Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information for

Co-crystal Engineering: A Novel Method to Get One-dimensional (1D) Carbon Nanocrystal of Corannulene-fullerene by Solution Process

Yu Wang,[a] Yang Li,[b] Weigang Zhu,[b] Jinyu Liu, [b] Xiaotao Zhang,*[a] Rongjin Li, [a]

Yonggang Zhen,[b] Huanli Dong[b] and Wenping Hu *[ab]

Contents

1. Experimental section

Materials: corannulene($C_{20}H_{10}$, 98%) was provided by professor Jay. S. Siegel; C_{60} was purchased from Sigma-Aldrich Company and directly used without further purification. Toluene (C_7H_8, HPLC) was purchased from Beijing Chemical Co. China. Deionized water (18.2 ΩM cm^{-1}) was made by a MilliQ (Millipore) water purification system.

Theoretical calculations: The molecular structure was firstly optimized based on the crystal structure got from the CCDC. The intermolecular potentials were calculated using UNI force field by Mercury software. And the glide planes are shown by Mercury software. Moreover, the calculations of the energy levels were using density functional theory (DFT) pw91.

Crystal Growth and Characterization: In a typical experiment, corannulene and C_{60} were mixed and dissolved in toluene with molar ratio 1:1. For preparation of cocrystals, the solution was directly dropped onto SiO_2 /Si wafer and let it evaporate slowly in a weighing bottle. Transmission electron microscopy (TEM) and selected area electron diffraction (SAED) were performed on a JEOL JEM-1011 electron microscope at an acceleration of 100 kV to gain a sufficient transmission. For preparation of TEM samples, toluene solution was directly dropped onto TEM grids and the cocrystals were observed in several minutes. The crystal structures were analyzed in an X-ray diffractometer (XRD, X-Pert, PANalytic, Netherlands) with Cu K radiation (40 kV, 30 mA). Atomic force microscopy (AFM) analysis was conducted on a Veeco Nanoscope IV Multimode AFM (Veeco, USA). The UV absorption spectrums of the crystals were conducted on a Cary 5000 UV-VIS-NIR (varian, USA) and the PL/EX spectra were collected on Horiba FluoroMax-4-NIR spectrophotometers. IR spectra were collected on a Tensor-27 fourier infrared spectrometer (Bruker, Germany). Raman spectra were collected on an inVia-Reflex raman spectrometer (Renishaw, UK) excited with a 785nm laser. Electron spin resonance (ESR) spectrum was collected on Bruker E500-10/12 instrument with microwave frequency of 9.5 GHz. The fluorescence lifetimes were collected on lifespec lifetime measurement equipment (Edinburgh Instruments Ltd).

Device Fabrication and Measurement: The cocrystal nanowires were grown by directly dropping the mixed toluene solution onto the BCB/SiO_2 /Si wafer. It has been reported that the capacitance of the substrates was 10 nF/cm^2. To reduce the influence of the solvent, cocrystals were heated at 60 °C in vacuum for 2 h. Then gold (Au) electrodes (50 nm thick) were thermally evaporated onto cocrystals, using “organic ribbon mask method”. All the devices measurements were recorded by a Keithley 4200 SCS analyzer and an iodine−tungsten lamp was used as a white light source. All measurements were performed at room temperature in air.

2. Structure informations of CCCs shown by Mercury.

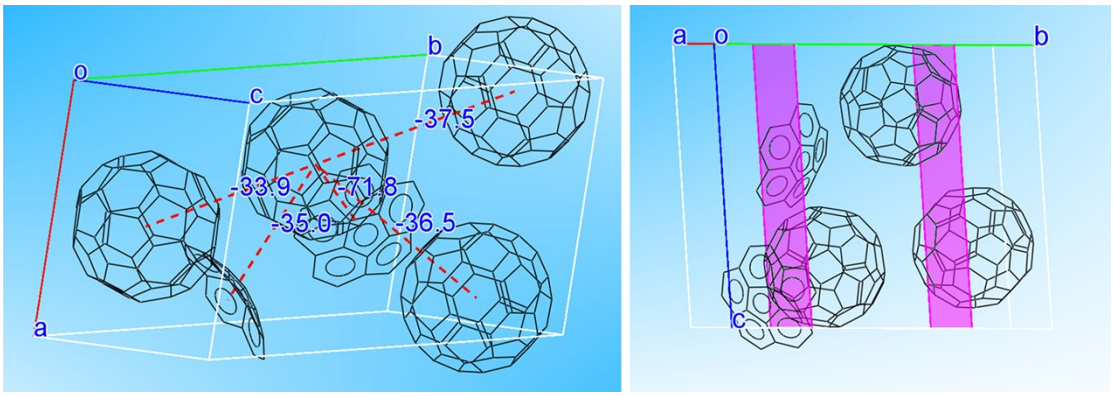

Figure S1. Five strongest interactions in cocrystal system (left) and glide planes of CCCs shown by Mercury (right).

