

Supporting Information for

Positioning growth of NPB crystalline nanowires on PTCDA nano-crystal template

*Hong Wang^a, Haiping Lin^b, Xing Fan^b, Stefan Ostendorp^c, Yandong Wang^b, Lizhen Huang^b, Lin Jiang^b, Youyong Li^b, Gerhard Wilde^c, Harald Fuchs^a, Wenchong Wang^{*a} and Lifeng Chi^{*b}*

a Physikalisches Institut and Center for Nanotechnology (CeNTech), Universität Münster, 48149 Münster, Germany

b Jiangsu Key Laboratory for Carbon-Based Functional Materials & Devices, Institute of Functional Nano & Soft Materials (FUNSOM), Joint International Research Laboratory of Carbon-Based Functional Materials and Devices, Soochow University, 199 Ren'ai Road, Suzhou, 215123, Jiangsu, PR China

c Institut Für Materialphysik, Universität Münster, 48149 Münster, Germany

Experimental Section

NPB and PTCDA were purchased from Sigma-Aldrich and used without further treatment. Si (100) substrates with a 300 nm thermally grown oxide layer were purchased from Silicon Materials. Au patterns were fabricated through EBL technique and subsequently coated with 4 nm Cr as adhesion layer and 50 nm Au by thermal evaporation, followed by a lift-off of the poly (methyl methacrylate) (PMMA) resist.

Thereafter the pre-patterned substrates were brought into a vacuum chamber for the organic molecules deposition. The temperature of the substrate was measured by thermocouples, and the deposition rate was monitored by reading of a nominal thickness on a quartz microbalance. The samples were taken out of the chamber and cut into several pieces for further steps after deposition of PTCDA molecules. A part of them were put back in the chamber again for the subsequent deposition of NPB molecules.

The morphology and topography of the samples were characterized by SEM, AFM and Optical Microscopy. The AFM images were analyzed by WSxM software and a larger size AFM images in the main text with Z range are presented in Figure S9 and S10. XRD measurements were performed in a θ -2 θ configuration with a Siemens D5000 X-ray diffractometer. With the heavily doped silicon wafer and the 300 nm oxide layer serving as gate and insulator, respectively, field-effect characteristic measurements were performed with a Keithley 4200 in air at room temperature.

All theoretical calculations in this work were performed using Vienna ab initio simulation packages (VASP)^{1, 2} with the projector-augmented wave (PAW)^{3, 4} method. The Perdew–Burke–Ernzerhof (PBE)^{5, 6} functional is used for the exchange and correlation interaction between electrons. The plane wave cutoff for this system was set to 400 eV. The Brillouin zone was sampled by a 1x1x1 Monkhorst–Pack k-point sampling for structural optimizations. The criterion of convergence of energy is set to 1×10^{-4} eV. The internal coordinates of each system are fully optimized until the

residual Hellmann–Feynman forces are smaller than 0.02 e V/\AA . The variations in vdW contributions of atoms in local chemical environment were evaluated by the method of Tkatchenko and Scheffler (DFT-TS).⁷

