Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information for

Donor-Acceptor Single Cocrystal of Coronene and Perylene Diimide: Molecular Self-Assembly and Charge-Transfer Photoluminescence

Chen Wang,[a] Jianlin Wang,[b] Na Wu,[a] Miao Xu,[a] Xiaomei Yang,[a] Yalin Lu [b,c] and Ling Zang[a,*]

[a.] Nano Institute of Utah and Department of Materials Science and Engineering, University of Utah, Salt Lake City, UT 84112, United States

[b.] National Synchrotron Radiation Laboratory, Synergetic Innovation Center of Quantum Information & Quantum Physics, University of Science and Technology of China, Hefei, Anhui, 230026, P.R. China

[c.] Laser Optics Research Center, Department of Physics, United States Air Force Academy, CO 80840, United States

Corresponding Author

*Email: lzang@eng.utah.edu.

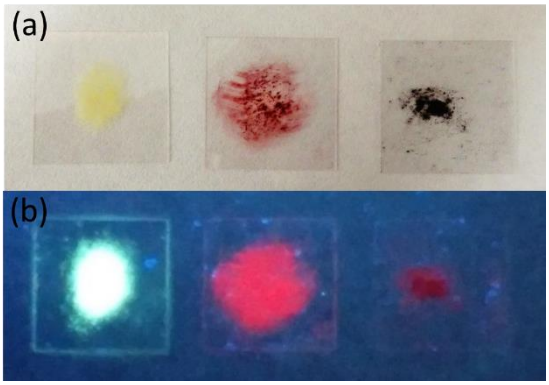

Figure S1. Photos taken on the solid coronene (left), PTCDI-C6 (middle) and the cocrystal (right) under white light (a) and 365 nm UV light (b).

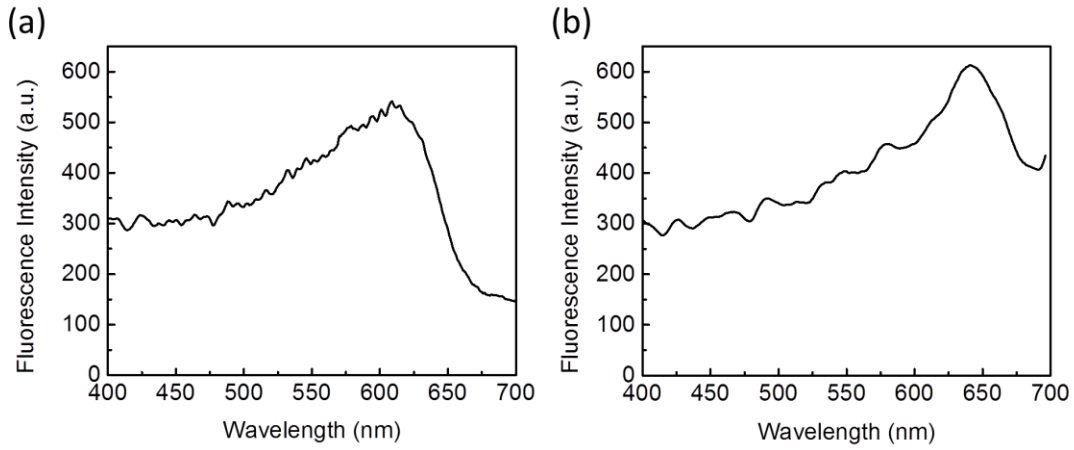

Figure S2. Excitation spectra of PTCDI-C6 (a) and the D-A cocrystal (b).

