Electronic Supplementary Material (ESI) for Nanoscale.

Dual-Functional Porous MOFs with Hierarchical Guest Encapsulation for Room-Temperature Phosphorescence and White-Light-Emitting

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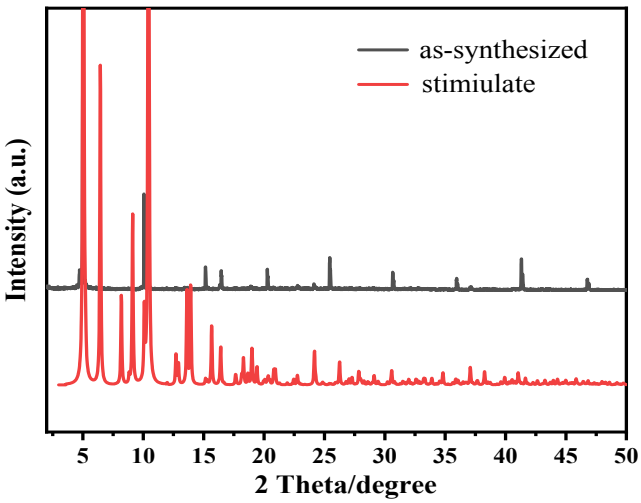


Figure S1. PXRD of PCN-921:as-synthesized (black line) and stimiulate (red line). Some diffraction peaks of the simulated curve are absent in the as-synthesized curve due to the crystal orientation. This phenomenon is consistent with the previous literature.[1]

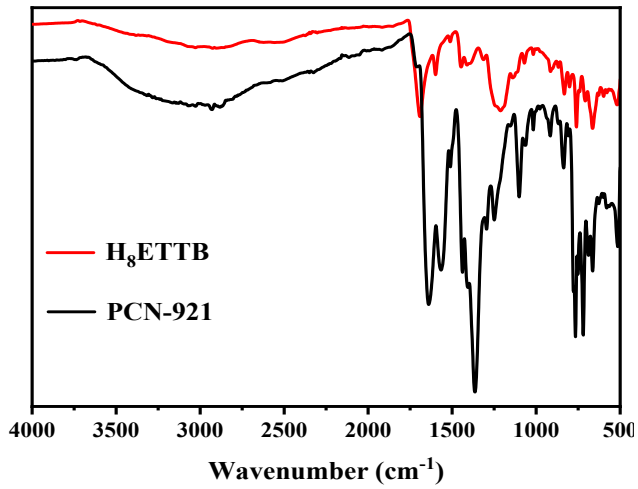


Figure S2. IR of H_8ETTB (red line) and PCN-921 (black line).

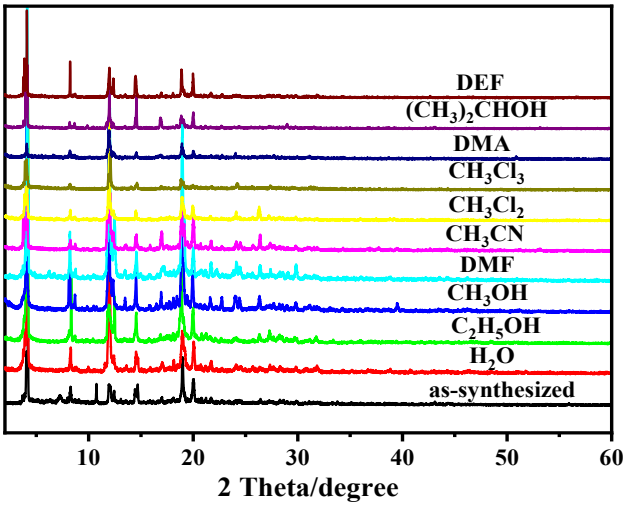


Figure S3. PXRD of PCN-921 MOF in different solvents.