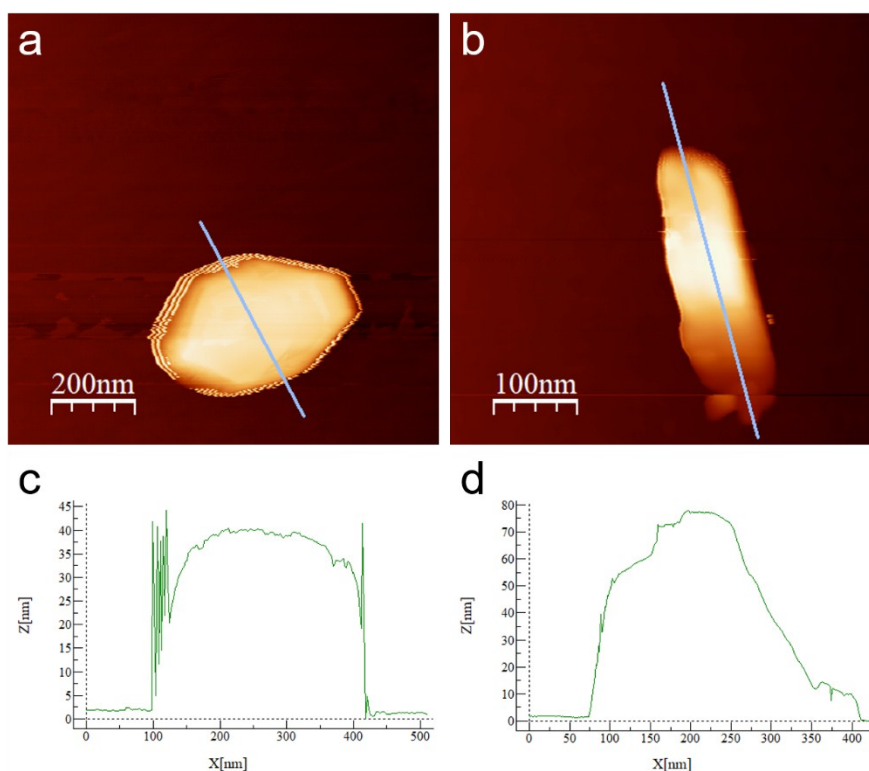


Figure S1. AFM images of (a) nano-sheet and (b) nano-rod PTCDA crystals and (c)-(d) corresponding profile curves of the lines marked in (a) and (b).

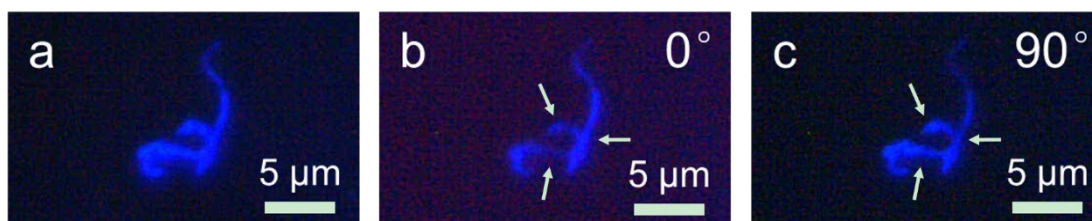


Figure S2. Fluorescence microscope images of NPB nanowires (a) without polarizer and with polarizer at a polarization angle of (b) 0° and (c) 90° . The images have large

variation in brightness of fluorescence under different conditions. Especially the brightness of the positions marked by white arrows change a lot by using different polarization angles.

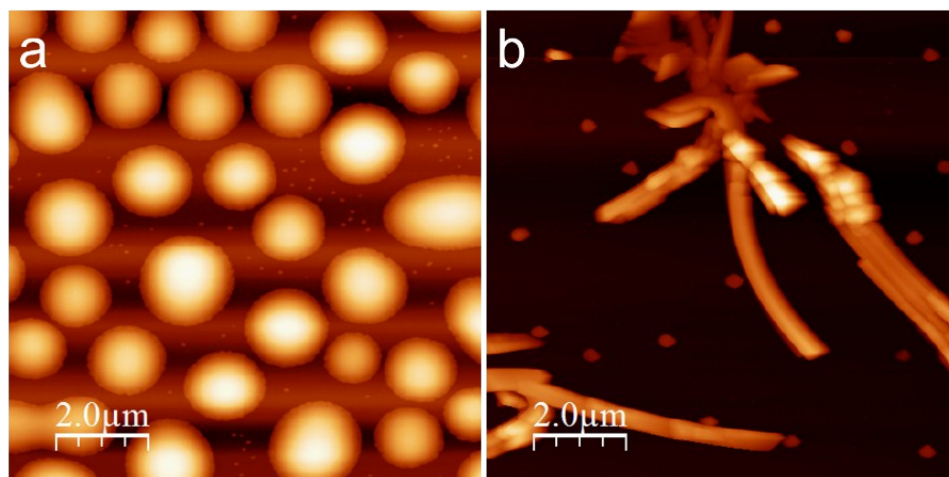


Figure S3. AFM images of (a) NPB islands on bare SiO₂ and (b) NPB nanowires grown on PTCDA nano-crystals/SiO₂.