3. XRD spectrum of cocrystals

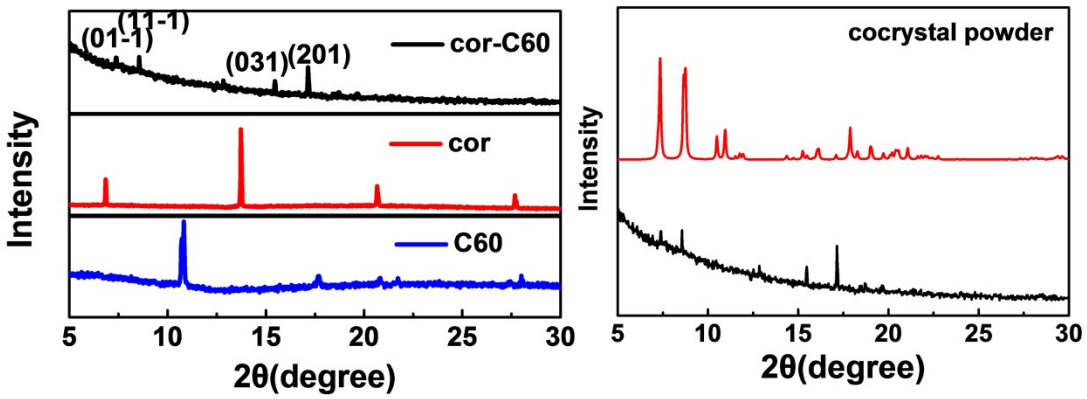

Figure S2. XRD spectrum of cocrystal nanowires.

4. UV spectrum and emission spectrum of corannulene, C_{60} and mixed solution.

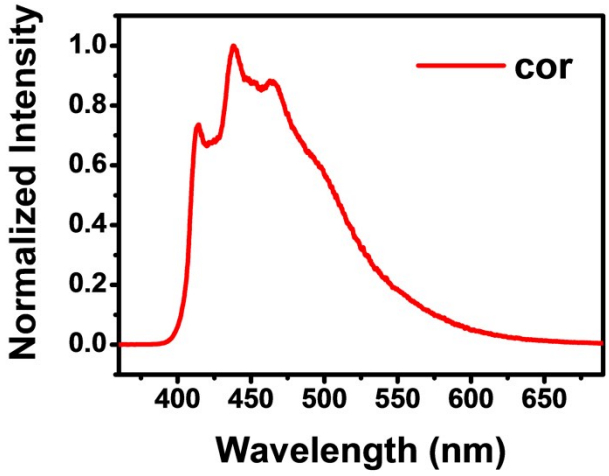

Figure S3. Emission spectrum of corannulene crystal.

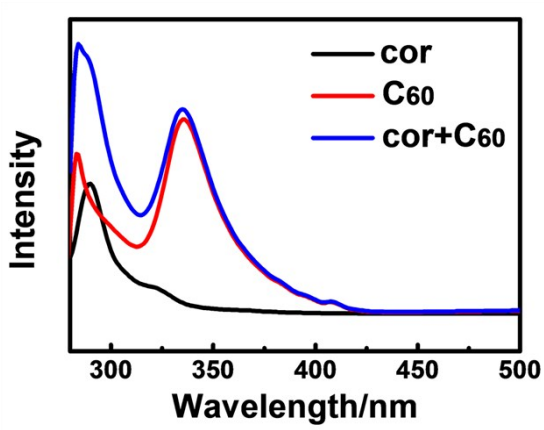

Figure S4. UV spectrum of corannulene, C_{60} and their mixed solution in toluene.

