Perylenediimide Nanowires and Their Use in Fabricating Field-Effect Transistors and Complementary Inverters

Alejandro L. Briseno,[1,*] Stefan C. B. Mannsfeld,[2] Colin Reese,[2] Jessica M. Hancock,[1] Yujie Xiong,[1] Samson A. Jenekhe,[1,3,*] Zhenan Bao,[2,*] and Younan Xia[1,*]

[1]*Department of Chemistry, University of Washington, Seattle, WA 98195*
[2]*Department of Chemical Engineering, Stanford University, Stanford, CA 94305*
[3]*Department of Chemical Engineering, University of Washington, Seattle, WA 98195*
E-mail: xia@chem.washington.edu; abriseno@u.washington.edu; jenekhe@u.washington.edu; zbao@u.washington.edu
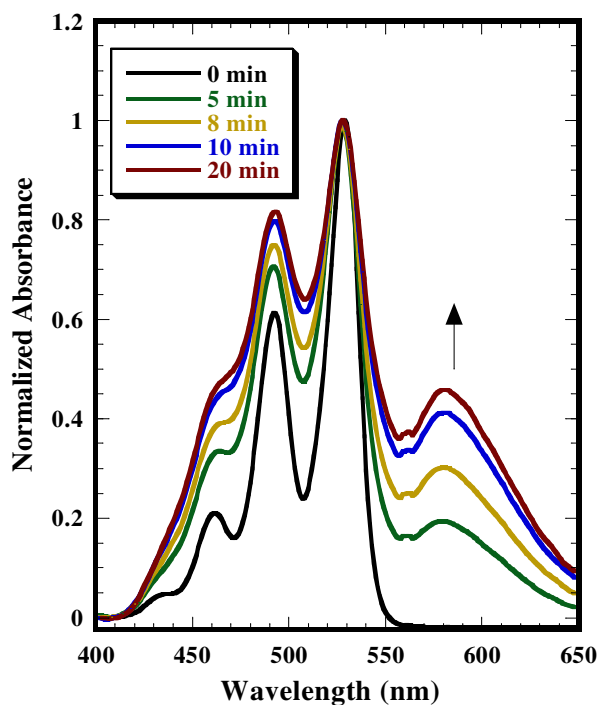
Figure S1. Normalized absorption spectra recorded at different times during the self-assembly of PTCDI-C8 nanowires at the interface between a 3.6 x 10^{-4} M PTCDI-C_8 chloroform solution and methanol. Similar trends are also observed in the spectra for self-assembly of PTCDI-C_5 and PTCDI-C_{13} nanostructure. The UV-Vis absorption spectra were recorded on a Perkin-Elmer model Lambda 900 UV/vis/near-IR spectrophotometer.
