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Supporting Information

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Carbon Nanotubes for Photovoltaics: From Lab to Industry

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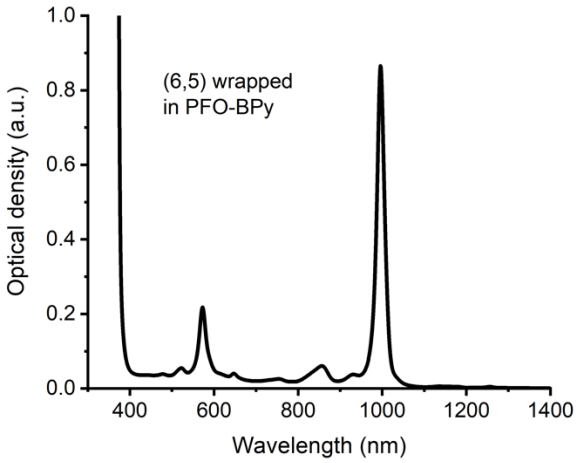

Figure S1. PFO-BPy wrapped (6,5) in toluene using a shear force mixing approach and the CoMoCAT raw soot. The method in ref[1] is used to estimate the concentration and a 4 mm path length cuvette.

In our experiments, 41 mg of CoMoCAT raw soot (~ €750/g) is added to 110 mL of toluene (~ €45/L) with 55 mg of poly[(9,9-dioctylfluorenyl-2,7-diyl)-alt-co-(6,6'-(2-2'-bipyridine))] (PFO-BPy) (~ €670/g) and shear force mixed or sonicated to produce a suspension which is centrifuged to produce ~1 – 2 mg of (6,5). Neglecting the additional mass associated with the polymer this places the price of (6,5) from polymer extraction in the laboratory at roughly €36,000 – 73,000/g.

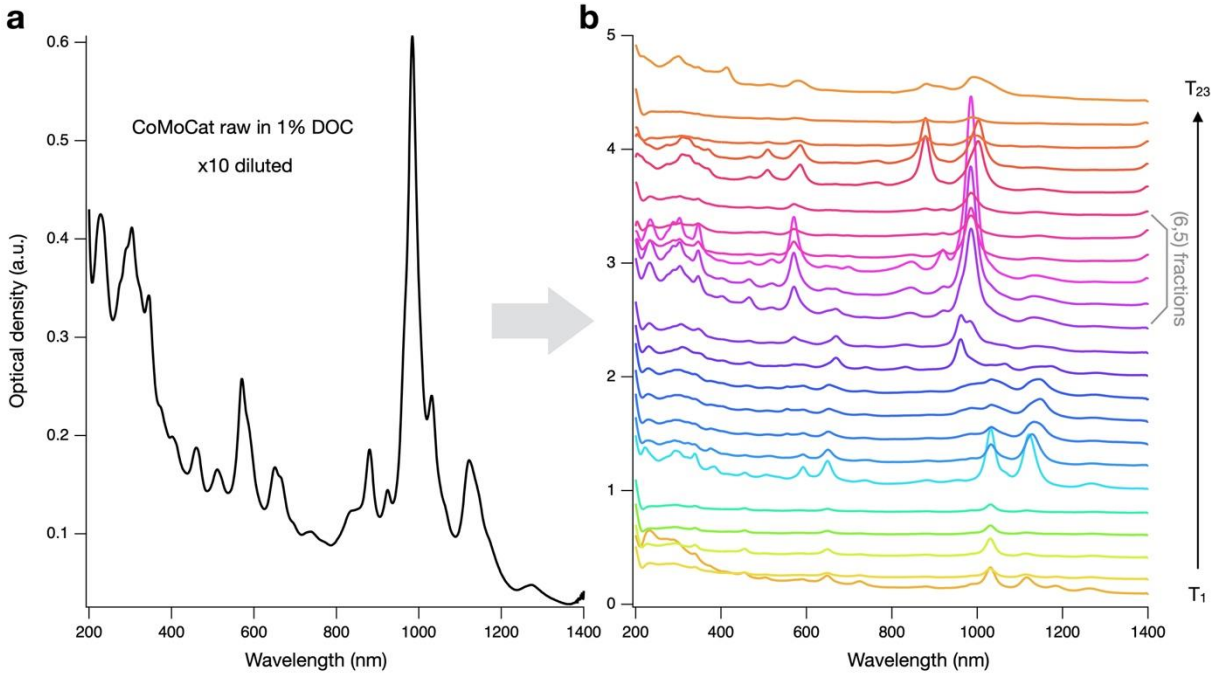

Figure S2. (a) CoMoCAT raw suspension as the parent material for ATPE sorting. (b) All the top phases from T_1 to T_{23} by ATPE. T_{13}, T_{14}, T_{15}, T_{16}, T_{17} and T_{18} are (6,5) enriched fractions. The method in ref[1] is used to estimate the concentration and a 2 mm pathlength cuvette.

In our research laboratory, a practical limit of 300 mL with a CNT concentration of ~1 mg/mL and is defined by a centrifuge rotor capable of supporting six 50 mL falcon tubes, each of which initially contain ~5 – 10 mg of SWCNTs. The current batch size is thus ~ 30 – 60 mg of raw CNT soot, which is very close to mass processed by polymer extraction and allows for an easy comparison. In our ATPE approach, 30 – 60 mg of CoMoCAT soot is dispersed in 120 mL of water with 2 % DOC (~ €0.7/g) and a 3-step process,[2] requiring a total of 180 mL 20 % m/v Dextran (~ €1.2/g) and 200 mL 25 % m/v PEG (~ €0.05/g), 6 g SDS (~ €0.5/g) and 3 g SC (~ €1.25/g), is used to obtain 6 – 12 mg of (6,5). The cost for (6,5) from ATPE is therefore ~ €8,300 – 13,000/g.

References

[1] M. Zheng, B. A. Diner, *J. Am. Chem. Soc.* **2004**, 126, 15490.
[2] H. Li, G. Gordeev, O. Garrity, S. Reich, B. S. Flavel, *ACS Nano* **2019**, 13, 2567.