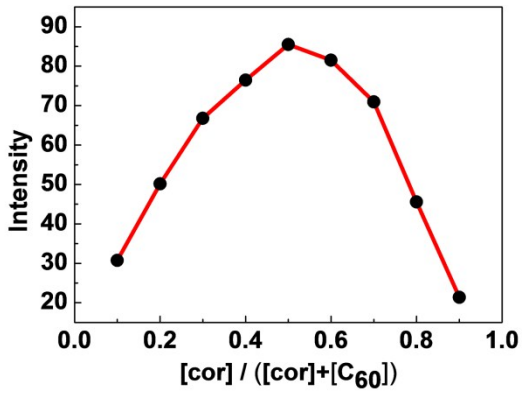

Figure S5. Job's plot of the corannulene and C_{60} mixed solution in toluene (λex=290nm, λmax=427nm).

5. Typical photoelectric properties of cocrystal nanowire devices.

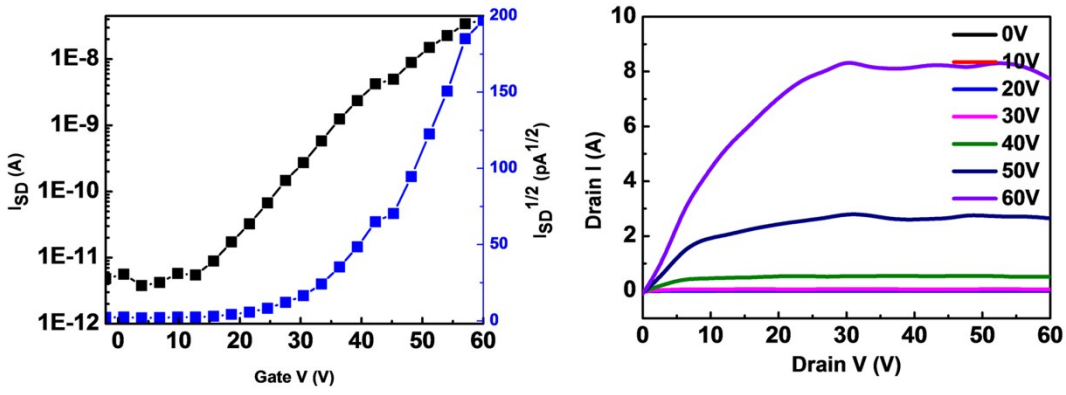

Figure S6. A typical cocrystal nanowire transfer characters (left) and its corresponding output curve (right). (V_{DS}=60V, W=0.80 μm , L=5.06 μm, μ_e= 0.11 $cm^2V^{-1}s^{-1}$)

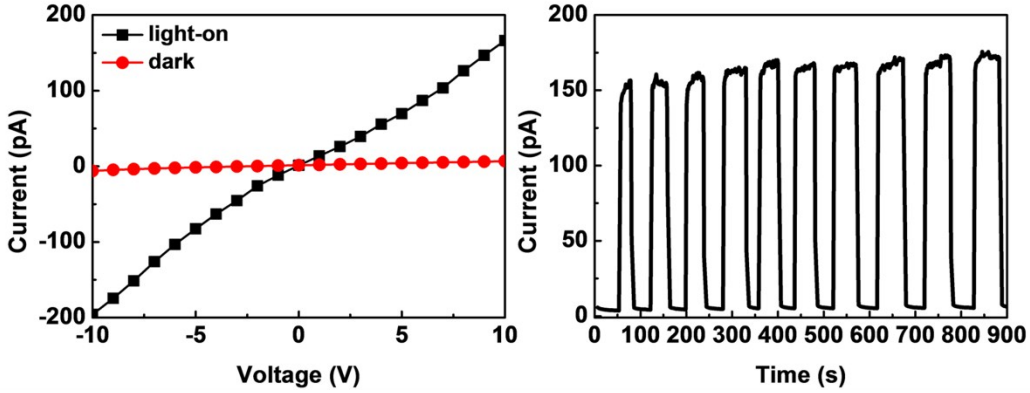

Figure S7. A typical cocrystal nanowire current-voltage (I-V) curves (left) and its corresponding on/off switch curve (right). (I_{on}/I_{off}=33.96)