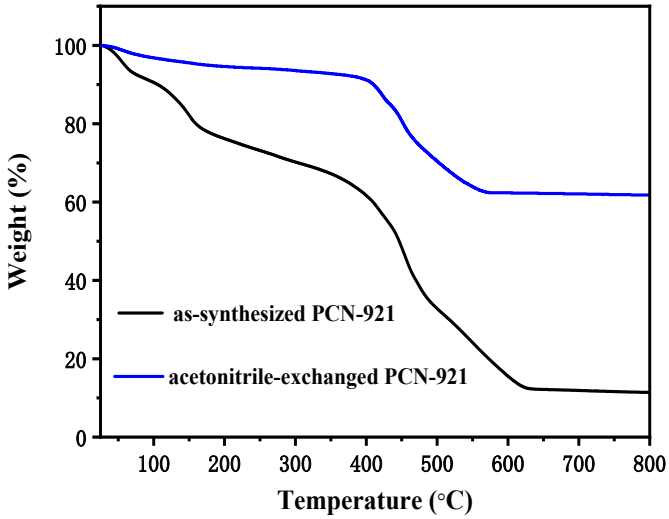


Figure S4. TGA of PCN-921 MOF before (black line) and after (blue lline) acetonitrile-exchanged.

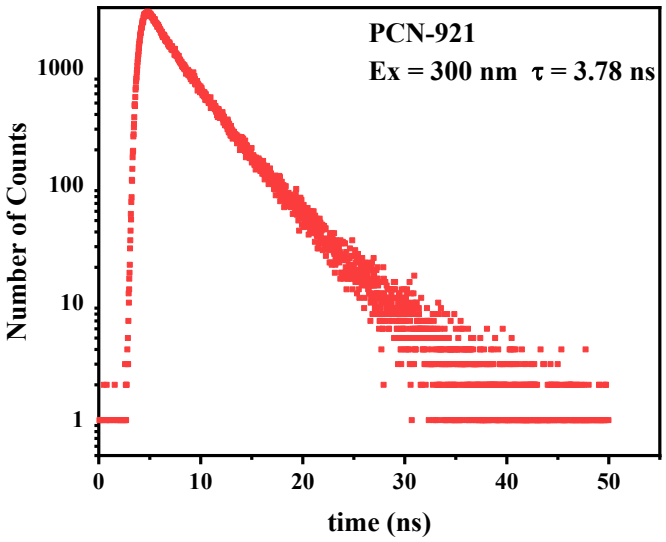


Figure S5. Fluorescence lifetime 3.78 ns of PCN-921 at Ex: 300 nm.

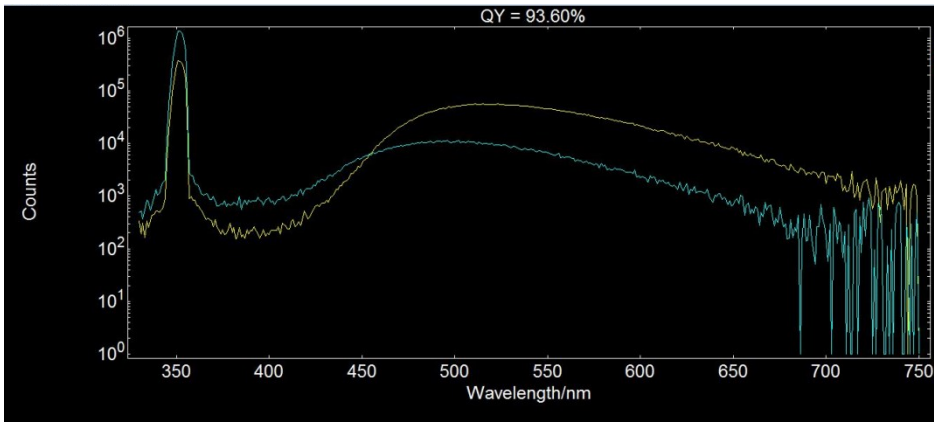


Figure S6. Quantum yield 93.6% of PCN-921 MOF.

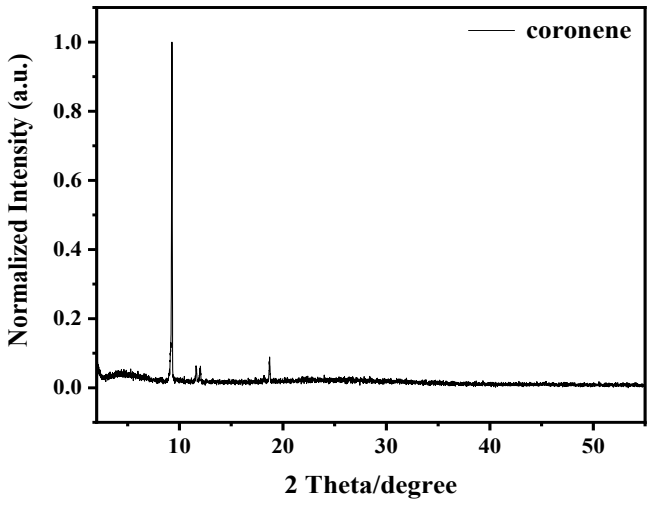


Figure S7. PXRD of coronene.

