Supporting Information

Perylene diimide derivative dispersed in LDH as a new efficient red-emitting phosphor for LED applications

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Sections :

Section 1: experimental section

1. Synthesis of *N*,*N*′-bis(2,6-diisopropylphenyl)-1,6,7,12-tetra-[4-(sulfuric acid)phenoxy]perylene -3,4,9,10-tetracarboxydiimide (TSP)

1.1. *N*,*N*′-Bis(2,6-diisopropylphenyl)-1,6,7,12-tetrachloroperylene-3,4,9,10-tetracarboxydiimide (PDI-4Cl)

0.53 g of PTCD-4Cl (1 mmol) was stirred in 50 mL of propionic acid with 1.79 mL of 2,6-diisopropylaniline (10 mmol) in a 100 mL three-necked round-bottomed flask. The reaction was completed at 160 °C for 16 h under nitrogen and then cooled down. The resulting solution was slowly transferred into 300 mL of methanol. An orange precipitate was then filtered and washed several times with methanol and then vacuum dried at 40 °C overnight. The crude product (0.76 g, yield: 90 %) was purified by column chromatography on silica gel using DCM as the eluent. The ^{1}H NMR spectrum is identical to that recorded in reference [12].

1.2. N,N′-Bis(2,6-diisopropylphenyl)-1,6,7,12-tetraphenoxy-perylene-3,4,9,10-tetracarboxydiimide (P-4OH)

0.76 g of PDI-4Cl (0.90 mmol) was dispersed in 50 mL of NMP with 0.68 g of phenol (7.20 mmol) and 0.50 g of K_2CO_3 (3.6 mmol) in a 100 three-necked round-bottomed flask. The setup was flushed with nitrogen, the temperature was raised to 120 ^{o}C and the reaction mixture was stirred for 16 h. After cooling to room temperature, the mixture was added dropwise to 500 mL of a 5% HCl solution. The red precipitate obtained was filtered off and then washed with distilled water until a neutral pH was obtained. The paste was vacuum dried at 40 °C overnight. As before, the obtained product P-4OH (0.85 g, yield: 88 %) was purified by column chromatography on silica gel using DCM as the eluent. The ^{1}H NMR spectrum is identical to that recorded in reference [12].

1.3. *N*,*N*′-Bis(2,6-diisopropylphenyl)-1,6,7,12-tetra-[4-sulfo)phenoxy] perylene-3,4,9,10-tetra carboxydiimide (TSP)

0.85 g of P-4OH (0.79 mmol) was added to 25 mL of concentrated sulfuric acid in a three-neck round flask and then stirred at room temperature for 24 h under sealed condition. After reaction, 50 mL of distilled water was added dropwise to the resulting solution. A deep black-red precipitate was filtered, then washed with DCM and vacuum dried at 40 °C overnight, yielding the desired product TSP (0.94 g, yield: 85 %). ^{1}H NMR (400 MHz, DMSO-d6, 298 K): 7.93 (s, 4H), 7.64 (d, 8H), 7.41 (t, 2H), 7.28 (d, 4H), 7.00 (d, 8H), 2.68 (m, 4H), 1.01 (d, 24H) ppm (Figure S1).

