

Supporting Information

for

Synthesis and Luminescent of Octacarboxy Cubic Polyhedral Oligosilsesquioxanes Coordinated with Terbium

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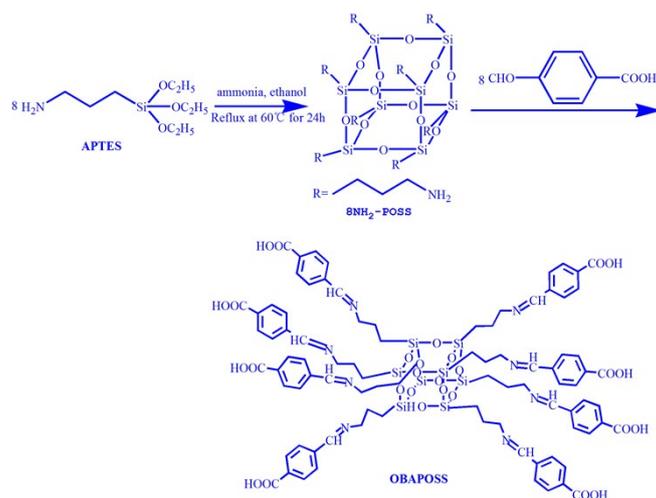
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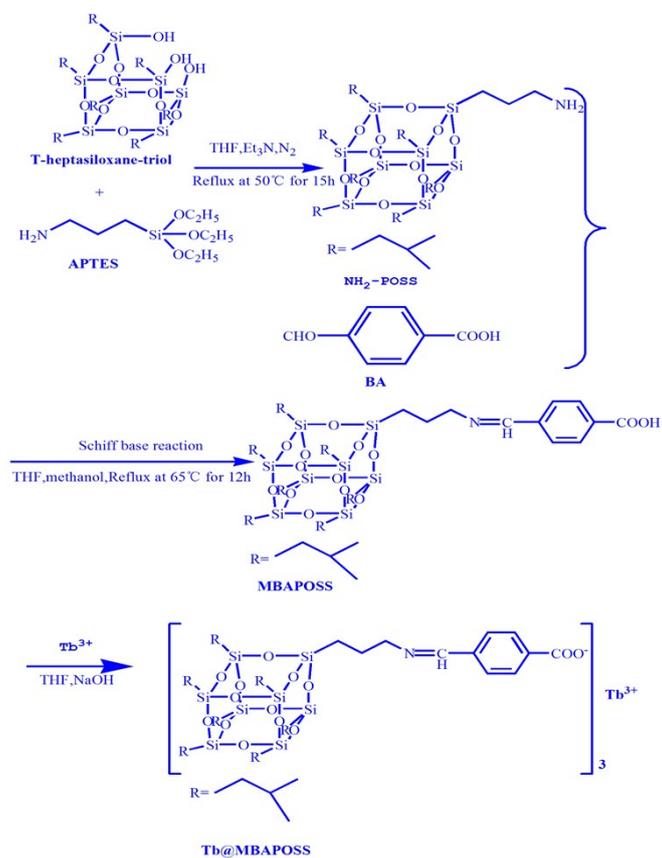
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Scheme S1. Synthesis procedures of the functionalized OBAPOSS.



Scheme S2. Synthesis procedures of the functionalized Tb@MBAPOSS.