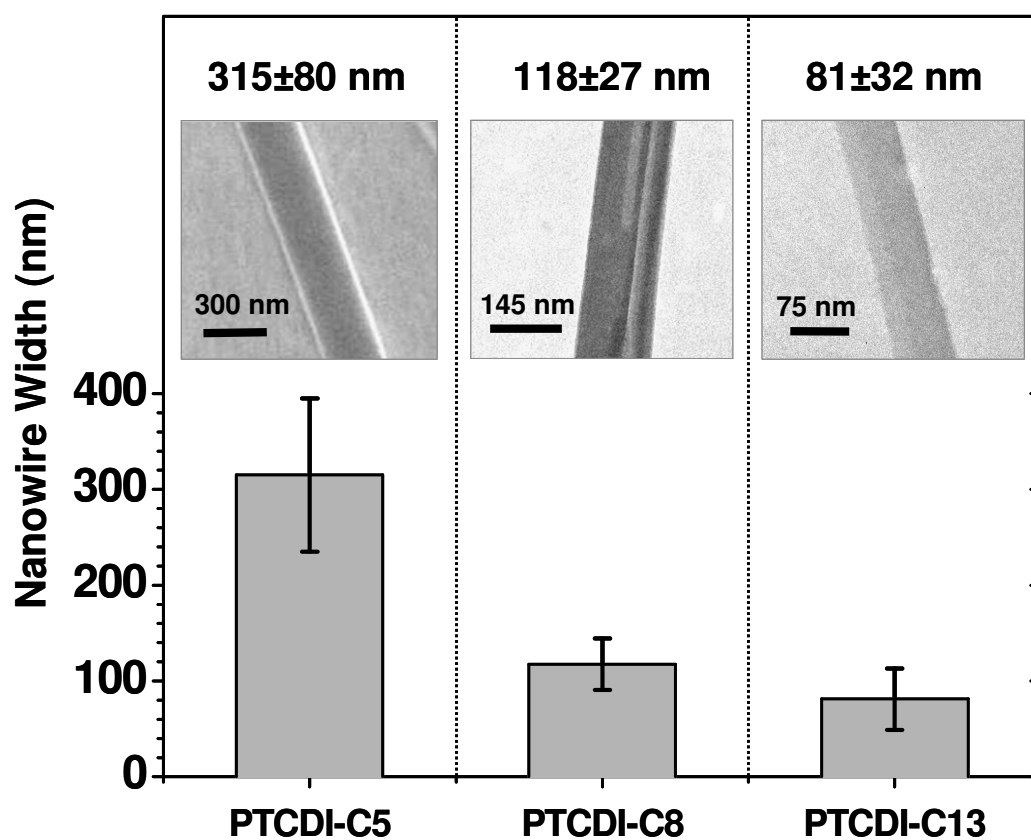
Figure S2. Average nanowire width plotted as a function of PTCDI alkyl chain. The insets give representative SEM images of the nanowires.
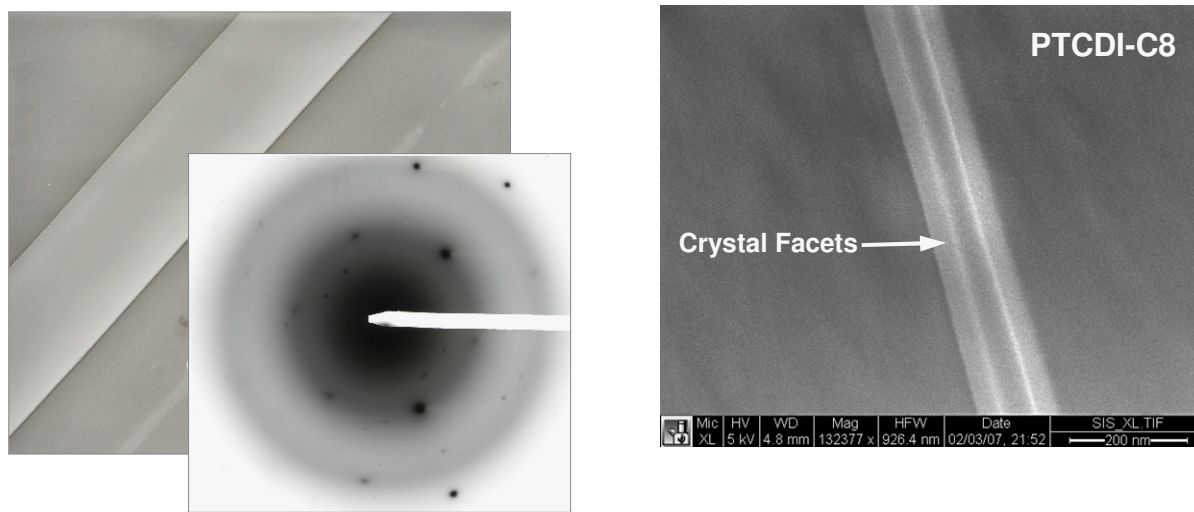
Figure S3. TEM image and corresponding electron diffraction pattern (inset) from a single-crystal PTCDI-C$_8$ nanowire. Although we were still able to acquire faint TEM diffraction spots from a single nanowire, the weak signal prevented precise structural analysis and we could only conclude the nanowires are highly crystalline in nature. The SEM image to the right clearly shows the crystal facets of a PTCDI-C$_8$ single-crystal nanowire.
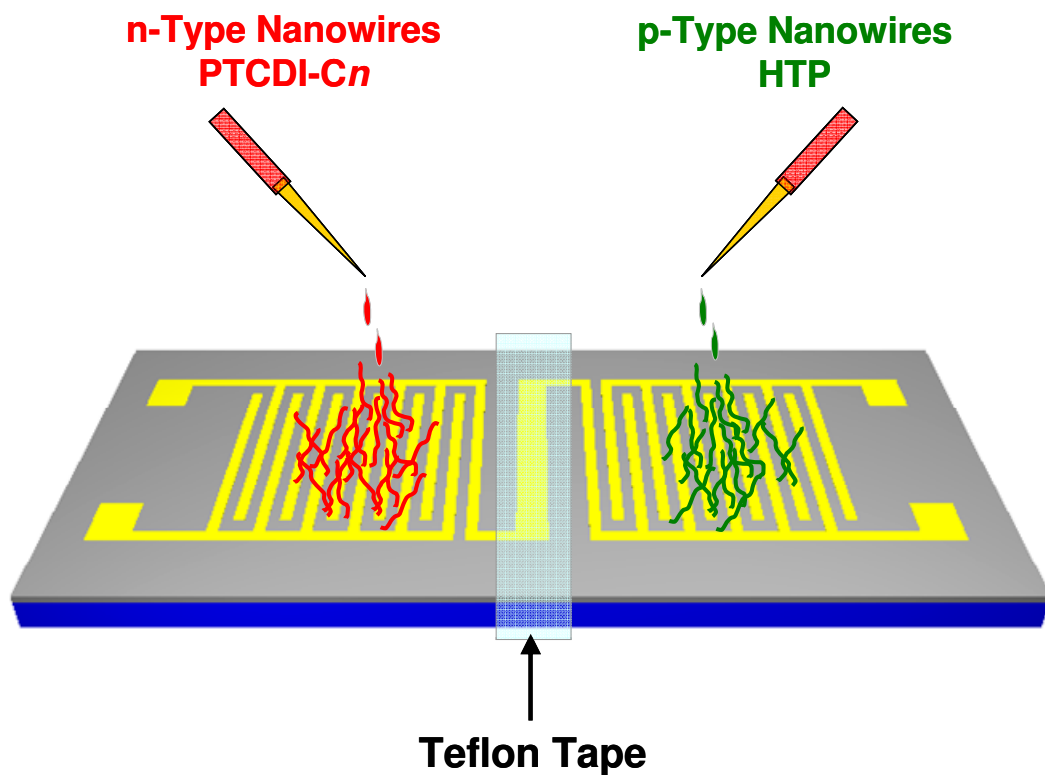
Figure S4. Nanowires were drop cast onto individual transistor devices from a suspension in methanol by separating the devices with Teflon tape. The devices were placed in a vacuum oven for several hours to allow complete drying and then annealed at ~130 °C prior to electrical measurements. All measurements were made under ambient conditions with a standard semiconductor probe station.