Section 2: supplementary figures

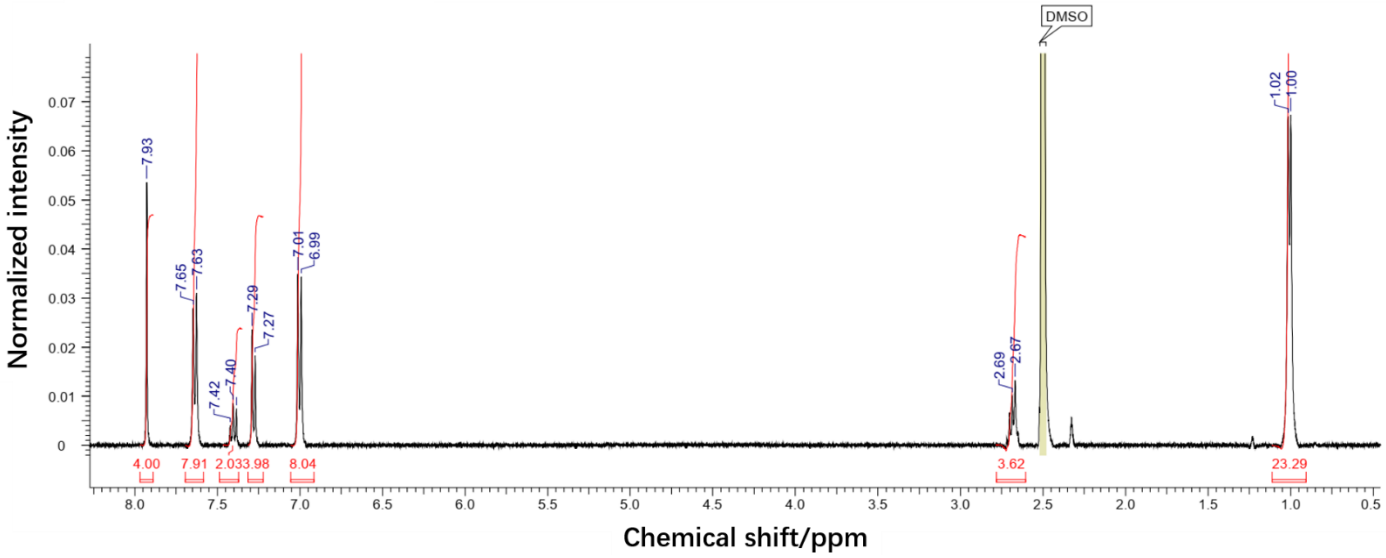

Figure S1. ^{1}H NMR spectrum of TSP.

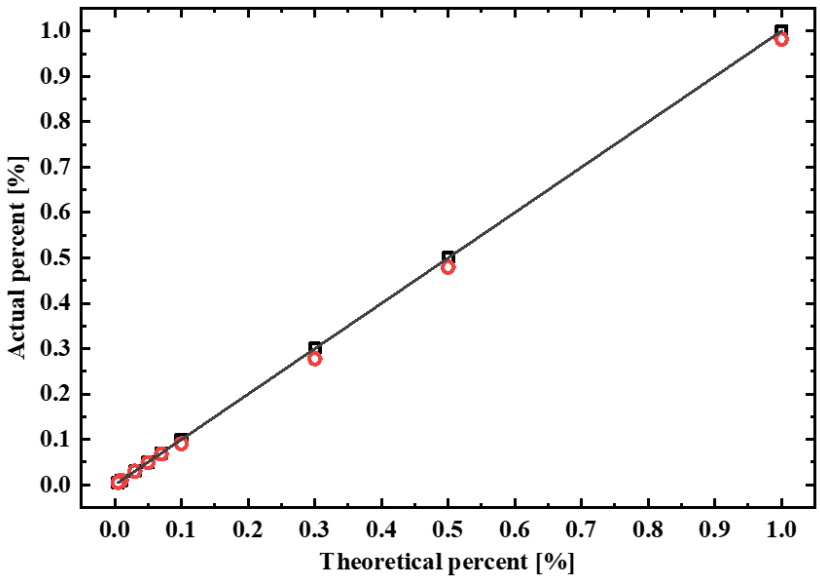

Figure S2. Variation in actual percent as a function of theoretical percent of TSP in LDH calculated by UV-vis spectra (black circles refer to the theoretical points; red circles are the actual points).