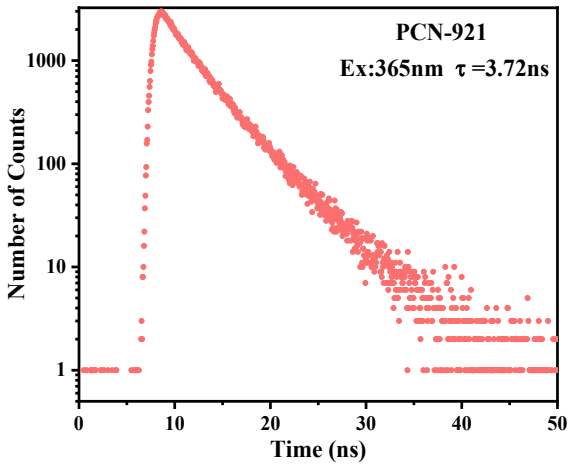


Figure S8. Phosphorescent lifetime 3.72 ns of PCN-921 MOF.

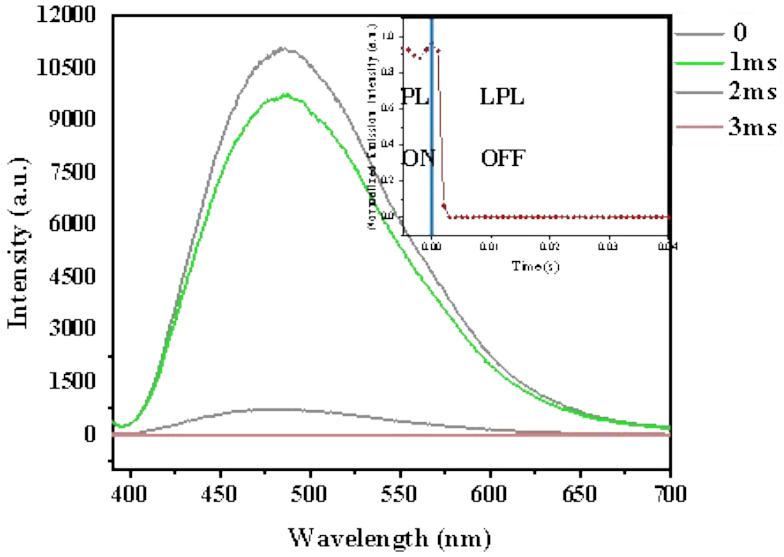


Figure S9. The instantaneous phosphor of PCN-921. There is almost no long afterglow.

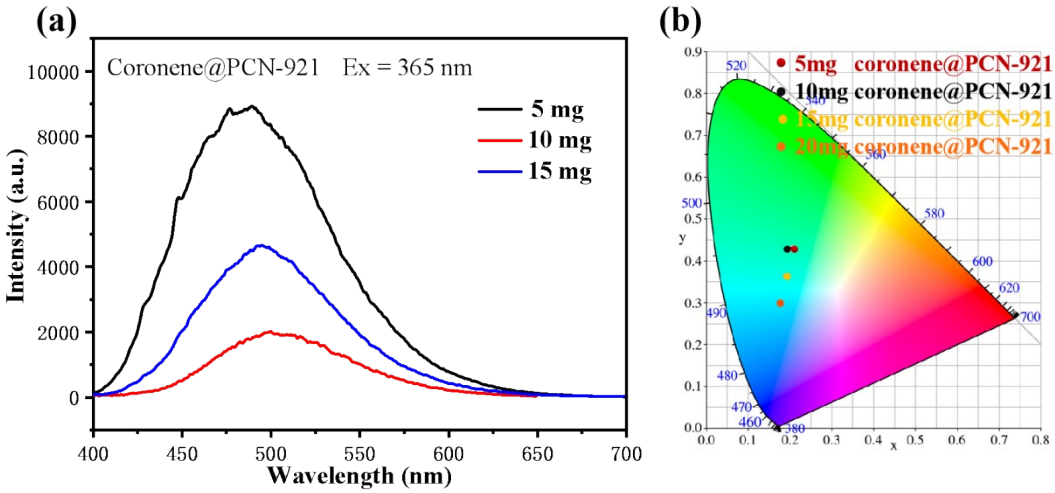


Figure S10. (a) fluorescence of package x mg-coronene@PCN-921 with different contents. (b) CIE: 5mg coronene@PCN-921 (0.30,0.39) (Brick red), 10mg coronene@PCN-921 (0.28,0.38) (Black), 15mg coronene@PCN-921 (0.26,0.36) (Origin), 20mg coronene@PCN-921 (0.25,0.29) (Red).