6. AFM image of a cocrystal nanowire

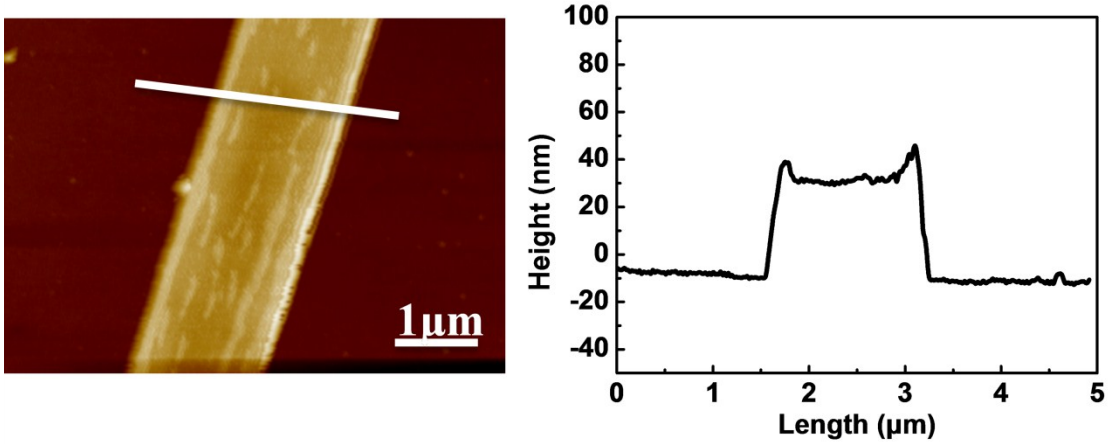

Figure S8. AFM analysis result of a cocrystal nanowire. The height of the cocrystal is around 52 nm.

7. Energy levels of corannulene and C_{60} calculated by DFT

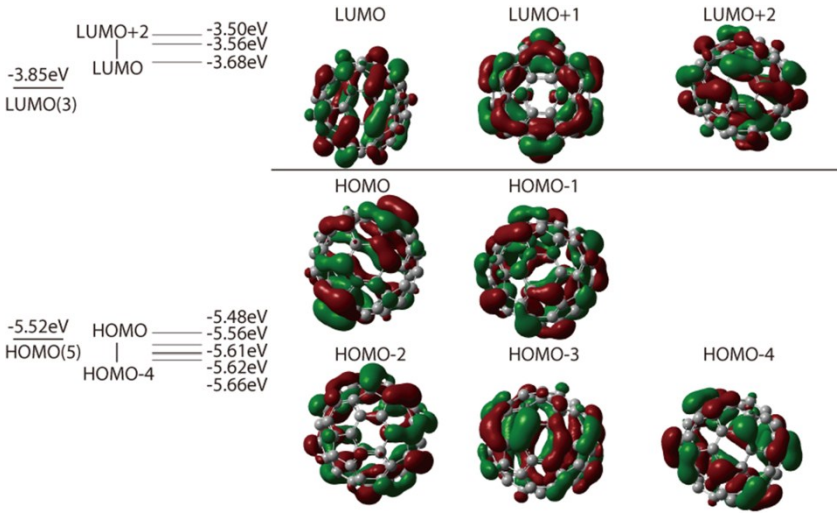

Figure S9. Energy levels of C_{60} before (left) and after (right) crystallization.

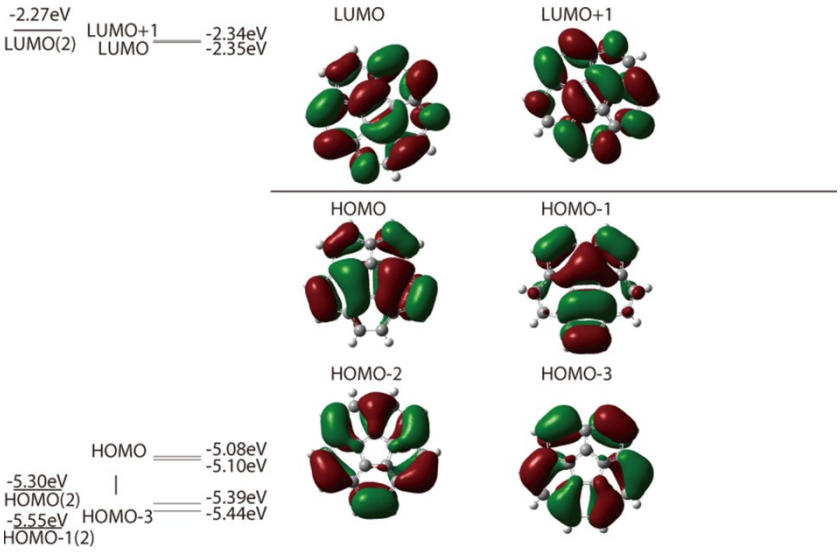

Figure S10. Energy levels of corannulene before (left) and after (right) crystallization.