lattice parameter variation. An equivalent 2θ shift is observed for the three peaks of the CuI templated pentacene film compared to CCDC 665900 (Figure 2c). This is attributed to a compressive structural force due to the induced flat-lying orientation. Further experimental work will be conducted to determine the crystal structure of the experimental powder used as well as to refine the crystal structure of the templated films.

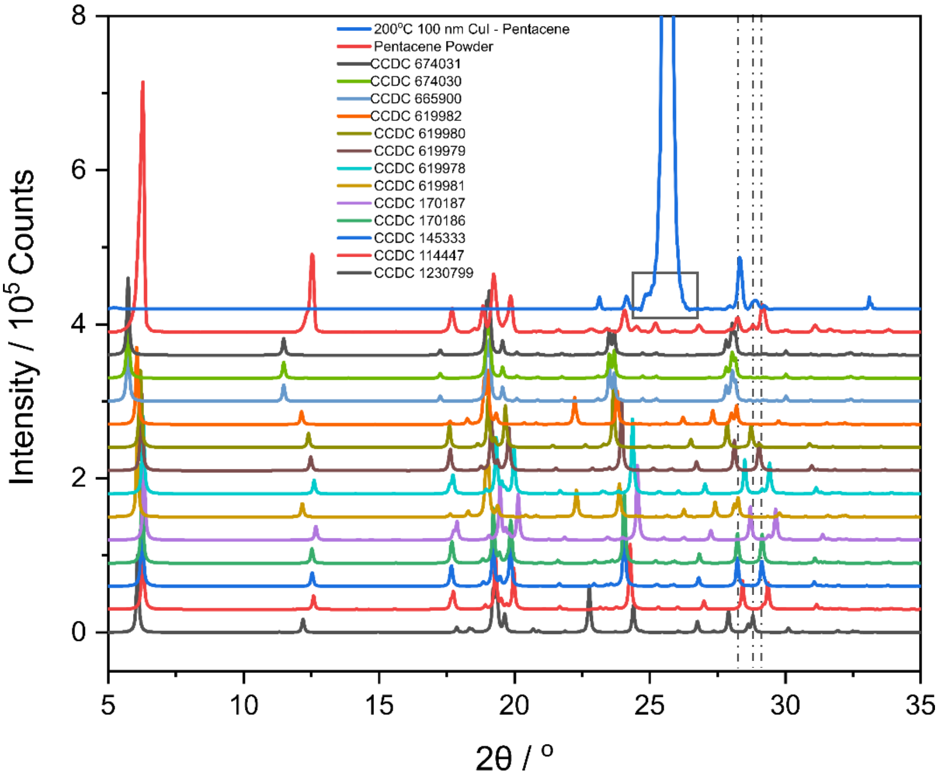

Figure S2: Comparison of the experimental diffraction patterns of pentacene powder and 200°C CuI templated pentacene film with all available literature powder patterns of pentacene.[1, 3-8]

Note 3

The SEM cross-section images of the templated pentacene films are presented in Figure S3. The images provide insight into the changes in morphology as a result of the introduction of the templating layers. Both the pure pentacene and PTCDA-templated pentacene samples present similar morphologies which agrees well with the top view images in Figure 1a and Figure 5a. The PTCDA-templated pentacene film cross-section is rougher than the other films due to the cleaving of the sample. For both pentacene films templated with CuI grown at different temperatures, grains appear to extend as platelets normal to the substrate, resulting in a higher roughness in comparison to those in Figure S3 a and b. This is due to the pentacene grain stacking axis rotating to a perpendicular alignment to the substrate surface.