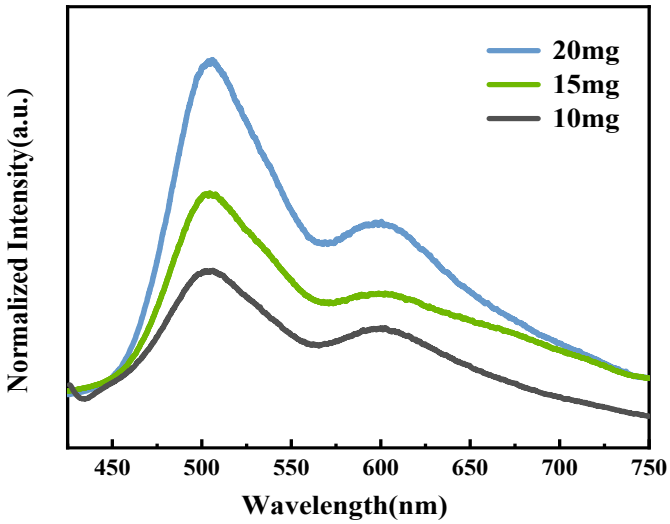


Figure S11. Phosphorescence of different amounts of coronene were capsulated.

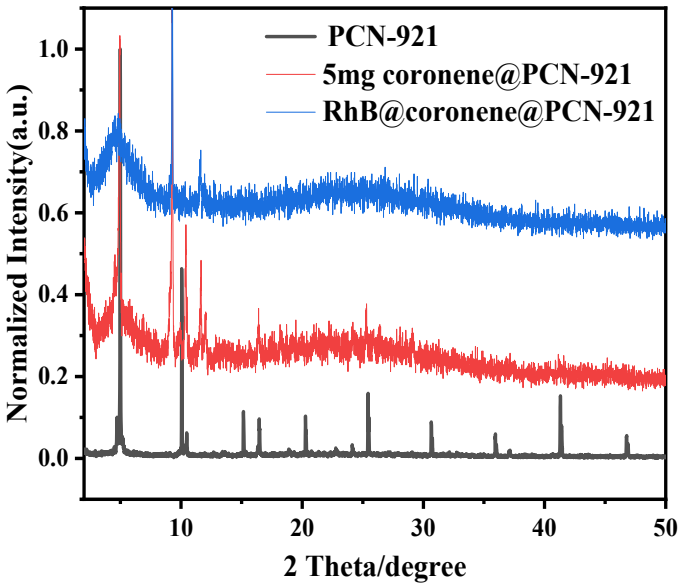


Figure S12. PXRD of PCN-921 (black line), 5mg coronene@PCN-921 （red line) and 0.06wt% RhB@coronene@PCN-921 (blue line).

