Supporting Information

Pure white light emission from Rare Earth free intrinsic Metal Organic Framework and its application in WLED

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SI 1. Crystallographic Data for$ZnipaPy_2$:

Empirical formula	$C_{18}H_{17}N_5O_6Zn$
Formula weight	464.73
Temperature/K	100
Crystal system	Monoclinic
Space group	$P2_1/c$
a/Å	8.617(8)
b/Å	22.95(2)
c/Å	10.243(9)
α/°	90
β/°	102.365(15)
γ/°	90
Volume/Å^3	1978(3)
Z	4
ρ_{calc}g/cm^3	1.560
μ/mm^{-1}	1.288
F(000)	952.0
Crystal size/mm^3	0.16 × 0.12 × 0.08
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.5 to 46.6
Index ranges	$-9 \leq h \leq 9$, $-25 \leq k \leq 25$, $-11 \leq l \leq 10$
Reflections collected	12204
Independent reflections	2855 [R_{int} = 0.1647, R_{sigma} = 0.1503]
Data/restraints/parameters	2855/0/271
Goodness-of-fit on F^2	1.002
Final R indexes [I>=2σ (I)]	R_1 = 0.0597, wR_2 = 0.1312
Final R indexes [all data]	R_1 = 0.1372, wR_2 = 0.1807
Largest diff. peak/hole / e Å^{-3}	0.53/-0.83

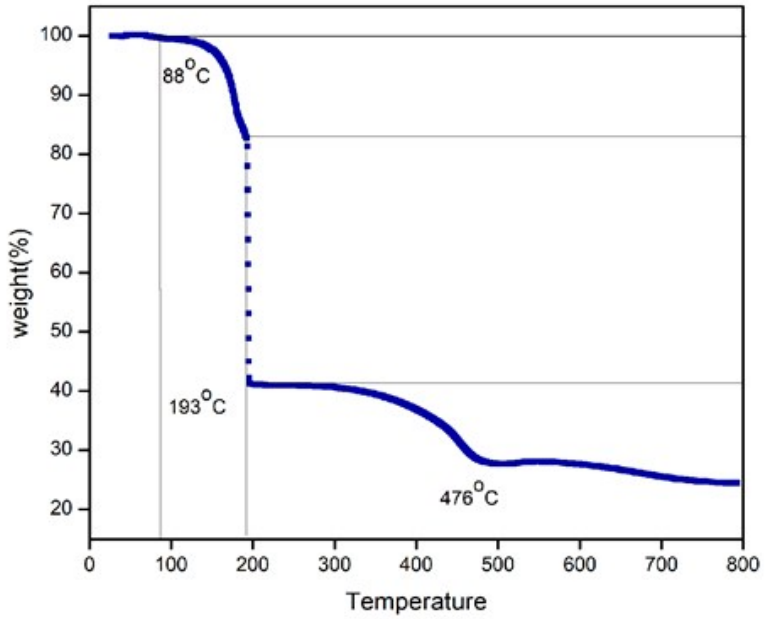

Figure SI2: Thermogravimetric analysis (TGA) of $ZnipaPy_2$

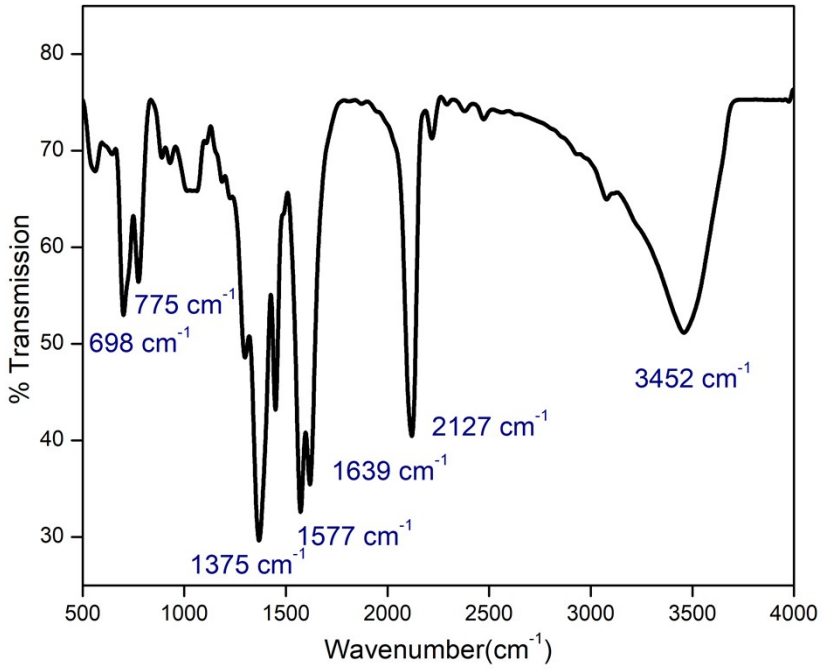

Figure SI3: FT-IR spectrum of $ZnipaPy_2$.