Table S1. OFET data of our best-performing PTCDI-C$_n$ nanowire transistors fabricated by drop-casting from a methanol suspension. The average mobilities are reported in the text of the manuscript and measured over at least 8 individual transistor devices. The threshold voltages are average values and the gain corresponds to the highest values achieved from our complementary inverters.

	Mobility, μ_e [cm^2/V s]	Threshold voltage [V$_T$]	I_{on}/I_{off}	Gain
PTCDI-C$_5$	1.2×10^{-4}	17.7	10^2	3.5
PTCDI-C$_8$	0.027	14.8	10^3	9
PTCDI-C$_{13}$	0.011	17.6	10^4	11

Structure refinement data and crystallographic information for PTCDI-C$_8$. A red needle of 0.59 mm x 0.09 mm x 0.07 mm in size was mounted on a glass capillary with oil. Data was collected at -143 °C with two sets of exposure as follows:

Scan	Type	Scanlength (deg.)	start (deg.) ϑ	φ	Ω	κ	
1	φ	182.0		3.70	-1.5	160	0
2	Ω	86.5		3.70	-25.9	-200.1	74.1
3	Ω	81.5		3.70	94.1	-195.1	74.1

Crystal-to-detector distance was 30 mm and exposure time was 40 seconds per degree for all sets. The scan width was 2°. Data collection was complete to 88.4% to 25° in ϑ. A total of 26468 partial and complete reflections were collected covering the indices, h = -5 to 4, k = -10 to 10, l = -22 to 23. 2497 reflections were symmetry independent and the R$_{int}$ = 0.1651 indicated that the data was of less than average quality (0.07).