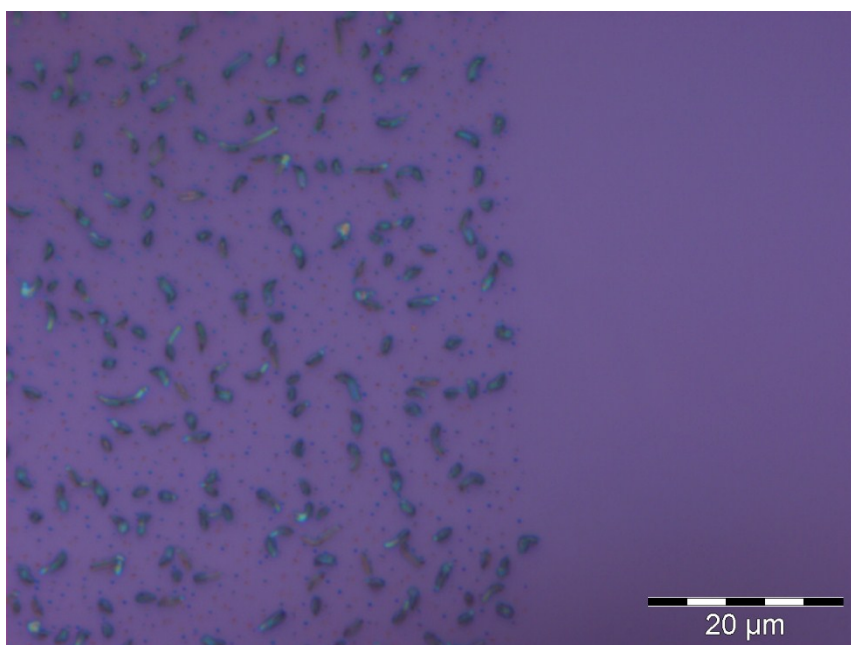


Figure S4. Microscope image of NPB deposited at the substrate temperature of 240 °C. Left part: with PTCDA nano-crystal, right part: without PTCDA nano-crystal. NPB forms crystals on SiO₂ surface in the presence of PTCDA nano-crystals, while no

aggregation of NPB molecules is detected on the bare SiO_2 . This confirms that NPB have stronger interaction with PTCDA (102) plane than that of NPB- SiO_2 .

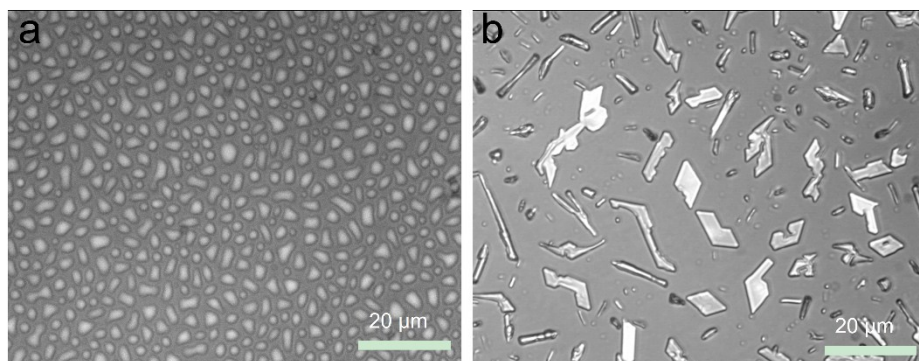


Figure S5. Optical images of 5, 11-Bis (triethylsilylethynyl) anthradithiophene (TES-ADT) deposited on (a) bare SiO_2 and (b) PTCDA / SiO_2 surface at elevated temperature. In comparison to dome-shaped amorphous islands on bare SiO_2 surface (a), TES-ADT micro-crystals with well resolved facets are obtained by presence the PTCDA nano-crystals (b).