Absorption Spectroscopy:

Absorption spectroscopy of $ZnipaPy_2$ was measured by dissolving the solid sample in acetonitrile solvent.

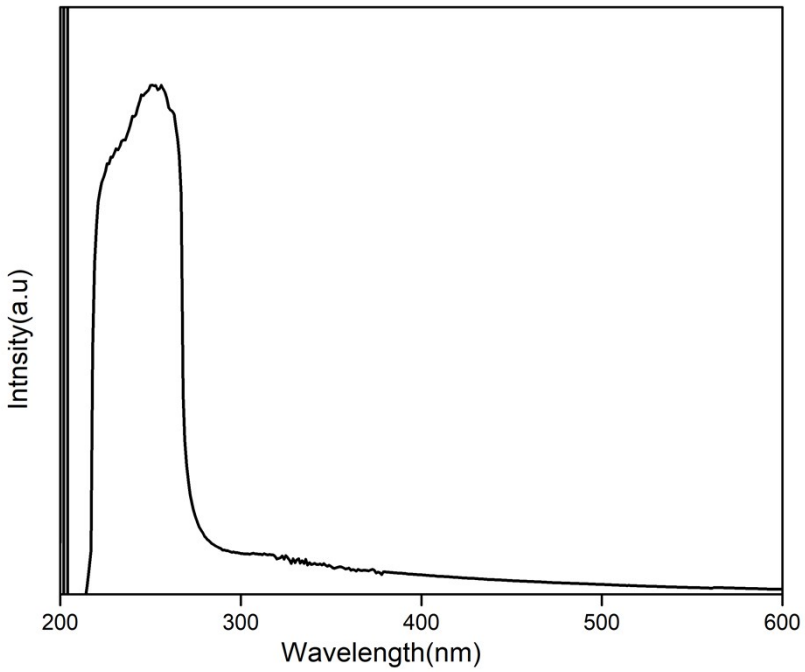

Figure SI4: Absorption Spectrum of $ZnipaPy_2$

Photoluminiscence emission intensity comparision:

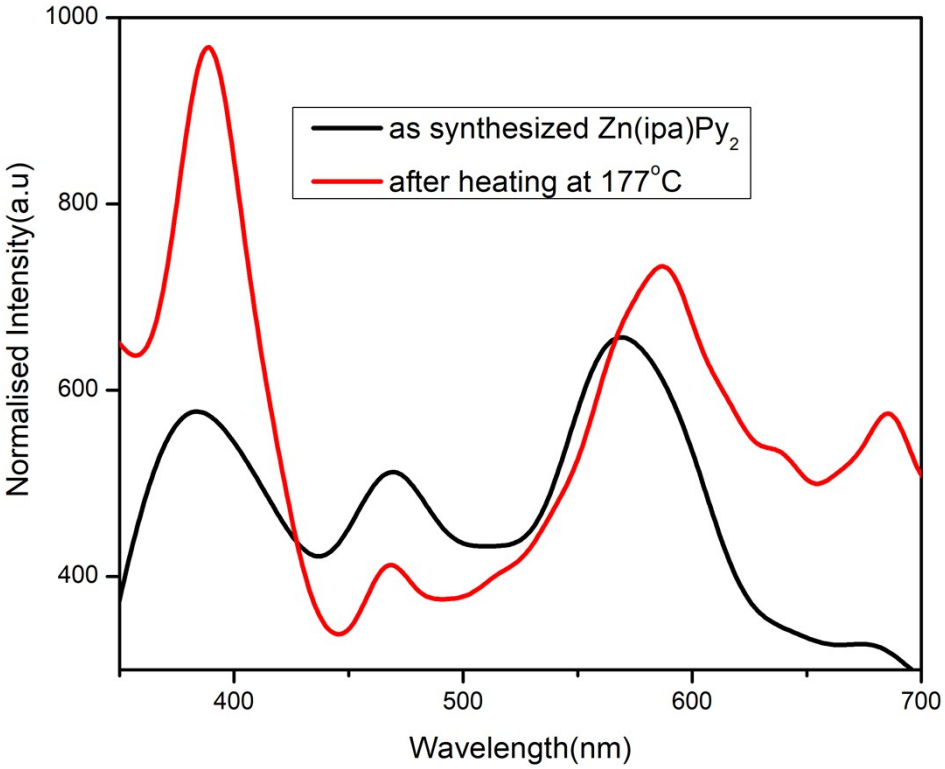

Figure SI5: Comparison of photoluminescence intensities of as synthesised MOF and after heating it at 177°C.

