A Strong Donor-Acceptor System Based on a Metal Chalcogenide Cluster and Porphyrin

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Table S1 Crystal Data and Structural Refinement Parameters for **1** and **2.**

	1	**2**
formula	$C_{44}H_{48}Ge_4N_8O_5S_{10}$	$C_{44}H_{62}Ge_4MnN_8O_{13}S_{10}$
fw	1380.11	1576.91
cryst size (mm^3)	0.05 × 0.10 × 0.20	0.08 × 0.15 × 0.16
cryst syst	monoclinic	orthorhombic
space group	*P* $2_1/m$	*Pbcn*
a (Å)	10.8645(10)	22.056(2)
b (Å)	18.2548(14)	21.656(2)
c (Å)	14.0599(11)	25.966(2)
α (deg)	90.00	90.00
β (deg)	99.670(8)	90.00
γ (deg)	90.00	90.00
V ($Å^3$)	2748.9(4)	12402.5(19)
Z	2	8
ρ_{calcd} (g cm^{-3})	1.628	1.689
F(000)	1360	6392
μ (mm^{-1})	2.592	2.515
T (K)	223(2)	223(2)
reflns collected	15794	49983
unique reflns	5001	10915
observed reflns	2474	4535
no. params	312	608
GOF on F^2	1.015	1.185
R_1 [I>2σ(*I*)]	0.0647	0.0786
$_wR_2$ [I>2σ(*I*)]	0.0967	0.1541

Table S2 The energy (eV) of the frontier molecular orbitals of **1** and **2**.

	1		**2**	
	α	**β**	**α**	β
LUMO+1	–3.16577	–3.49367	–2.81366	–3.23761
LUMO	–3.36061	–3.65667	–3.09638	–3.2904
HOMO	–4.45178	–3.92687	–4.25695	–3.91817
HOMO–1	–4.63845	–4.35382	–4.40199	–4.2213
Δ*E**	1.09	0.27	1.16	0.63