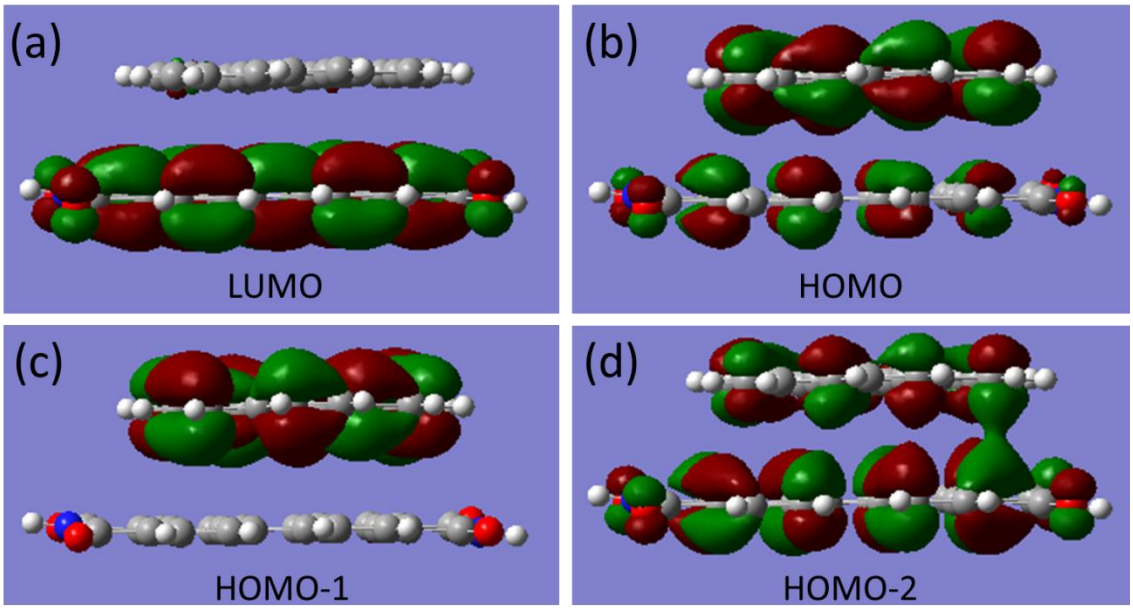

Figure S3. The calculated LUMO (a), HOMO (b), HOMO-1 (c) and HOMO-2 (d) for the D-A stack of coronene and PTCDI. The stacking geometry was adapted from the single crystal data and the calculations were performed with density-functional theory (B3LYP/6-311g**) using the Gaussian 03 package.

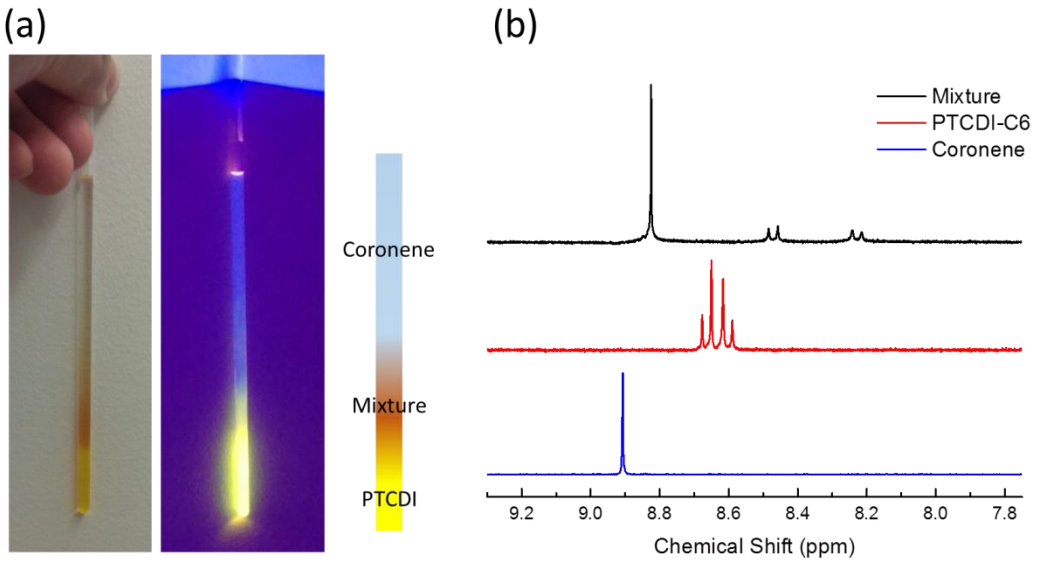

Figure S4. (a) Photos taken on the mixed chloroform solutions of coronene and PTCDI-C6 (both 1 mmol·L^{-1}) in a NMR tube under white light (left) and 365 nm UV light (right). (b) ^{1}H-NMR spectra measured from the coronene (blue), PTCDI-C6 (red) and the cocrystal (black) solutions in $CDCl_3$ (ca. 2 mmol·L^{-1}).

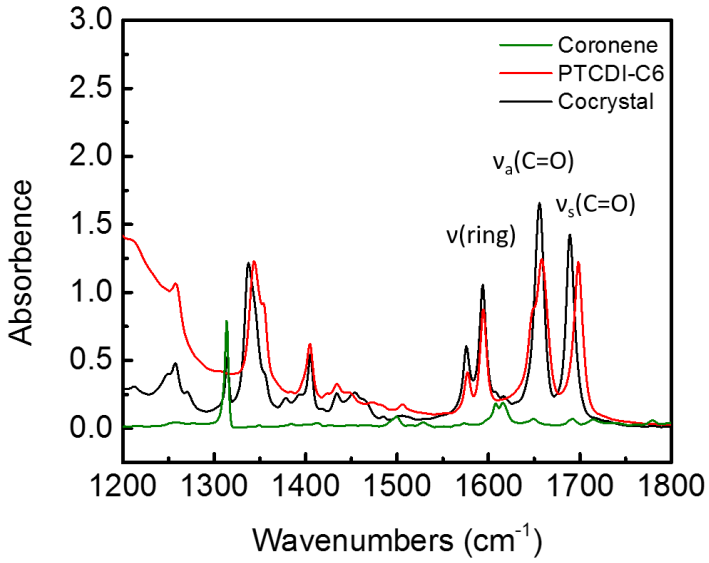

Figure S5. FT-IR spectra of coronene (green), PTCDI-C6 (red), and the cocrystal (black).