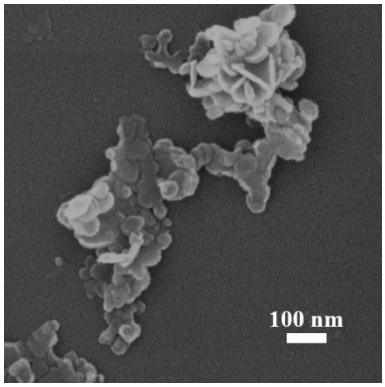

Figure S3. SEM image of TSP-LDH sample

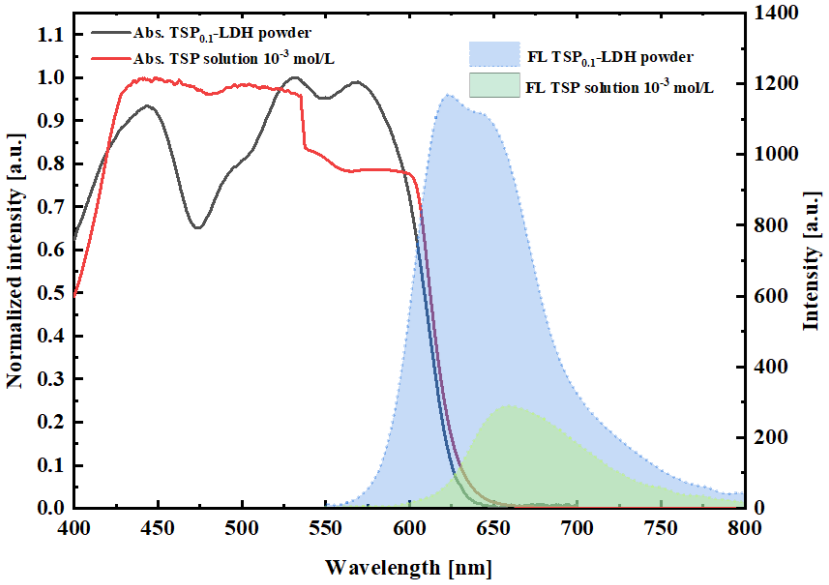

Figure S4. UV-vis absorption and emission spectra of TSP aqueous solution (10^{-3} mol/L) and $TSP_{0.1}$-LDH powder.

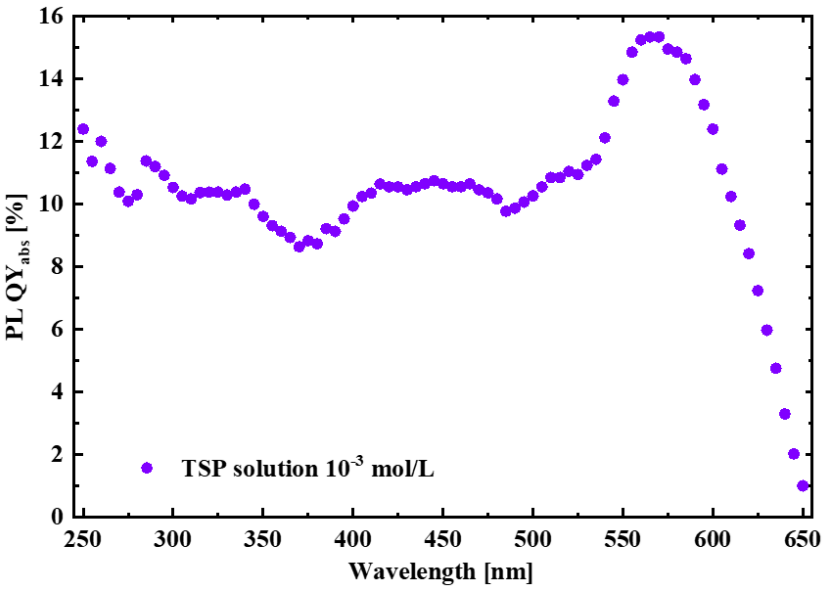

Figure S5. Variations in PL QY$_{abs}$ of TSP aqueous solution (10^{-3} mol/L) as a function of excitation wavelength.