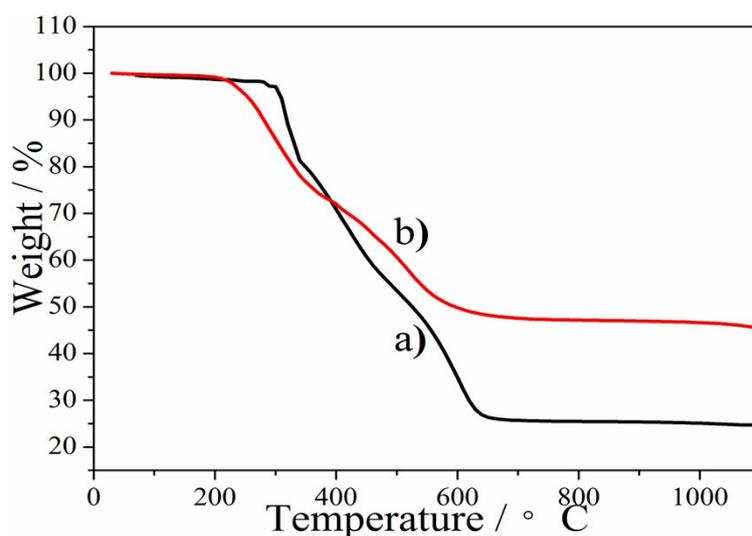


Figure S1. The thermogravimetric analysis of a) OBAPOSS and b) MBAPOSS.

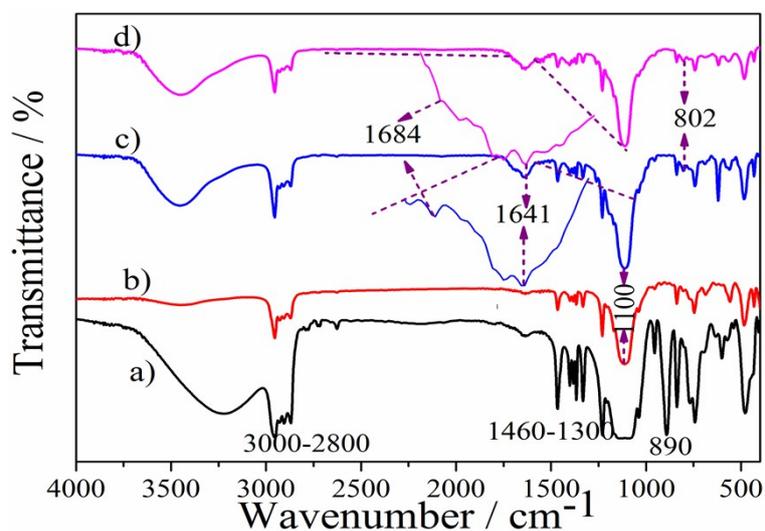


Figure S2. FT-IR spectra of a) T, b) NH₂-POSS, c) MBAPOSS and d) Tb@MBAPOSS.

As shown in Figure S2, the FT-IR spectra of all the samples show peaks at 3000-2800 and 1460-1300 cm^{-1} , which can be assigned to the stretching and bending modes of the isobutyl moieties. In addition, an intense peak at 1110 cm^{-1} can be attributed to asymmetric stretching of Si-O-Si, and the band at 802 cm^{-1} can be assigned to Si-C rocking. The FT-IR spectra of T (Figure S2a) show two bands at 3250 and 890 cm^{-1} may be assigned to stretching and bending of Si-OH, respectively, which were no longer seen in the IR spectrum of NH₂-POSS, indicating that the cage was completely condensed. In addition, a intense peak at about 1641 cm^{-1} assigned to the C=N stretching can be observed in MBAPOSS and Tb@MBAPOSS spectrum (Figure S2

c&d). In addition, the bands at 1684 cm^{-1} belong to stretching vibrations of carboxyl in MBAPOSS. After coordinated with Tb^{3+} , the characteristic stretching vibrations of carboxyl at 1684 cm^{-1} almost completely disappeared. This phenomenon indicates that the Tb^{3+} is successfully coordinated to OBAPOSS.