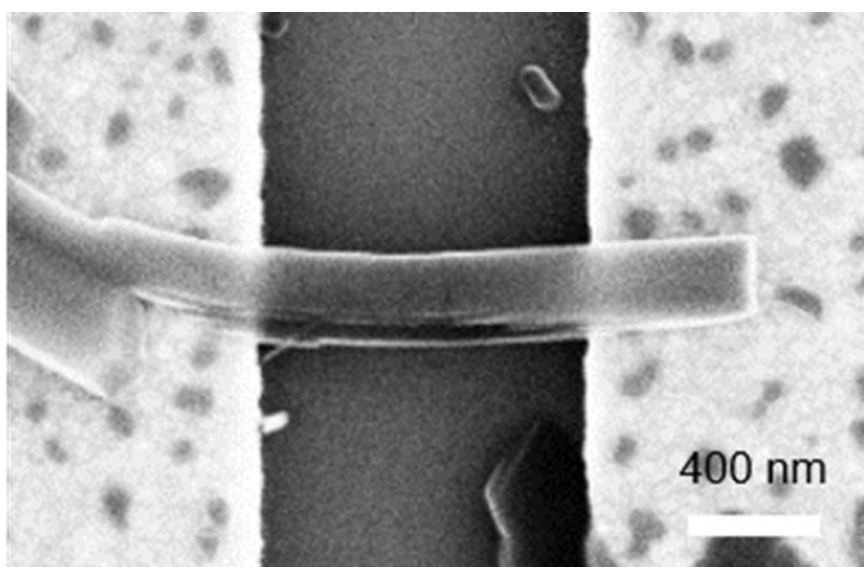


Figure S6. High resolution SEM image of a NPB nano-wire bridged source and drain electrodes.

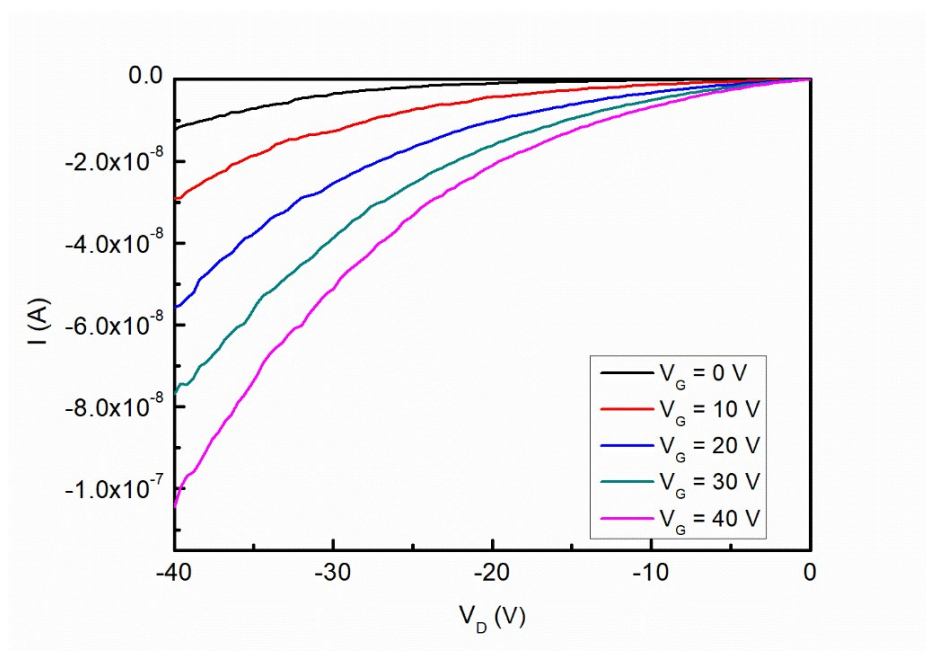


Figure S7. Output curves of a typical NPB nanowire OFET.