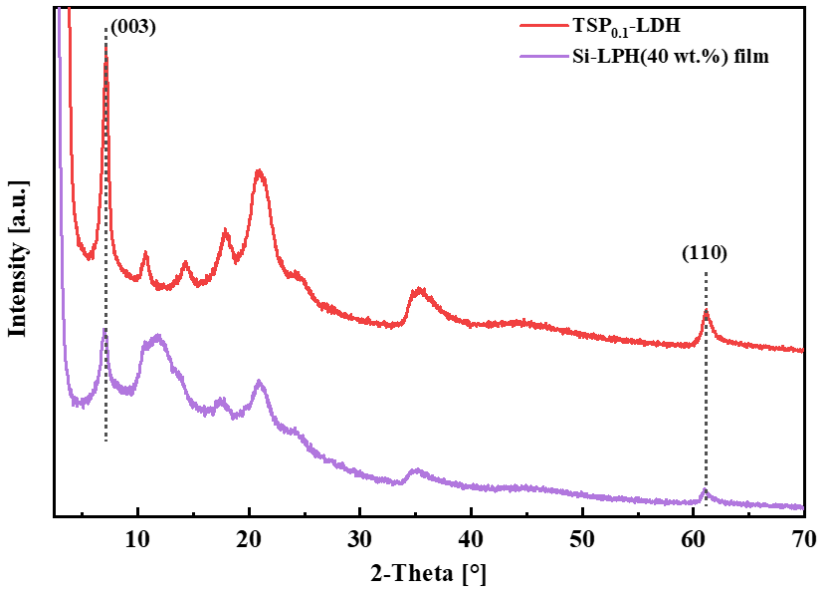

Figure S6. PXRD patterns of TSP$_{0.1}$-LDH powder and Si-LPH (40 wt.%) film.

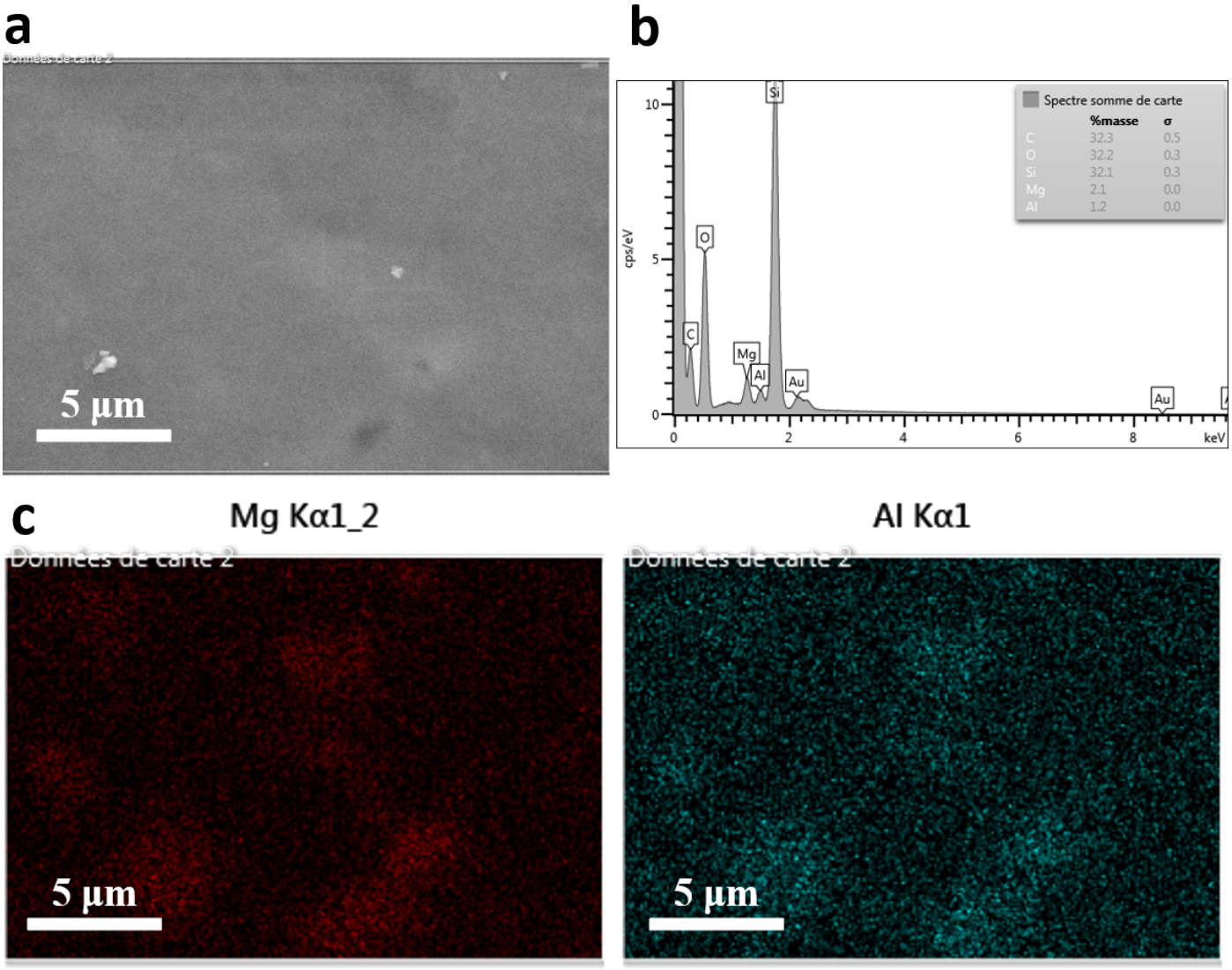

Figure S7. (a) SEM image and (b, c) EDX analysis of Si-LPH (40 wt%) film (the EDX analyzed area corresponds to the whole SEM image, the red dots refer to Mg and the blue to Al).

