Supporting Information

Lanthanide Directed Luminescent "Soft" Coordination Polymer Gels: White Light Emission, Anticounterfeiting and Thin-film Based Sensing

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Experimental section:

Materials Used. 5- Amino isophthalic acid, and 1,3,5-benzenetricarbonyl trichloride were bought from Sigma-Aldrich. Poly(methyl methacrylate) was bought from tokyo chemical industry. 4- Dimethylaminopyridine was purchased from Sisco Research Laboratories (SRL). All the metal salts and solvents were purchased from Central Drug House (CDH) and utilized without further purification. The solvents N,N-dimethyl sulfoxide (DMSO), N, N-dimethylacetamide (DMA) and tetrahydrofuran (THF) were used without further distillation.

Characterization. Malvern Panalytical Empyrean diffractometer (with $\lambda = 1.5418$ Å, Cu Ka radiation) was utilized for powder X-ray diffraction (PXRD) measurement. The morphology of the luminescent CPGs was explored by the ZEISS GEMINISem500 field emission scanning electron microscope attached to an EDX spectroscopy detector. To record the SEM images, a small amount of dried form of CPGs (i.e., xerogels) was sprinkled onto a double-sided carbon tape mounted onto an aluminium SEM stub. The as-synthesized luminescent materials were further studied through a transmission electron microscope (a JEOL-JEM-F200) operating at 200 kV. To record the TEM images, a minimal amount of xerogel was dispersed in 1 mL ethanol, subsequently sonicated for 30 min, and then xerogel containing ethanol drop-casted on a TEM grid. The MCR 302-Anton Paar rheometer was used for rheological studies. To confirm the gel property of the assynthesized luminescent CPGs, the storage modulus (G') and loss modulus (G'') values were obtained against angular frequency and shear strain on a 9 mm diameter parallel plate at room temperature. FTIR analysis was carried out by PerkinElmer spectrum 400 in ATR mode. The UV-vis spectra were recorded by Shimadzu UV2500 spectrophotometer. Thermogravimetric analysis was performed under a nitrogen atmosphere at a scan rate of 10 °C/min by SDT Q600 (TA Instruments). A Horiba TCSPC spectrometer equipped with a picosecond pulsed diode laser

and an MCP-PMT detector was used to record time-resolved photoluminescence data for Tb@BTT and after adding TNP in the Tb@BTT. Edinburg FSP 920 Instrument was used for measuring lifetime of the Eu@BTT and Eub@BTT CPGs.

Recyclability test. After each cycle of the sensing experiment, the material was washed multiple times with tetrahydrofuran, followed by acetone to remove the dissolved TNP and NP from the dispersed solution. The xerogel material was collected through filtration. Prior to reuse, the obtained material after filtration was kept in a vacuum oven at 50 °C for 12 h.

Methods:

Quenching efficiency was calculated with help of the following equation, expressed by

$$(1 - (I/I_0)) \times 100 \%$$
(Eq-S1)

Stern-Volmer equation was utilized for the quantitative analysis of the quenching analysis, which is expressed as,

$$I_0 / I = K_{sv}[Q] + 1$$
 (Eq-S2)

The low detection of limit was calculated using $3\sigma/k$ equation (where σ = standard deviation of repetitive blank measurements and k is the slope of the line) where K_{sv} is the Stern-Volmer (S-V) constant or quenching effect coefficient (M⁻¹), and the molar concentration of the quencher is denoted by Q.¹

Quantum yield measurement:

Here, we have utilized the Parker-Rees method² to calculate the quantum yield of the prepared luminescent materials, using a 0.5 M H₂SO₄ solution of quinine sulphate as a standard reference. The formula for this calculation is provided as follows:

 $\Phi_{\rm s} = (A_{\rm r}F_{\rm s}n_{\rm s}^{2}/A_{\rm s}F_{\rm r}n_{\rm r}^{2}) \Phi_{\rm r}$ (Eq-S3)

In this equation, Φ_r represents the quantum yield of the quinine sulfate reference solution, while Φ_s represents the quantum yield of the sample. The absorbance maxima were kept under 0.1 to minimize the reabsorption of fluorescent light that passed through the materials. The values of A_r and A_s correspond to the absorbance of the reference and sample, respectively, whereas F_r and F_s refer to the integrated area of fluorescence intensity for the reference and sample, respectively. The refractive indices of the reference and sample are represented by n_r and n_s , respectively.³ Table S1 contains the relevant photophysical parameters and quantum yield values.

Table S1. Photophysical parameters of the as-synthesized materials and Quinine Sulfate,

required for quantum yield calculation

Sl. No.	Sample Name	Excitation Wavelength λ _{ex} (nm)	Absorbance (A)	Area of Integrated Fluorescence Intensity (F)	Quantum Yield (Φ)
1	Quinine Sulphate	310	0.095	2.254E8	0.540
2	Tb@BTT	321	0.071	5.044E7	0.175
3	Eu@BTT	321	0.048	9.110E6	0.047
4	EuTb@BTT	321	0.055	2.242E7	0.100

Excited State Calculation: All the theoretical calculations were performed with the help of Density Functional Theory (DFT), by using the Gaussian 16 package of programs. The molecular geometry of BTT ligand was optimized using B3LYP functional in conjunction with 6-31+G(d,p) basis set, as shown in Figure S7. The impact of solvent was not taken into account to match the solid-state experimental setting. Based on the optimized singlet ground state geometry, the energy of the triplet excited state of BTT ligand was calculated to be 30068 cm⁻¹ using the time-dependent DFT (TDDFT) approach.



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