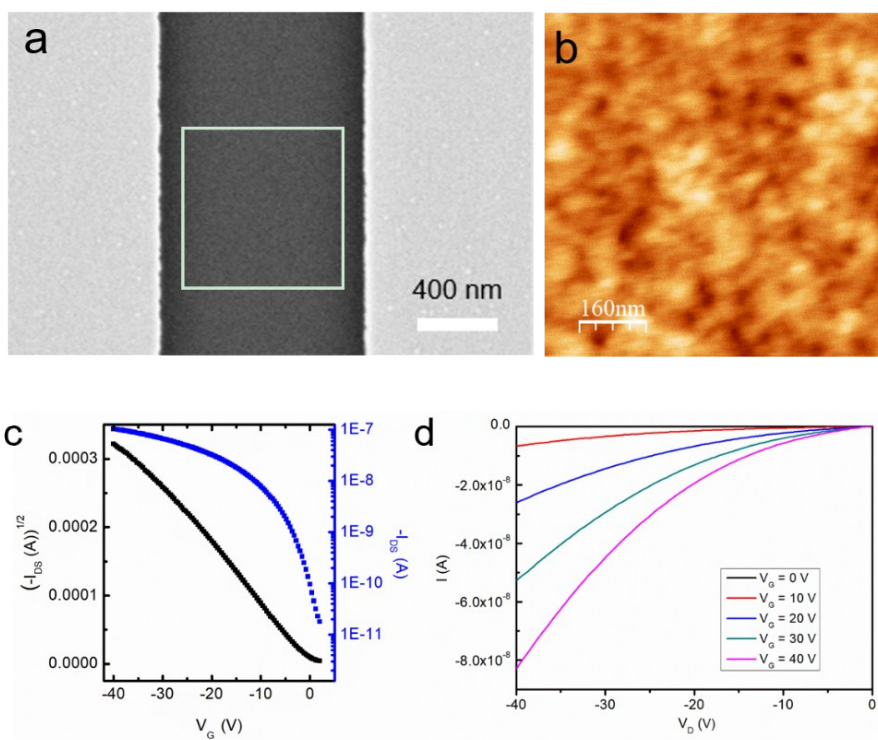


Figure S8. (a) SEM image of the NPB amorphous film OFET. (b) AFM image of the NPB film marked in (a). (c) Transfer and (d) output curves of the NPB amorphous film OFET, where the length and width of the channel are $1 \mu\text{m}$ and $400 \mu\text{m}$ respectively.