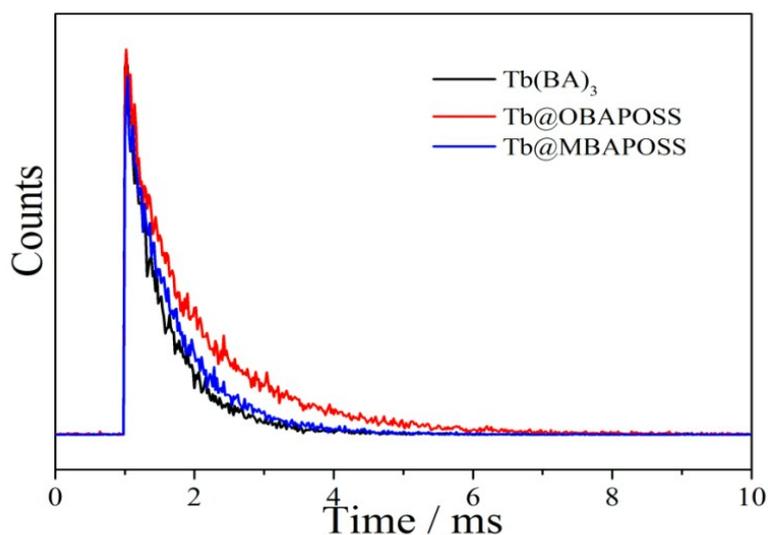


Figure S3. Decay curve of Tb@OBAPOSS (red line), Tb@MBAPOSS (blue line) and $\text{Tb}(\text{BA})_3$ (black line) measured at room temperature using an excitation of 300 nm and monitored at 544 nm, which can be well-fitted by mono-exponential function.

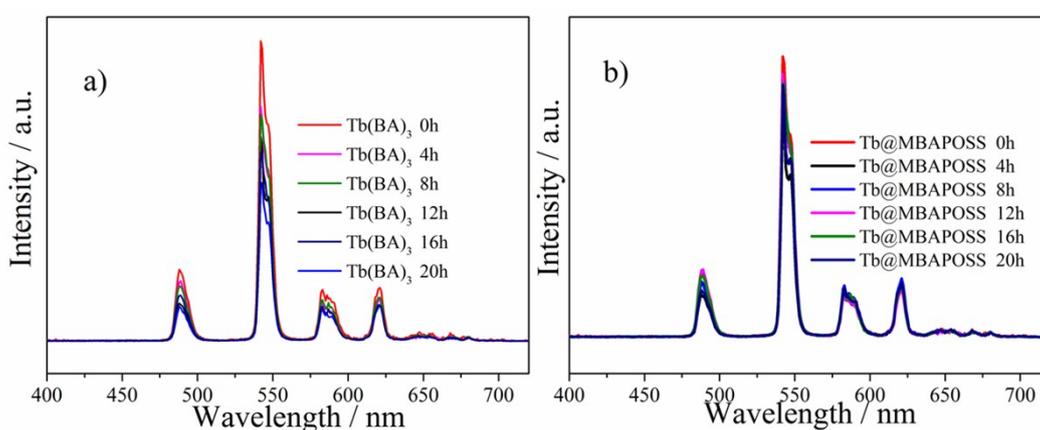


Figure S4. Changes of emission luminescence spectra of a) $\text{Tb}(\text{BA})_3$, b) Tb@MBAPOSS monitored at 544 nm at different exposure time under UV light irradiation ($\lambda_{\text{ex}} = 300\text{ nm}$).

Table S1. Changes of decay time of the 5D_4 state of $Tb(BA)_3$, $Tb@MBAPOSS$ and $Tb@OBAPOSS$ under UV irradiation

Time / h	0	4	8	12	16	20
$\tau_{Tb(BA)_3}/ms$	0.51	0.54	0.50	0.44	0.40	0.37
$\tau_{Tb@MBAPOSS}/ms$	0.54	0.49	0.48	0.49	0.50	0.49
$\tau_{Tb@OBAPOSS}/ms$	0.91	0.92	0.91	0.90	0.89	0.90

Table S2. Changes of the quantum yield of $Tb(BA)_3$, $Tb@MBAPOSS$ and $Tb@OBAPOSS$ under UV irradiation