Indexing and unit cell refinement indicated a triclinic P lattice. The space group was found to be P $\bar{1}$ (No.2).

The data was integrated and scaled using hkl-SCALEPACK. This program applies a multiplicative correction factor (S) to the observed intensities (I) and has the following form:

$$S = (e^{-2B(\sin^2\theta)/\lambda^2})/\text{scale}$$

S is calculated from the scale and the B factor determined for each frame and is then applied to I to give the corrected intensity (I$_{corr}$).

Solution by direct methods (SHELXS97) produced a complete heavy atom phasing model consistent with the proposed structure.

All hydrogen atoms were located using a riding model. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares.

The unit cell consists of only one complete molecule where the center of symmetry of the space group located between C9 and its symmetry related one trans to it in the aromatic ring in the molecule center relates one half of the molecule (enumerated) to the other (not enumerated). The packing thus is a simple pi to pi stack along the a-axis (4.6757Å long). The shortest distance between the slightly tilted molecule planes is 3.797 Å. It is remarkable that the C8 chains show little or no librative motion and not a hint of disorder often observed for this type of ligand.
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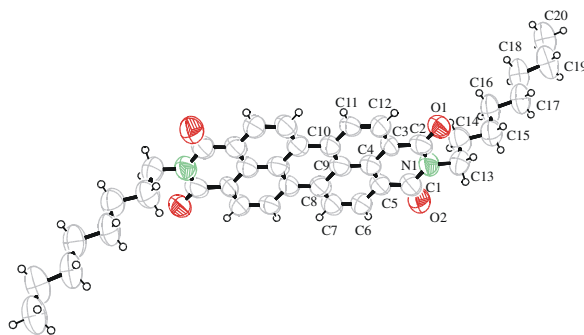
ORTEP diagram with thermal ellipsoids at the 50% probability level.
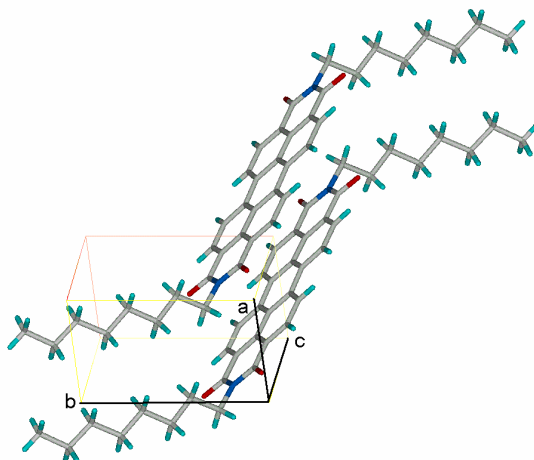
Packing diagram

Indexing of the crystals via orienting the needles on the 4-circle diffractometer identified the {010} and {001} faces. The {100}faces were not developed. The needles were strongly elongated along [100] and slightly flattened towards the {001} faces. Similarly, the Bravais-Friedel; Donnay-Harker predicts the existence of these faces and that of {100}. The absence of [100] is directly linked to the much elongated (nanowire-like) growth along the *a*-axis. The structure (cif) was edited for publication, however, because the biggest needle of suitable quality found was still very thin and in the absence o Å f strongly scattering atoms the dataset lacks the usually required completeness to a scattering angle of 25 degrees in ϑ.
The x-ray crystal structure was determined by:
Dr. W.Kaminsky: tel. (206) 543 7585
(X-ray lab): tel. (206) 543 0210
E-mail: kaminsky@wintensor.com

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