

Supplementary Figure S1 Scheme of synthesis of the H₆TATPT ligand.



Supplementary Figure S2 Photograph of crystals of compound 1.



Supplementary Figure S3 Crystal structures of compound 1. (a) The coordination environment of Cd^{2+} ion and its connectivity with TATPT ligands, C gray, O red, N blue, Cl green and Cd orange. (b) Coordination mode of TATPT ligand. (c) Ball and stick representations show the 3D structure in 1 viewed along the *a*-axis. The orange and blue spheres represent the void inside the cages. (d) Polyhedral representations of the crystal structure viewed along a axis in which the cuboid represented the $Cd_2(\mu_2-Cl)(CO_2)_8$ secondary building unit (SBU).



Supplementary Figure S4 TG profile. TG profile of compound **1** under nitrogen gas atmosphere with a heating rate of 10 °C·min⁻¹. The inset is the TG profile of desolvated **1** from 50 to 280 °C under nitrogen gas with a heating rate of 2 °C·min⁻¹.



Supplementary Figure S5 Photographs of 1 and samples after ion exchange with transition metals. (a) As-synthesized 1. (b) $Cu^{2+} \supseteq 1$. (c) $Co^{2+} \supseteq 1$. (d) $Ni^{2+} \supseteq 1$. (e) $Zn^{2+} \supseteq 1$.



Supplementary Figure S6 PXRD patterns. PXRD patterns for 1 and transition metal ion exchanged 1. simulated, black; as-synthesized 1, yellow; $Co^{2+} \supseteq 1$, blue; $Ni^{2+} \supseteq 1$, red; $Zn^{2+} \supseteq 1$, green; $Cu^{2+} \supseteq 1$, purple.



Supplementary Figure S7 ¹**H NMR spectrum**. The ¹H NMR spectrum in dmso-d₆solution taken after ion exchange experiment.



Supplementary Figure S8 photoluminescence spectrum of ligand. Solid photoluminescence spectrum of H₆TATPT ligand at room temperature ($\lambda_{ex} = 370$ nm).



Supplementary Figure S9photoluminescence spectrum of 1.Solidphotoluminescence spectrum of compound 1 at room temperature uponexcitation at 370 nm.



Supplementary Figure S10 photoluminescence spectra of $[Ir(ppy)_2(bpy)][PF_6]$. Room temperature photoluminescence spectra of $[Ir(ppy)_2(bpy)][PF_6]$ in DMF solvent (top) and in solid state (bottom) upon



Supplementary Figure S11 PXRD patterns. PXRD patterns for **1** (simulated, black; as-synthesized**1**, yellow) and [Ir(ppy)₂(bpy)]⁺ encapsulated **1** with different concentrations of [Ir(ppy)₂(bpy)]⁺ (0.52wt%, olive; 1.04wt%, violet; 3.5wt%, red; 3.7wt%, green; 4.5wt%, blue; 7.5wt%, cyan; 8.8wt% pink).



Supplementary Figure S12 Photographs of 1 and [Ir(ppy)₂(bpy)]⁺@1 (under natural light (left) and laboratory UV light (365 nm, right)). (a) As-synthesized 1.
(b) 3.5wt% contained [Ir(ppy)₂(bpy)]⁺@1. (c) 8.8wt% contained [Ir(ppy)₂(bpy)]⁺@1.



Supplementary Figure S13 Photographs of crystals. Photographs of a single crystal of a freshly

grown $[Ir(ppy)_2(bpy)]^+@1$ (left) and crushed fragments of the same crystal (right).



Supplementary Figure S14 Optical spectra. The absorption spectrum of 1 (blue), and emission spectrum of the $[Ir(ppy)_2(bpy)]^+$ complex excited at 370 nm (green).



Supplementary Figure S15 Optical spectra. The absorption spectrum of the $[Ir(ppy)_2(bpy)]^+$

complex (red), and emission spectrum of **1** excited at 340 nm (black).



Supplementary Figure S16 Fluorescence decay profiles. Fluorescence decay profiles of **1** and $[Ir(ppy)_2(bpy)]^+@1$ at $\lambda_{ex} = 370$ nm and $\lambda_{em} = 425$ nm: black, after fitted; red, compound **1**; blue, 3.5% $[Ir(ppy)_2(bpy)]^+@1$; green, 8.8% $[Ir(ppy)_2(bpy)]^+@1$.



Supplementary Figure S17 Temperature-dependent photoluminescence spectra. Photoluminescence spectra of white-emitting $[Ir(ppy)_2(bpy)]^+@1$ at different temperatures: black, 298K; red, 318K; green, 338K; blue, 358K; violet, 378K; dark yellow, 388K; wine, 398K; gray, 408K; pink, 423K. All measurements were performed on solid samples at an excitation wavelength λ_{ex} of 370 nm.