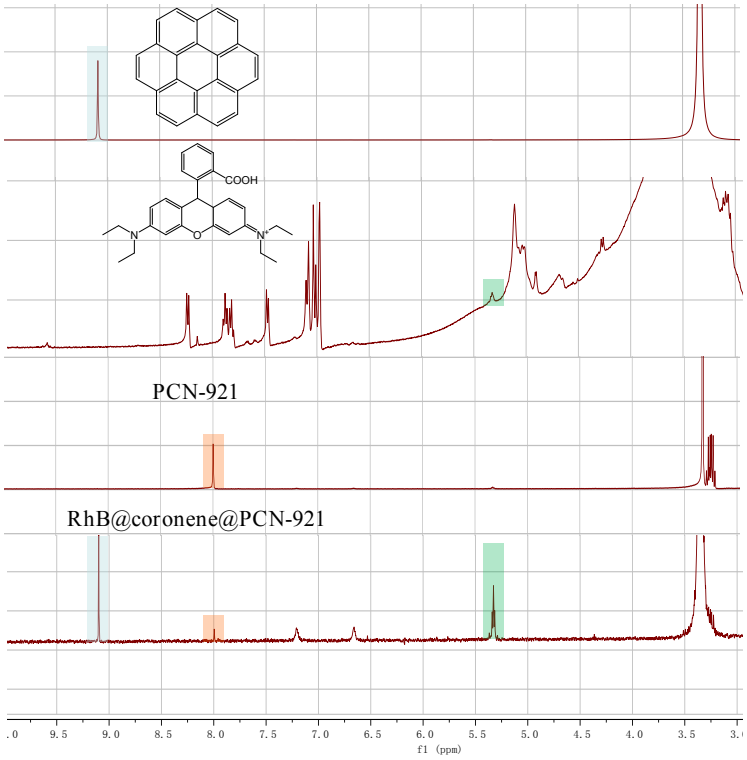


Figure S13. ^{1}H NMR spectra of coronene, RhB, PCN-921, and RhB@coronene@PCN-921 contained DMSO-d6.

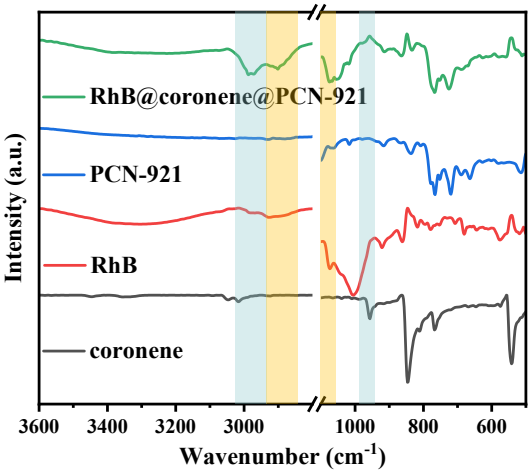


Figure S14. IR of coronene, RhB, PCN-921, and RhB@coronene@PCN-921.

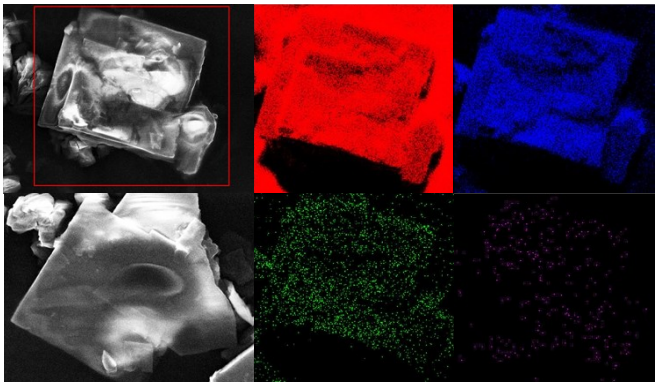


Figure S15. SEM-EDS mapping of RhB@coronene@PCN-921.

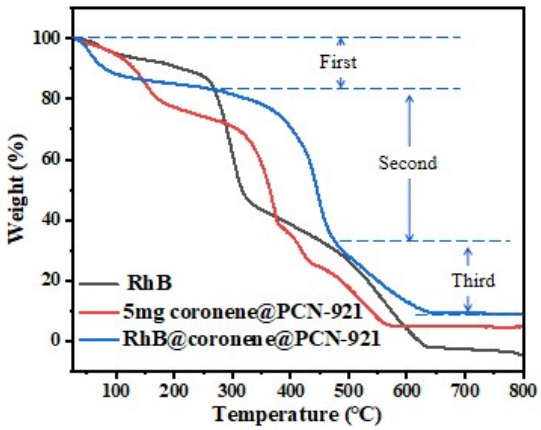


Figure S16. TGA of RhB, 5mg coronene@PCN-921 and RhB@coronene@PCN-921.