*energy gap $\Delta E = E_{LUMO} - E_{HOMO}$

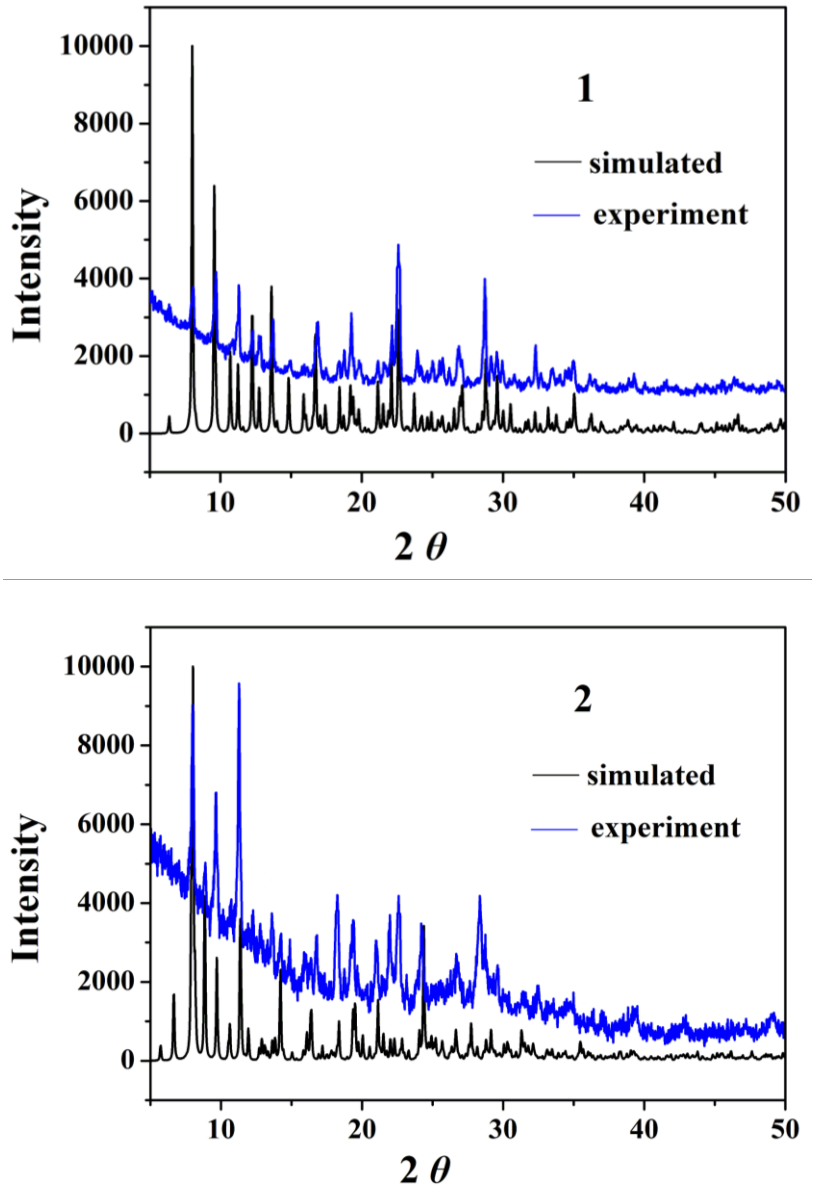

Figure S1 The experimental bulky sample powder XRD pattern and the calculated pattern from the crystal data of compounds **1** and **2**.