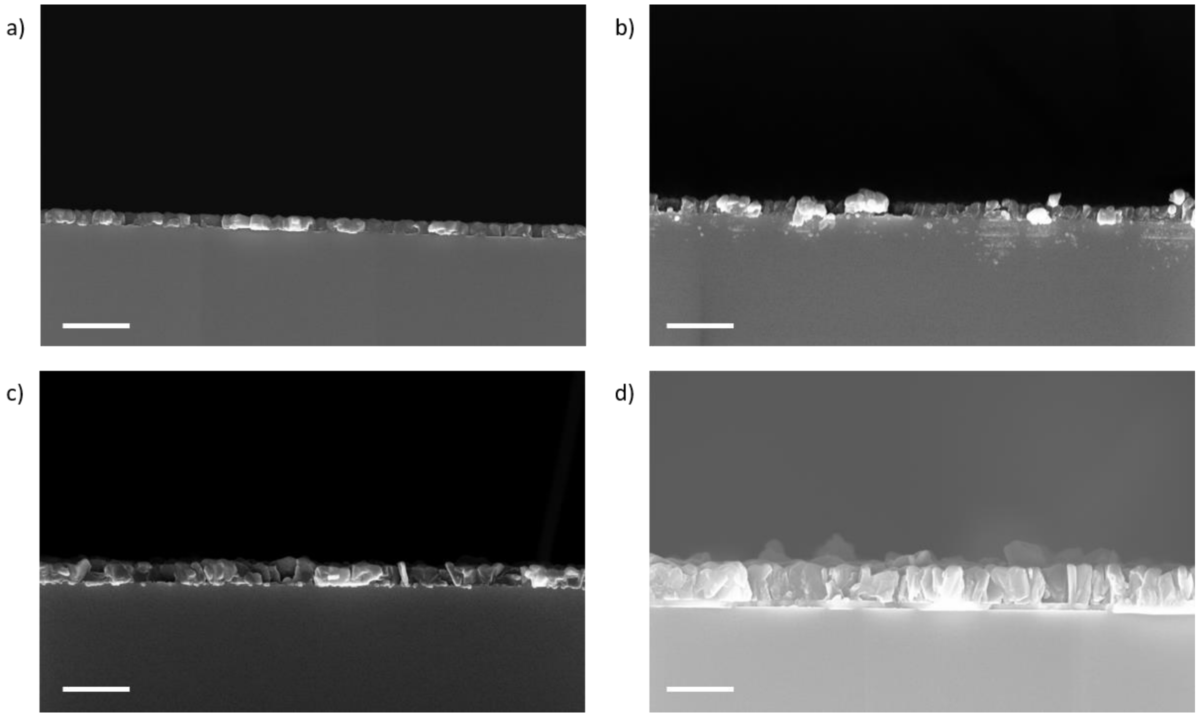

Figure S3: Cross section SEM images of a) 200 nm pentacene, b) 20 nm PTCDA - 200 nm pentacene, c) 20°C 20 nm CuI - 200 nm pentacene and d) 200°C 100 nm CuI - 200 nm pentacene on silicon. All scare bars are set to 1 µm.

Note 4

As mentioned in the main text, contact potential difference images of the pure pentacene, 200°C 100 nm CuI-templated pentacene and 200°C 100 nm CuI samples were taken and are presented in Figure S4. The topographical images of the films were taken simultaneously and are also presented to determine the presence of any influence the topography has on the measured V_{CPD}. For all three images (Figure S4a, b, c) presented, the contact potential is observed to be highly homogeneous throughout the entire image area regardless of any variation in height or roughness of the films. Thus, the topography of the films is found to have a negligible effect on the measured contact potential difference.