Time / h	0	4	8	12	16	20
$\Phi_{Tb(BA)_3}/ms$	25.3%	24.5%	22.1%	20.9%	18.2%	16.3%
$\Phi_{Tb@MBAPOSS}/ms$	31.4%	30.2%	30.8%	29.1%	29.7%	28.9%
$\Phi_{Tb@OBAPOSS}/ms$	39.8%	39.2%	40.1%	39.0%	39.5%	39.0%

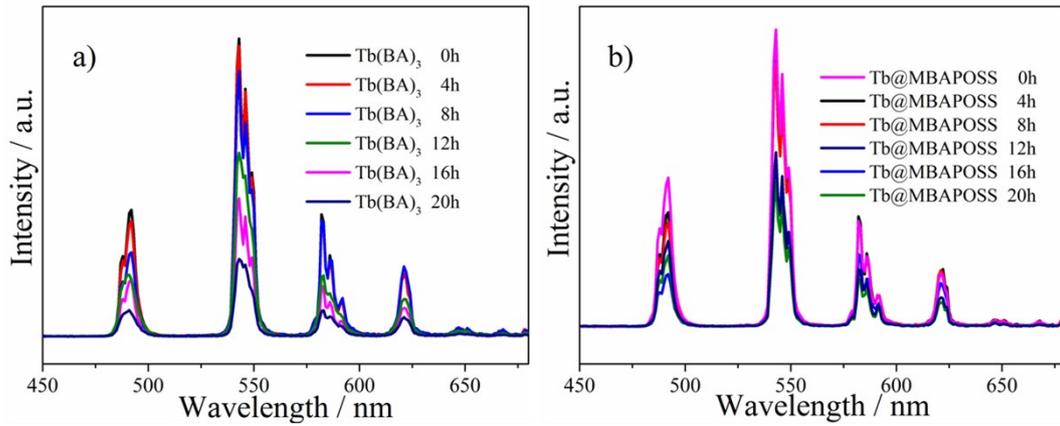


Figure S5. Changes of emission luminescence spectra of a) $Tb(BA)_3$, b) $Tb@MBAPOSS$ monitored at 544 nm at different exposure time at 120 °C ($\lambda_{ex} = 300$ nm).

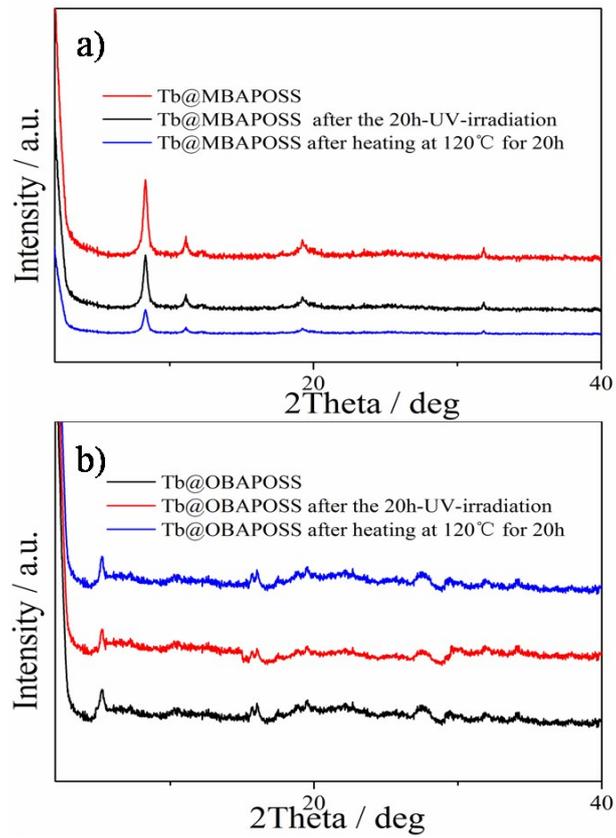


Figure S6. The P-XRD of a) Tb@MBAPOSS and b) Tb@OBAPOSS after 20h-UV-irradiation and heating at 120 °C for 20 h.