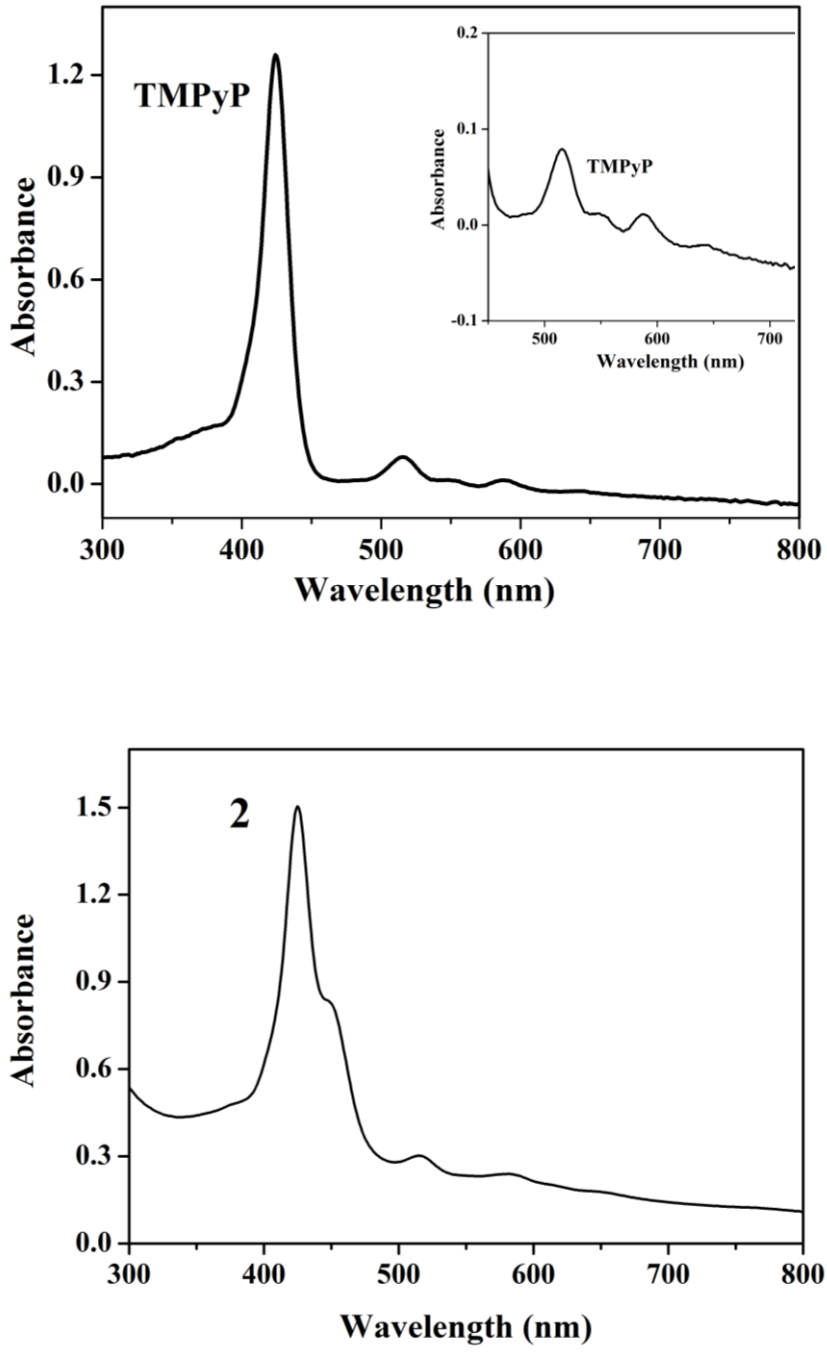

Figure S2 The UV-Vis absorption of compounds $TMPyP(PF_6)_4$ (6.0×10^{-6} mol·L^{-1}) and **2** (1.0×10^{-5} mol·L^{-1}) in DMSO.

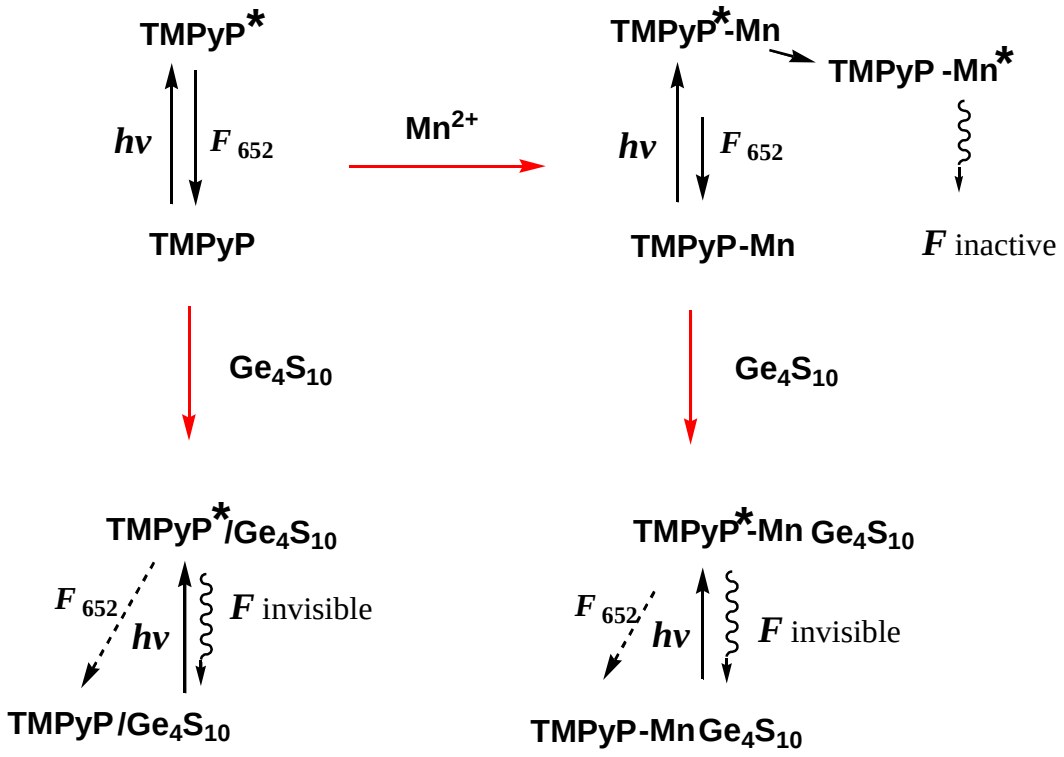

Figure S3 Schematic diagrams of the energy states and transfer pathways for the fluorescence quenching.