

Supplementary Information

Size-dependent cathodoluminescence properties of 5,5'-di(4-biphenyl)-2,2'-bithiophene nanocrystals

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S1. Crystal structure information on a BP2T single crystal.

When crystals are grown by solution growth or physical vapor transport methods, BP2T molecules grow into thin single crystals. Typically, parallelogram-shaped single crystals are obtained. Regarding the crystal structure of the BP2T crystals, previous study reported that the BP2T molecules crystallizes in monoclinic form ($P21/c$, $a = 0.57081$ nm, $b = 0.76036$ nm, $c = 5.2869$ nm, $\beta = 97.147^\circ$).¹ Figures S1(a) and S1(b) show three-dimensional crystal structure of BP2T crystal and crystal structure indicating unit-cell projections on ab -plane, respectively. The transition dipole moment makes an angle of 5° with respect to the c -axis. The confined fluorescence inside the BP2T single crystal is propagated through the crystal and observed from the end faces, as shown in Fig. 2(b).

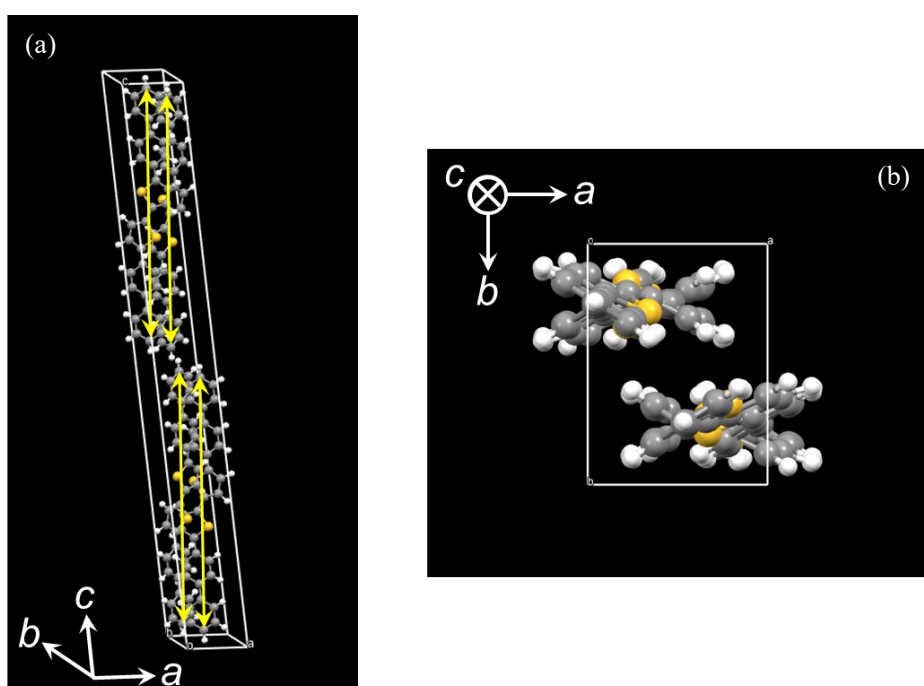


Figure S1. (a) Three-dimensional crystal structure of BP2T crystal. Transition dipole moments are depicted by yellow arrows. (b) Crystal structure indicating unit-cell projections on ab -plane.

Reference

1. H. Mizuno, I. Ohnishi, H. Yanagi, F. Sasaki, and S. Hotta, *Adv. Mater.* 2012, **24**, 2404-2408.

S2. TEM characterization of BP2T nanocrystals.

To demonstrate that a single nanocrystal has a crystalline nature, we showed TEM images and SAED patterns of four nanocrystals with different sizes in total. Figure S2 shows TEM images of the BP2T nanocrystals and corresponding SAED patterns. The nanocrystal sizes were estimated to be approximately 310 nm, 60 nm, 40 nm, respectively, from the TEM images. For Fig. S2(e), the size was determined for the nanocrystal surrounded by white dashed circle. For the nanocrystal with 310 nm in size (Fig. S2(a)), the bright spots in the SAED pattern corresponded to the (0 2 0) and (0 1 20) planes. For the 60 nm-sized nanocrystal (Fig. S2(c)), the bright spots corresponding to the (1 0 -24) plane were observed. In the nanocrystal with the size of 40 nm (Fig. S2(e)), we observed the bright spots correspond to the (0 4 12) plane. The distinct bright spots without ring pattern indicating an amorphous in the single BP2T nanocrystals revealed that the prepared nanocrystals have crystalline nature.

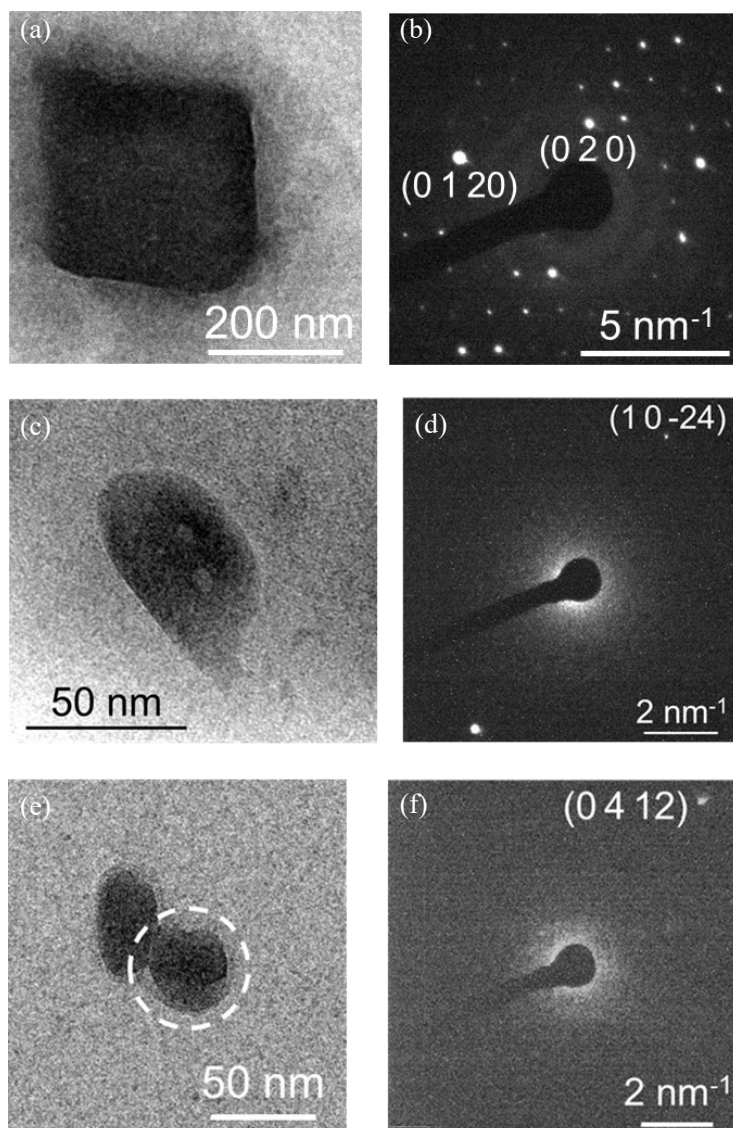


Figure S2. TEM images of BP2T nanocrystals ((a), (c), (e)) and corresponding SAED patterns ((b), (d), (f)).