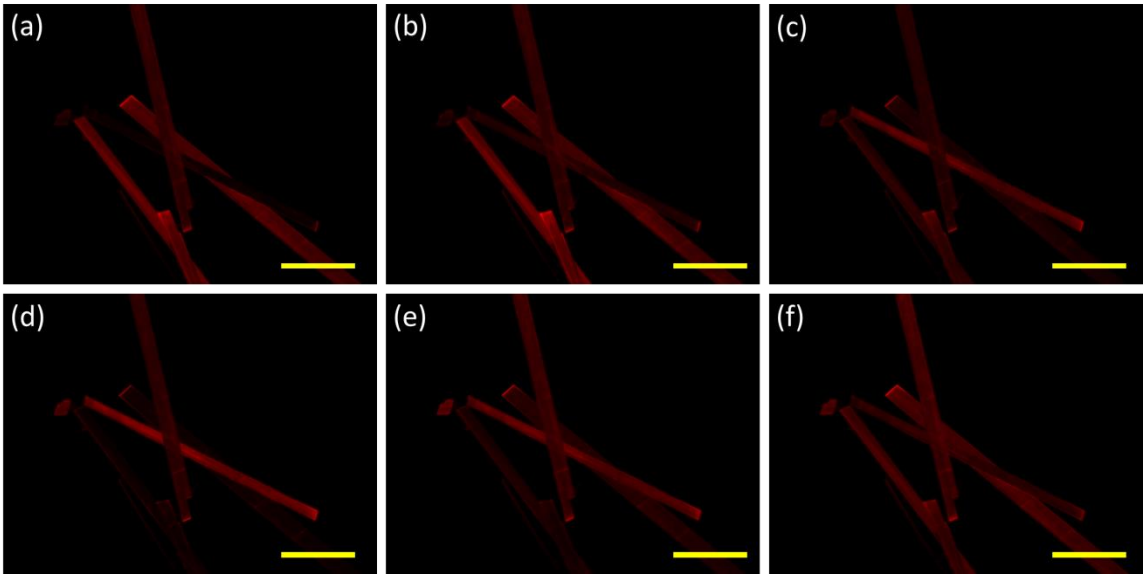

Figure S6. Fluorescence images recorded on multiple cocrystal microfibers at different polarization. The zero angle was defined as the horizontal direction of the images in (a) and increased by 30° each image to (f). Scale bar is 100 μm.

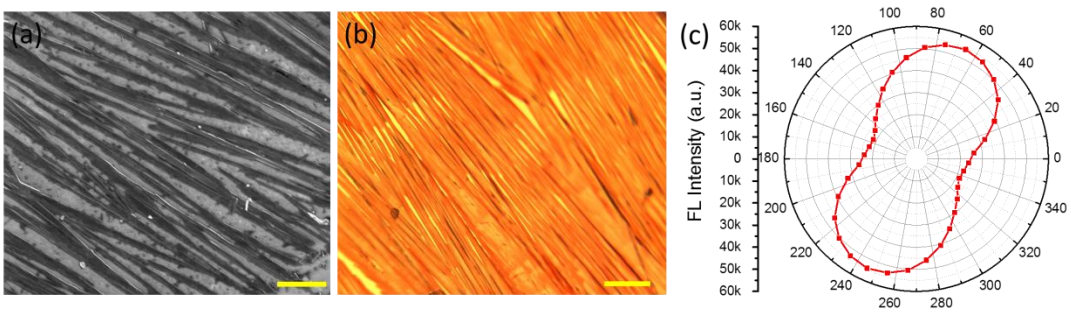

Figure S7. (a) SEM image and (b) optical microscope image taken on a microfibers array fabricated on a glass substrate (scale bar = 100 μm). (c) Polar plot of fluorescence intensity measured on the whole fibers array as a function of the angle between the fluorescence polarization direction and the average long axis of fiber.

Table S1. Calculated transition energies of the cocrystal.

E_{vert}	Contribution
S_0->S_1	1.86 eV (f=0.05) H-2->L (7%) H-1->L (2%) H->L (90%)
S_0->S_2	1.97 eV (f=0.08) H-1->L (98%) H->L (2%)
S_0->S_3	2.45 eV (f=0.34) H-2->L (92%) H->L (8%)
S_0->S_4	2.99 eV (f=0.002) H-3->L (100%)

Table S2. The Miller index, energy and area ratio of exposing facets calculated by the Material Studio 7.0 software package.

hkl	dhkl	E_{total} (a.u.)	Total facet area (%)
{ 0 0 1}	13.61278	-21.0286	49.84477
{ 0 1 1}	8.927946	-38.0045	23.82977
{ 1 0 0}	7.01556882	-58.58129668	15.1445656