DFT study in support of Photoluminescence Spectra:

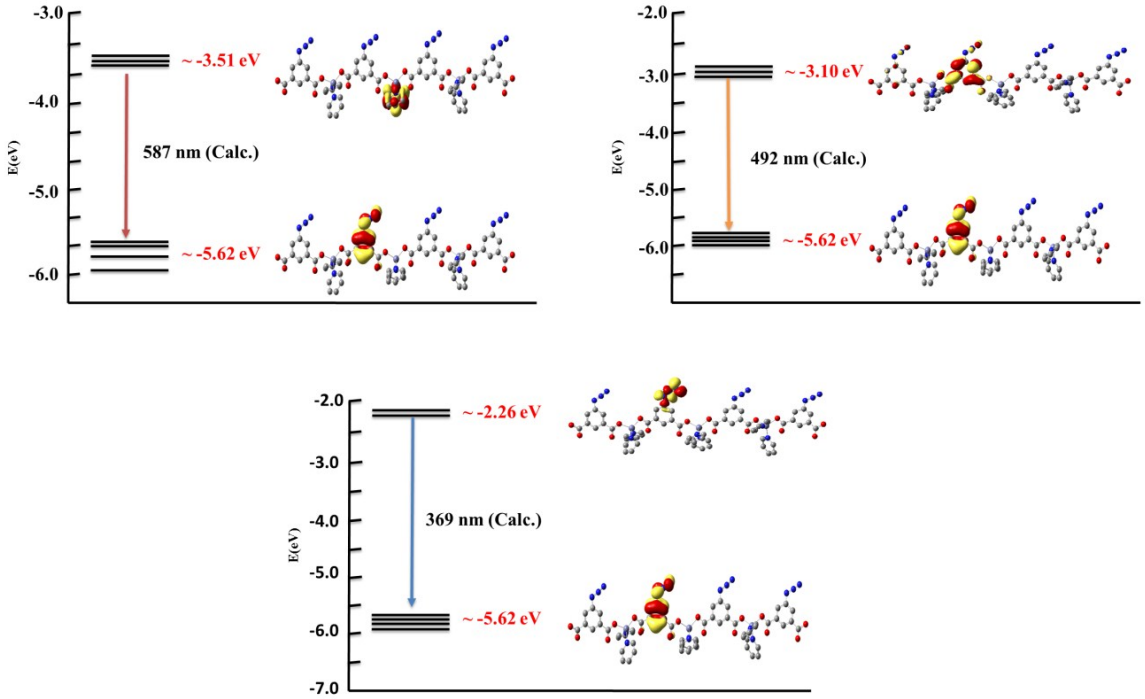

Figure SI6: The possible transitions shown by DFT.

Photoluminescence Excitation spectra:

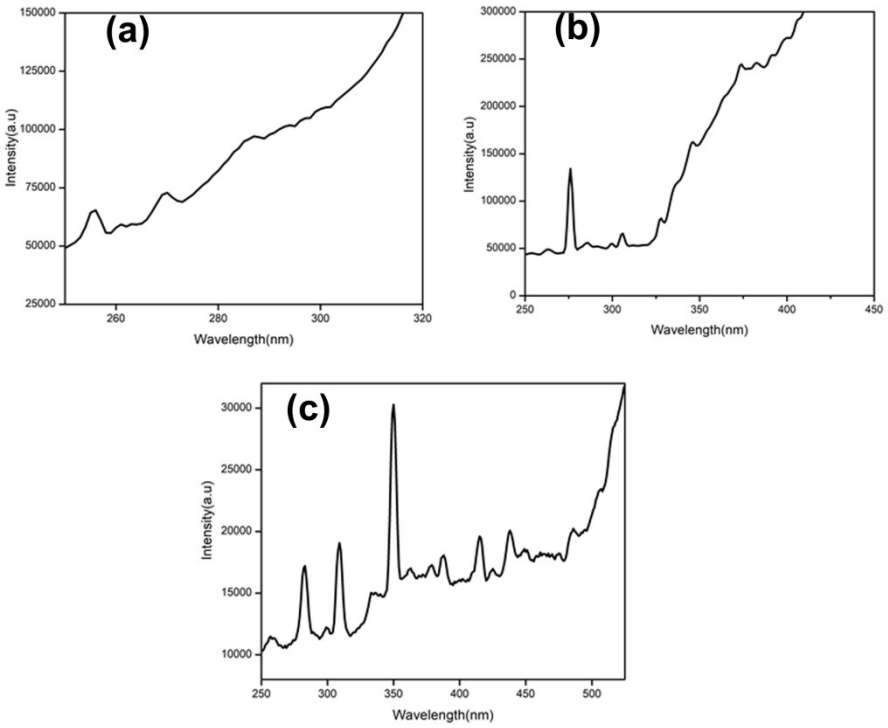

Figure SI7: Photoluminescence excitation spectra monitoring (a) 385 nm emission (b) 468 nm emission (c) 593 nm emission peaks.