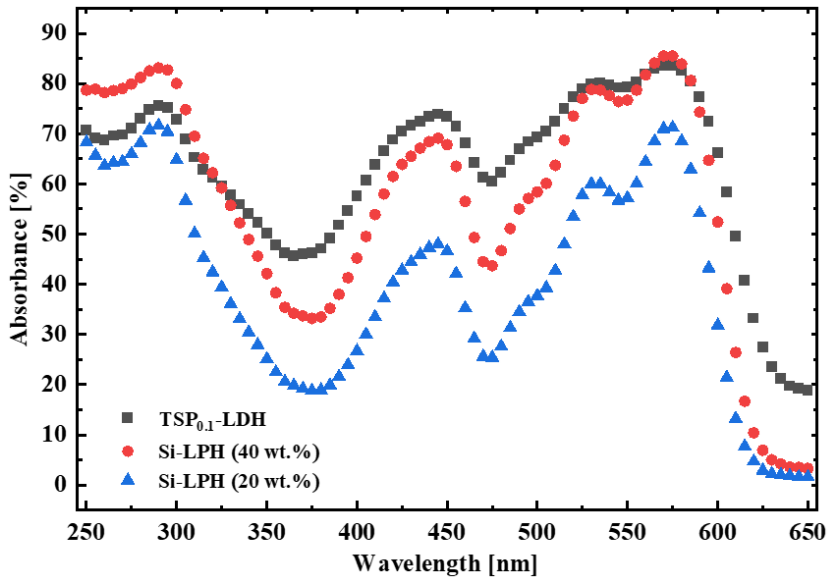

Figure S8. Comparison between absorbance spectra of Si-LPH composite film (20 wt.%) (blue line), Si-LPH composite film (40 wt.%) (red line) and $TSP_{0.1}$-LDH powder (black line).

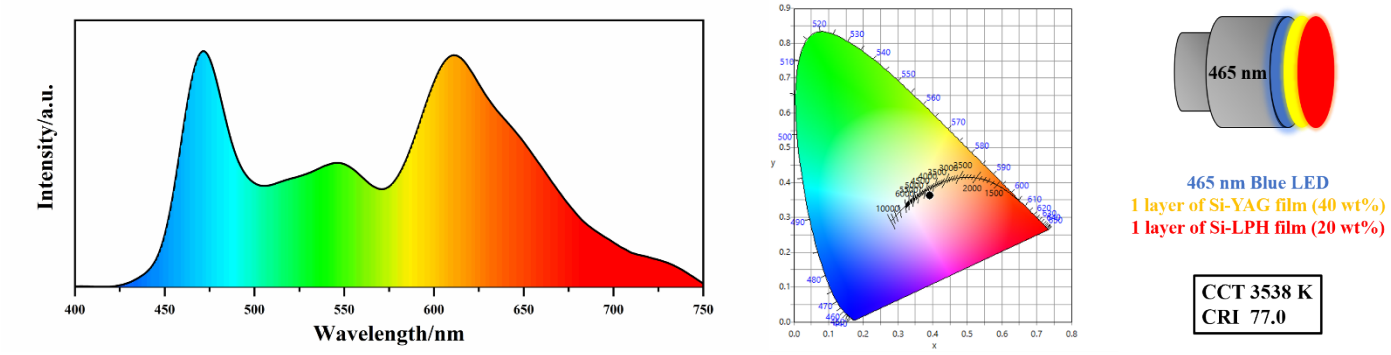

Figure S9. Emission spectra and photometric parameters of white LED prototypes designed using combinations of a commercial blue LED (465 nm) with configuration: Si-YAG film and Si-LPH film (20 wt.%).