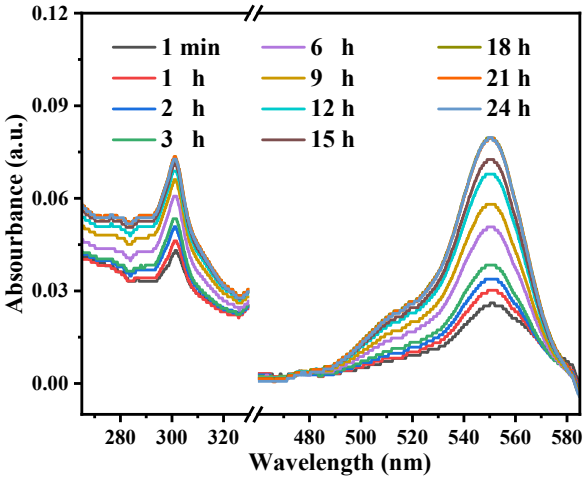


Figure S17. UV-Vis leaching test of RhB@coronene@PCN-921.

Table S1. Fluorescence lifetime 3.78 ns of PCN-921 MOF.

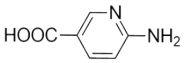
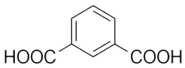
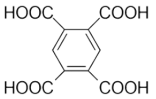
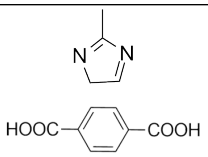
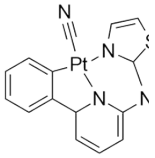
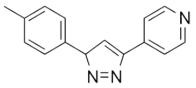
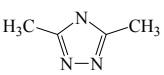
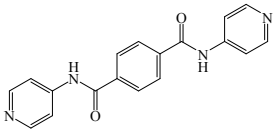
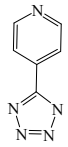
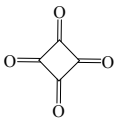
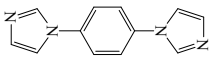
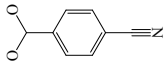
Param	Valuens	Std. Dev.ns	Param	Value	Std. Dev.	Rel.%
τ_1	2.4750	0.06896	B1	1744.662	90.1142	41.20
τ_2	4.6931	0.08466	B2	1312.974	94.8295	58.80
			A	0.182		
			χ^2	1.124		

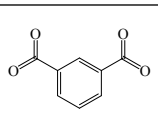
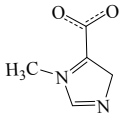
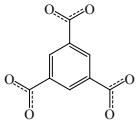
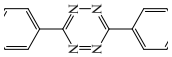
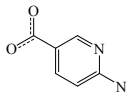
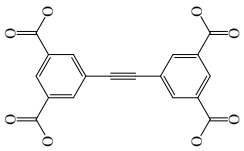
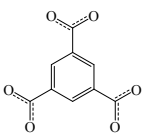
Fitting Range Low 198

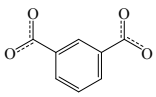
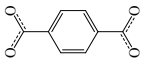
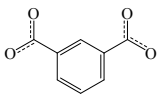
Fitting Range High 1640

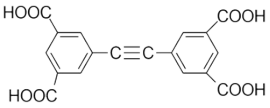
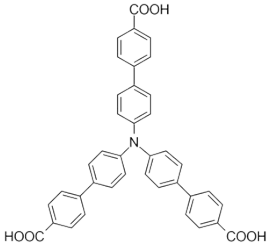
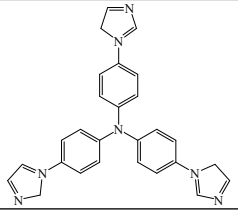
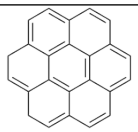
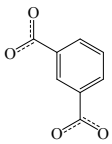
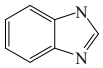
Table S2. The encapsulated guest molecules in RTP and WLED MOFs materials.

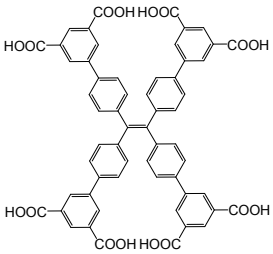
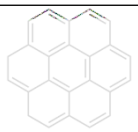
Name	Ligand	Coordinated metal ions	Guests	Phospho r-escence lifetime (ms)	LED(Q Y)	Ref.