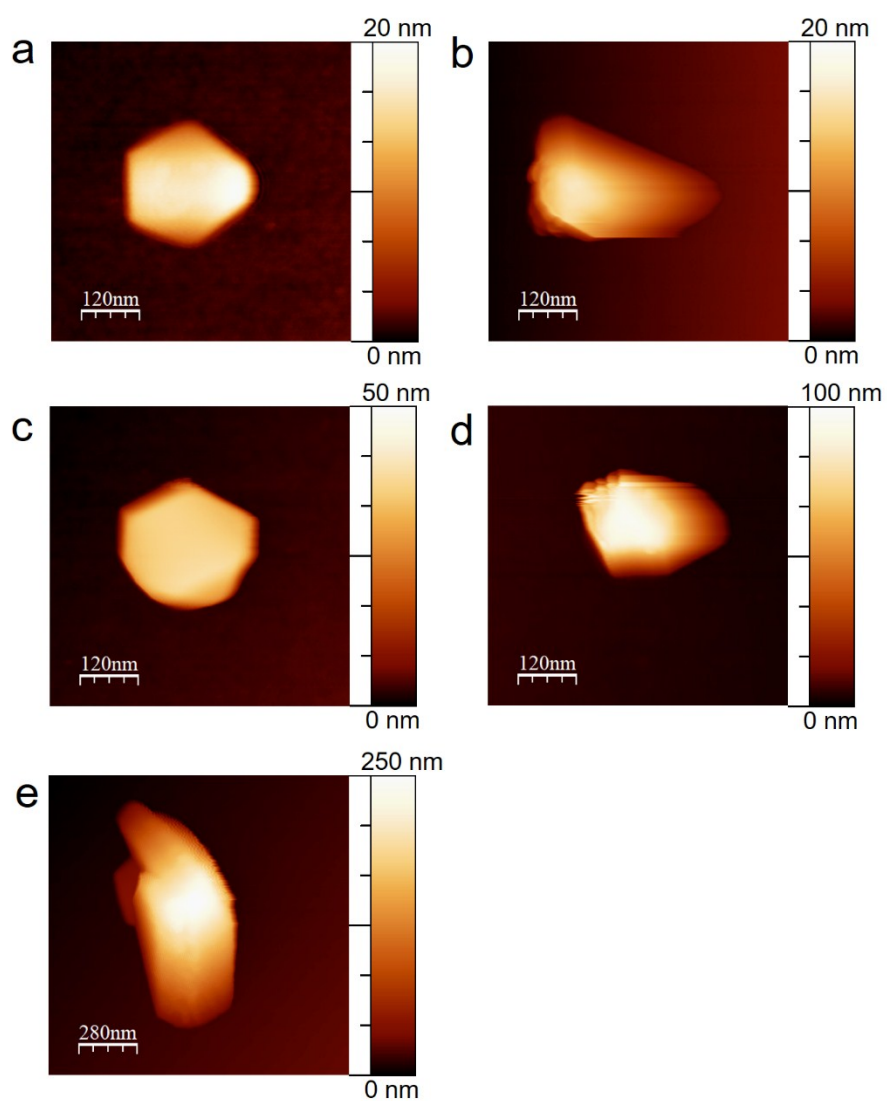


Figure S9. AFM images with Z range in Figure 3.

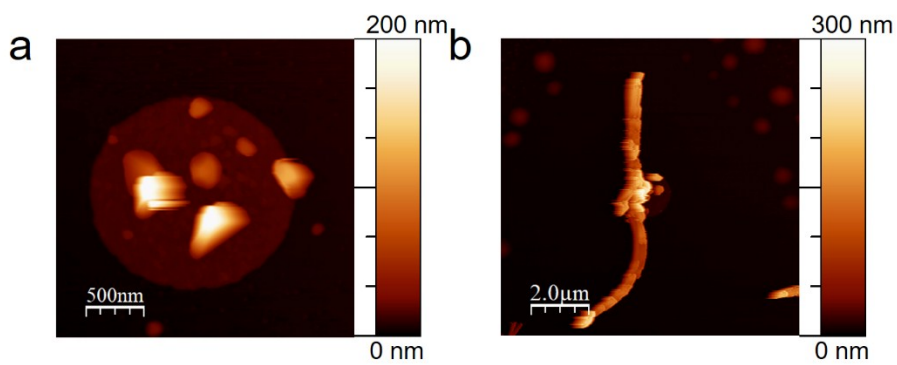


Figure S10. AFM images with Z range in Figure 4.

References

- 1 G. Kresse and J. Furthmüller, *Comp. Mater. Sci.*, 1996, **6**, 15-50.
- 2 G. Kresse and J. Furthmüller, *Phys. Rev. B*, 1996, **54**, 11169-11186.
- 3 G. Kresse and D. Joubert, *Phys. Rev. B*, 1999, **59**, 1758-1775.
- 4 P. E. Blöchl, *Phys. Rev. B*, 1994, **50**, 17953-17979.
- 5 A. Tkatchenko and M. Scheffler, *Phys. Rev. Lett.*, 2009, **102**, 073005.
- 6 J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.*, 1996, **77**, 3865-3868.
- 7 J. P. Perdew, J. A. Chevary, S. H. Vosko, K. A. Jackson, M. R. Pederson, D. J. Singh and C. Fiolhais, *Phys. Rev. B*, 1992, **46**, 6671-6687.