Supplementary Figure S18 Photographs of the white LED fabricated using a UV InGaAsN LED chip and white phosphor of 3.8 wt% [Ir(ppy)₂(bpy)]⁺@1. (a) Without current. (b) After applying a forward current of 150 mA.



Supplementary Figure S19 PXRD patterns. PXRD patterns for 1 and transition metal exchanged 1: as-synthesized 1, red; Eu³⁺@1, green; Tb@1, blue; Eu/Tb@1, orange.



Supplementary Figure S20 HRMS spectrum for the ligand (H₆TATPT). High resolution mass spectra (HRMS) were recorded on Bruck microTof using ESI method. (ESI) m/z calcd for C₂₇H₁₈N₆O₁₂ [M+H]⁺: 619.1016 found: 619.1058.



Supplementary Figure S21 ¹³C-NMR spectrum for the ligand (H₆TATPT,

 $C_{27}H_{18}N_6O_{12}$). Data were recorded on a Bruker AV400 NMR (400 MHz) at 25 °C.

Supplementary Table S1 Crystal data and structural refinement of compound **1**; for atomic coordinates, equivalent isotropic displacement parameters, bond lengths, angles, and anisotropic displacement parameters please see the CIF (CCDC code 916964).

Empirical formula	$C_{174}H_{288}N_{51}O_{78}Cl_3Cd_6\\$
Formula weight	5147.52
Temperature (K)	296
Crystal system	cubic
Space group	Fm-3m
Unit cell dimensions	
a (Å)	38.527(2)
b (Å)	38.527(2)
c (Å)	38.527(2)
α (°)	90
β (°)	90
γ (°)	90
Volume (Å ³)	57186.8 (6)
Z	8
Calculated density (mg/m ³)	1.196
F(000)	12600
Crystal size (mm ³)	$0.86 \times 0.44 \times 0.24$
$R_{ m int}$	0.0697
Goodness-of-fit on F^2	1.052
Final R indices $[I > 2\sigma(I)]$	$R_1 = 0.0896, wR_2 = 0.2749$

	The concentration of transition	The concentration of transition	
Transition metai	metal (wt%)	metal per formula	
Co	5.268	0.37	
Cu	7.021	0.46	
Ni	3.615	0.26	
Zn	4.307	0.28	

Supplementary Table S2 The concentration of Cu^{2+} , Co^{2+} , Ni^{2+} , and Zn^{2+} in compound 1.

Comula	CIE co	ordinate	The concentration of	
Sample	Х	Y	(respect to Cd wt%)	
1	0.175	0.145	0	
2	0.231	0.206	0.526	
3	0.254	0.239	1.04	
4	0.311	0.330	3.52	
5	0.322	0.352	3.73	
6	0.350	0.429	4.52	
7	0.371	0.468	7.50	
8	0.400	0.501	8.83	

Supplementary Table S3 The CIE coordinates of $[Ir(ppy)_2(bpy)]^+@1$ at various concentration of $[Ir(ppy)_2(bpy)]^+$.

Compound	Quantum yield	Reference number
PbL2 ^a	2-3%	26
Eu-SMOF-1 ^b	4.3%	25
ZJU-1:1.5%Tb ³⁺ , 2.0%Eu ^{3+c}	6.8%	12
$[AgL]_n nH_2O^d$	10.86%	23
Eu/Tb@1 ^e	11.3%	this work
$[Ir(ppy)_2(bpy)]^+@1^e$	20.4%	this work

Supplementary Table S4 Summary of the quantum yield of the reported white-emitting MOFs.

 $^{a}L2 = 2,5$ -bis((((S)-2-hydroxypropyl)thio)terephthalic acid

 b SMOF-1 = In(BTB)_{2/3}(OA)(DEF)_{3/2} (BTB = 1,3,5-Tris(4-carboxyphenyl)benzene, OA = oxalic acid,

DEF = N,N'-diethylformamide)

^cZJU-1 = Na₃[La(PDA)₃](H₂O)₁₂ (PDA = pyridine-2,6-dicarboxylate)

 $^{d}L = 4$ -cyanobenzoate

 ${}^{e}\mathbf{1} = [(CH_{3})_{2}NH_{2}]_{1.25}[(Cd_{0.5}Cl_{0.25})(TATPT)_{1/3}] \cdot DMF \cdot 1.5H_{2}O, (TATPT =$

2,4,6-tris(2,5-dicarboxylphenylamino)-1,3,5-triazine, DMF = N,N-Dimethylformamide)

eratures.						
Temperature (K)	298	378	388	398	408	423
Quantum yield (%)	20.7	21.1	20.1	19.7	18.5	17.9

Supplementary Table S5 Quantum yield of white-emitting $[Ir(ppy)_2(bpy)]^+@1$ at different ter

Supplementary Table S6 Correlated color temperature (CCT) and color rendering index (CRI) for white LED.

CCT		CIE		
(K)	CRI	х	У	
5409	84.5	0.30	0.35	