TCSPC Measurement:

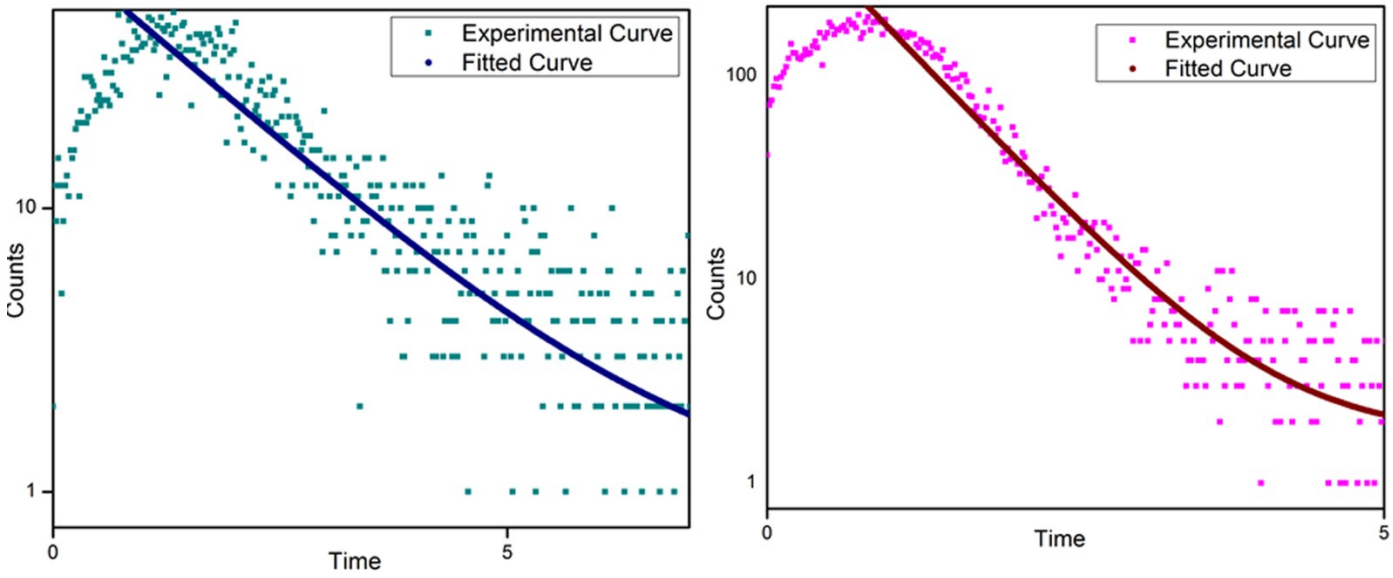

Figure SI8: Lifetime decay curve of $ZnipaPy_2$

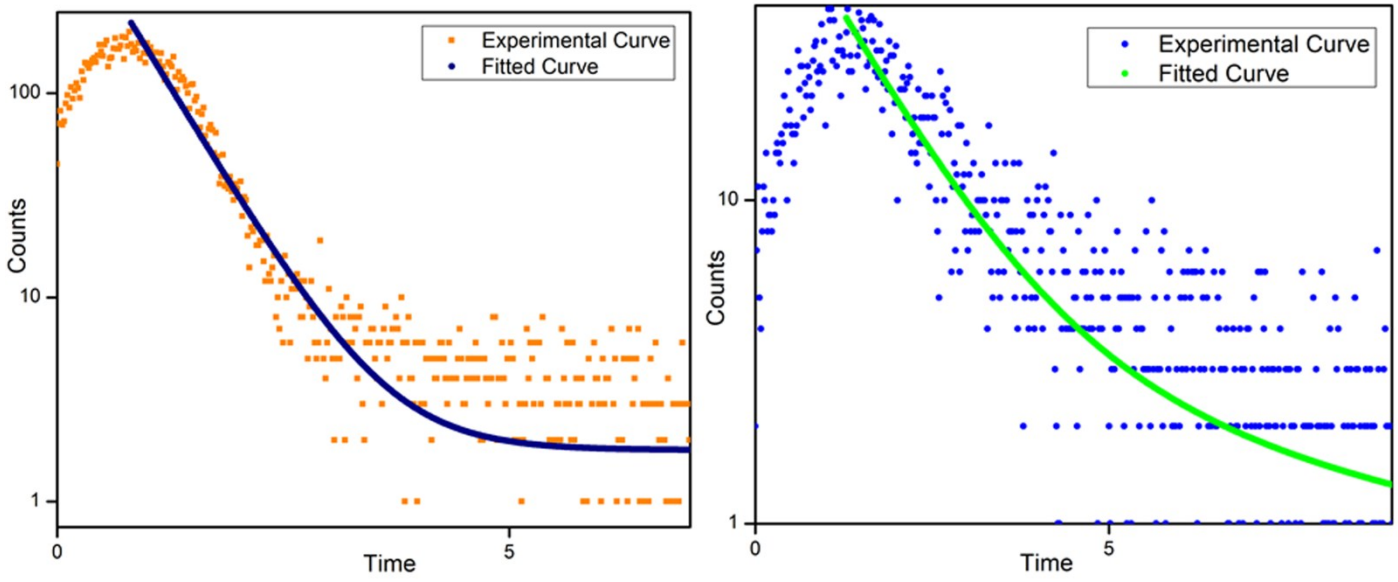

Figure SI9: Lifetime decay curve of the free ligand

HOMO –LUMO band position calculation:

To estimate the actual, the band alignment of the ZnipaPy2 material we have used cyclic voltammetry and Uv-Vis spectroscopy. The measurements were performed at room temperature under an inert atmosphere using a three electrode system consisting of a Pt wire as the counter and working electrodes and Ag/Ag+ as the reference electrode.The positions of LUMO orbital of the ZnipaPy2 was obtained from the onset reduction potential (E_{red}) using the followingequations[1].

$$E_{CB/LUMO} = -(E_{red} + 4.71)\ eV = -\ (-1.1 + 4.71)\ eV = -\ 3.61\ eV$$

