Supporting Information For

Temperature Dependent 2D Self-assembled Motif Transition of Copper-Phthalocyanine Derivates at Air/HOPG interface: An STM study

Yamin Wang^{a,b}, Hongbo Xu^{a,b}, HuanHuan Wang^a, Shouzhu Li^a, Wei Gan^{*a}, Qunhui Yuan^{*a}

^a Laboratory of Environmental Science and Technology, Xinjiang Technical Institute of Physics
& Chemistry; Key Laboratory of Functional Materials and Devices for Special Environments,
Chinese Academy of Sciences, Urumqi 830011, China. Fax: +86-991-3838957; Tel: +86-9913677875; E-mail: ganwei@ms.xjb.ac.cn and yuanqh@ms.xjb.ac.cn

^b University of Chinese Academy of Sciences, Beijing, 100049, P. R. China.

1. The procedure for the calculation of the Q^a/H^a ratio.

The calculation of the Q^a/H^a ratios in Table 1 and Table 2 in the main manuscript is based on the methods used in previous reports^[1,2]. The quartic and hexagonal domains are marked on the STM images by hand so that their areas can be presented as the number of pixels in each marked area, as shown in the figures in the second part of this supporting information. For one assembly film (one sample), normally several STM images with distinguishable quartic and/or hexagonal domains were obtained. The quartic and hexagonal areas from these STM images were summed up to get a Q^a/H^a ratio as one measurement. For each experimental condition at least 3 measurements (3 samples) were used and the Q^a/H^a values from these measurements were averaged to get the final Q^a/H^a ratio and its standard deviation. To be safe, all the standard deviations below 0.1 were marked as 0.1.

References:

- [1] T. Chen, W.-H. Yang, D. Wang and L.-J. Wan, Nat. Commun., 2013, 4.
- [2] M. O. Blunt, J. Adisoejoso, K. Tahara, K. Katayama, M. Van der Auweraer, Y. Tobe and S. De Feyter, J. Am. Chem. Soc., 2013, 135, 12068.
- 2. Typical STM images (three from more than ten for each case) of the CuPcOC₈ adlayer on HOPG surface obtained under different experiment conditions.



Figure S1. Typical STM images of the freshly prepared $CuPcOC_8$ adlayer formed under room temperature (25 ± 1 °C) on HOPG surface.



Figure S2. Typical STM images of the $CuPcOC_8$ adlayer stored for 3 days after the formation under room temperature.



Figure S3. Typical STM images of the $CuPcOC_8$ adlayer annealed at 55 °C for 30 minutes after the formation under room temperature.



Figure S4. Typical STM images of the $CuPcOC_8$ adlayer annealed at 75 °C for 30 minutes after the formation under room temperature.



Figure S5. Typical STM images of the $CuPcOC_8$ adlayer annealed at 90 °C for 30 minutes after the formation under room temperature.



Figure S6. Typical STM images of the freshly prepared $CuPcOC_8$ adlayer formed at 55 °C.



Figure S7. Typical STM images of the freshly prepared $CuPcOC_8$ adlayer formed at 60 °C.