Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C. This journal is © The Royal Society of Chemistry 2023

1	Supporting Information
2	
3	Manipulating the Transition of Aggregated States to Control the Photochromism in a New
4	Triphenylethylene Derivative
5	
6	Mingyao Shen, Yuxin Xiao, Cheng Huang, Rongjuan Huang, ^a Vonika Ka-Man Au* and Tao Yu*
7	
8	
9	
10	
11	
12	
13	

14 1 Synthesis and characterization of compounds

15 The details of the synthetic procedures for TrPE*o*I, TrPE*o*P and TrPE*o*PO are shown below. All the final 16 compounds were characterized by ¹H NMR spectroscopy, and High-resolution EI mass spectroscopy.

17 General chemical reagents and solvents were purchased from commercial suppliers, including Adamas-beta,

18 Energy Chemical, and Aladdin. All chemicals and solvents used were of analytical grade and all the

19 commercial reagents were used without further purification.

20 Synthesis of the compound TrPEoI

A mixture of 2-iodobenzylbromide (2.50 g, 8.42 mmol) and triethylphosphite (2.10 g, 12.63 mmol) was 21 added to a two-necked flask under an argon atmosphere and stirred at 85°C for 6 h. After the reaction was 22 23 completed, the mixture was cooled to room temperature to give crude reagent diethyl (2-24 iodophenyl)phosphate without further purification. Then the mixture of bis(4-fluorophenyl)methanone (2.20 g, 10.10 mmol) and t-BuOK (2.83 g, 25.25 mmol) in THF (70 mL) was added under an argon atmosphere 25 26 and an ice water bath. The resulting mixture was further stirred at ambient temperature for 3 h. Subsequently, THF of the mixture was removed by distillation under reduced pressure, the mixture was then poured into 27 water and extracted with CH₂Cl₂. Further purification was done by column chromatography on silica gel 28 with hexane as eluent. Yield: 2.52 g (71.60%). ¹H NMR (500 MHz, CDCl₃) δ = 6.78-6.85 (m, 3H), 6.90-29 6.95 (m, 2H), 6.99-7.07 (m, 5H), 7.30-7.36 (m, 2H), 7.83 (dd, J=7.9, 1.0 Hz, 1H); High resolution EI-MS: 30 31 418.0030 m/z found: 418.0024 [M]⁺.

32 Synthesis of the compound TrPEoP

Diphenylphosphine (1.18 g, 6.31 mmol) was added in a dropwise manner to a mixture of TrPEoI (2.40 g, 33 5.74 mmol), Pd(PPh₃)₄ (0.01 g, 0.09 mmol) and triethylamine (11.96 mL, 86.08 mmol) in degassed toluene 34 35 (30 mL) under an argon atmosphere. The resulting mixture was further refluxed and stirred for 24 h. After the mixture was cooled to room temperature and filtered, the filtrate was p_o oured into water and extracted 36 with CH₂Cl₂. Further purification was carried out by column chromatography on silica gel with CH₂Cl₂-37 hexane (1:4, v/v) as eluent. Yield: 1.56 g (57.05%). ¹H NMR (500 MHz, CDCl₃) δ = 6.70-6.76 (m, 2H), 38 39 6.78-6.86 (m, 3H), 6.91-6.97 (m, 3H), 6.98-7.08 (m, 2H), 7.10-7.15 (m, 2H), 7.28-7.37 (m, 11H); High resolution ESI-MS: 476.1505 m/z found: 477.1577 [M+H]+. 40

41 Synthesis of the compound TrPEoPO

42 To the TrPEoP (1.00 g, 2.39 mmol) in 20 mL CH₂Cl₂, 0.5 ml H₂O₂ aqueous (30 wt%) solution was added in 43 a dropwise manner. After stirring for 60 minutes at room temperature, the mixture was poured into 50 mL 44 water and extracted with CH₂Cl₂. Further purification was carried out by chromatography on silica gel with

- 45 ethyl acetate-hexane (2:1, v/v) as eluent. Yield: 0.87 g (84.17%). ¹H NMR (500 MHz, CDCl₃) δ= 6.69-6.76
 46 (m, 2H), 6.81-6.93 (m, 5H), 6.97-7.02 (m, 2H), 7.08-7.18 (m, 2H), 7.28-7.45 (m, 6H), 7.46-7.53 (m, 2H),
 47 7.73 (dd, J=11.7, 7.4 Hz, 4H); High resolution EI-MS: 492.1455 m/z found: 493.1533 [M+H]⁺.



Figure S1 ¹H NMR spectrum of TrPEoPO (in Chloroform-d).











Figure S3 High resolution EI mass spectrum of TrPEoPO.

57 2 Physical measurements and instrumentations

58 ¹H NMR spectra experiments were performed on a Bruker ADVANCE NEO 500 NMR spectrometer (500 59 MHz) at room temperature with Chloroform-d as solvent and tetramethylsilane (TMS) as the internal standard. High Resolution EI mass spectra were performed using a Thermo MAT95XP high resolution mass 60 spectrometer. The UV-vis absorption spectra of solution were performed on Hitachi U-3900. Steady-state 61 fluorescence spectroscopy and the fluorescence lifetimes of solids were measured using an Edinburgh 62 instrument FLS1000. The time dependent UV-vis reflectance spectra were carried out using an Ocean Optic 63 Maya2000PRO spectrometer with Ocean Optic reflection probes R600-125F. PXRD data were obtained on 64 a Bruker D8 Advance X-ray diffractometer with Cu Ka radiation. TGA was carried out on a Netzsch TG 65 209 F3 Tarsus at a heating rate of 10 °C•min⁻¹ under nitrogen flow of 20 mL•min⁻¹ from room temperature 66 to 800 °C. DSC curve was performed on a Netzsch DSC 214 at a heating rate of 10 °C•min⁻¹ under nitrogen 67 flow of 40 mL•min⁻¹ from room temperature to 220 °C. 68

69 3 Supplementary information





Figure S4 First-order kinetic plots for decoloring of TrPEoPO (a) in solution state at the wavelength of 460 nm and (b) in amorphous state at the wavelength of 500 nm. ($A_t=A_0 \exp(-kt)$, A_0 is the absorbance before decoloring (t = 0), and A_t is the

73 absorbance at the moment of decoloring time)