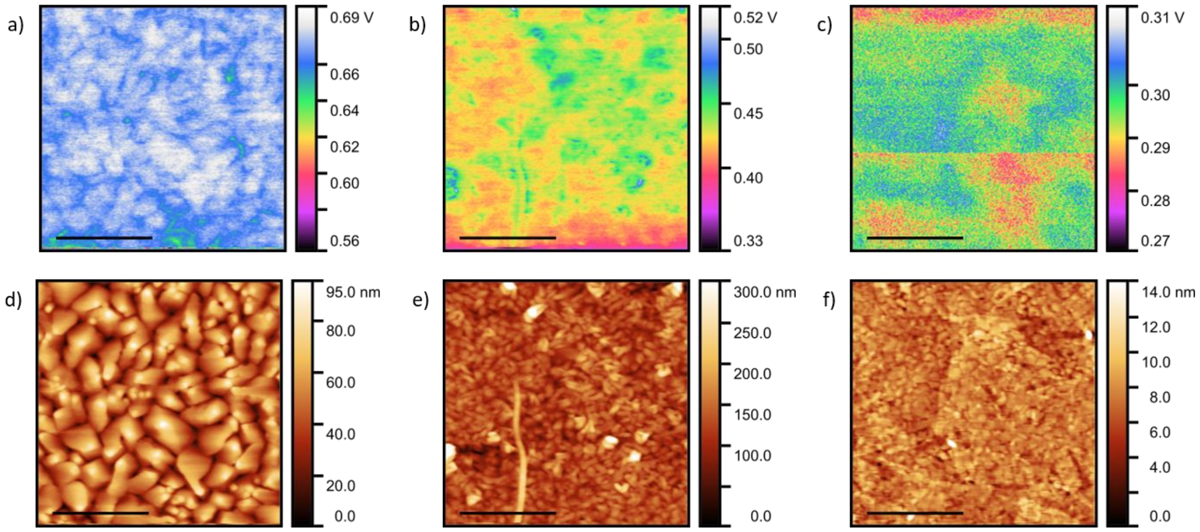

Figure S4: KPFM images of a) 200 nm pentacene, b) 200°C 100 nm CuI - 200 nm pentacene and c) 200°C 100 nm CuI. All scale bars are set to 2 µm.

Note 5

The UV-Vis spectra of the templated pentacene films and pure pentacene film are presented in Figure S6. An increase in absorption is observed for the 200°C 100 nm CuI-templated pentacene film which is deemed to be solely due to the intrinsic properties of pentacene with the spectra discussed in more detail in the main text

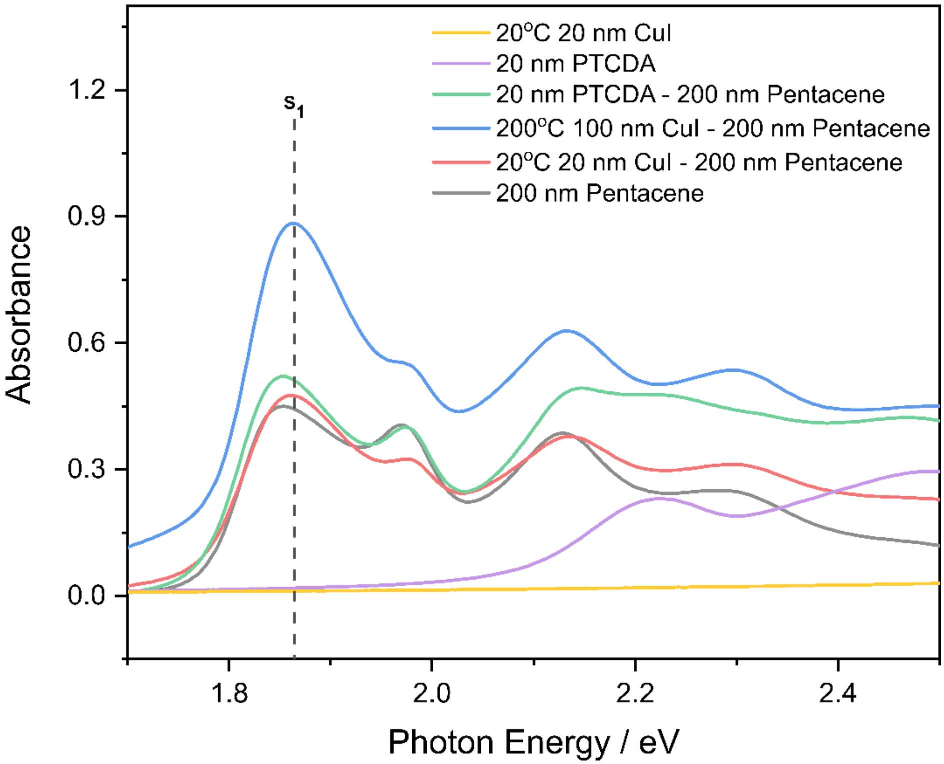

Figure S5: UV-Vis absorption spectra of 200 nm pentacene films deposited on 20 nm PTCDA, 20°C 20 nm CuI, 200°C 100 nm CuI and quartz. S_1 corresponds to the singlet-singlet transition and the peaks at higher energy correspond to the vibronic states of pentacene.

References

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