Here the potential is considered with respect to Ag/Ag^{+} reference electrode.

The difference between HOMO and LUMO was obtained from UV-Vis spectroscopy using standard method[2]. The Difference is found to be 2.09 eV. Therefore, The Position of HOMO would be (-3.61-2.09) eV = -5.70 eV.

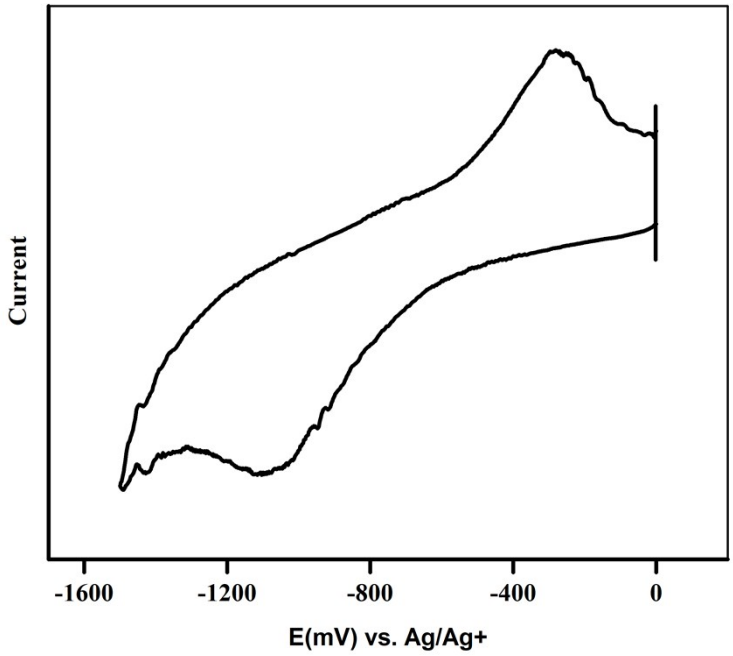

Figure SI10: CV diagram of $ZnipaPy_2$

Cyclic Voltammogram of the $ZnipaPy_2$ in acetonitrile solvent with tetrabutylammonium perchlorate as supporting electrolyte. The potential is reference with respect to Ag/Ag^+ reference electrode.

References:

1. M. K. Barman, P. Mitra, R. Bera, S. Das, A. Pramanik, and A. Parta, *Nanoscale*, 2017,**9**, 6791-6799

2. V. Srikant, and D. R. Clarke, *Journal of Applied Physics,* 1998**, 83,** 5447