Zn(II) based coordination polymer (CP)		Zn^{2+}	-	2000(10 K)	-	2
Eu-Cd-CP		Zn^{2+} Cd^{2+}	Eu^{3+}	454(RT)	-	3 3
{$(H_2Bpy)[Cd_3(BTC)_2]\cdot 2H_2O$}$_n$		Cd^{2+}	H_2Bpy^{2+}(H_2Bpy= deprotonated 4,4′-bipyridin)	Two months (RT)	-	4
ZIF-8 and MOF-5		Zn^{2+}		0.0184 (77K)	-	5
Cu_4I_4 and $[Cu_3Pz_3]_2$ (Pz=pyrazolate)		Cu^{+}	Cu_4I_4	0.0152 (50K)	-	6
$[Ag_3(dmtrz)_2(CN)]_n$		Ag^{+}	-	25.6 (RT)	-	7
Zn(II)-based MOFs		Zn^{2+}		0.15 (RT)	-	8
$[Cd_2(ptz)(squarate)(OH)(H_2O)_2]_n$		Cd^{2+}		0.13 (RT)	-	9
ZIF-8		Zn^{2+}	-	0.11 (RT)	White (4.73%)	10
$[(Ag_4I_4)(bix)]_n$ (bix=1,4-bis(imidazole-1-ylmethyl)benzene)		Ag^{+}	-	1.26 (10K)	-	11
$[AgL]_n\cdot nH2O$ (L = 4-cyanobenzoat		Ag^{+}	-	2.60 (RT)	White (10.86%)	12

e)						
$[Ag(tz)]_\infty$(tz= triazole)		Ag^+	-	4.59 (RT)	-	13
$[CdLi(IPA)_2](Me_2NH_2)$ (IPA = isophthalic acid, Me_2NH_2 = dimethylamine)		CdLi	-	32 (RT)	-	14
			Mn	1.6-10.5 (RT)	-	15
$[Cd(\mu\text{-}mimc)_2(H_2O)]_n$		Cd^{2+}	-	250 and 430 (10K)	-	16
$\{[Cd_3(\mu_5\text{-}btc)_2(\mu\text{-}pbptz)]\cdot 2DMF\}_n$		Cd^{2+}		170 and 760 (10K)	-	17
$[Zn(\mu\text{-}6ani)_2]_n$		Zn^{2+}	-	430-1110(10 K)	-	2
		Cd^{2+}	-	340-830 (10K)	-	17
				290(RT)		17
$[Pb_2(EBTC)(DMSO)_3]$	 EBTC	Pb^{2+}	-	4.17 (10K)	-	18
Cd(II)-based		Zn^{2+}	-	202(RT)	-	19
		Cd^{2+}	-	75(RT)		19
[Zn(TPA)(DMF)]	TPA	Zn^{2+}	pyridine	472(RT)	-	20

Zn(II)/Cd(II)-based		Zn^{2+}	-	1796 (77K)	-	19
				1321 (293K)		19
				94 (413K)		19
		Cd^{2+}	-	324 (293K)	-	19
Zn/Cd-terephthalate (TPA)		Zn^{2+}	-	472(293 K)	-	20
				106 (373K)	-	20
				30 (293K)		20
				475 (293K)	-	19
		Cd^{2+}	-	158(293 K)	-	19
Cd-Eu\Tb\Gd-CPs		Cd^{2+}	-	489 (77K)	-	21
			$Eu_xCd_{1-x}O_7$	427 (293K)	-	21
				10.54 (413K)	-	21
			$Tb_xCd_{1-x}O_7$	312 (293K)	-	21
				57.66 (293K)		21
Ln-CPs		Cd^{2+}	Eu^{3+}	10.54 (RT)	-	21
			Tb^{3+}	57.66 (RT)	-	21
zinc iso-phthalic acid (IPA) based MOF (denoted as Y346)		Zn^{2+}	rhodamine B	926.56 (RT)	-	22
				97.55 (RT)		22

$NH^+/Na^+/K^+$-TPA		NH_4^+	-	586(RT)	-	23
		Na^+		504(RT)		23
		K^{+-}		585(RT)	-	23
$[Pb_2(EBTC)(DMSO)_3]$		Pb^{2+}	-	4.17 (RT)	-	18
Cd-TCPA		Cd^{2+}	$[(CH_3)_2NH_2]^+$ cations, which are generated from in situ decomposition of DMF	472 (RT)	White	24
$\{[Cd_2(tipa)_2Cl_4]\cdot 6\ DMF\}_n$		Zn^{2+}	-	-(77K)	-	25
		Cd^{2+}				25
C@Zn(ZIF-8)		Zn^+		7400 (RT)	-	26
				22400 (RT)		26
C@Zn(ZIF-8)		Zn^{2+}	Gd[(Pyr)4cyclen] (Pyrpyrenol)	(77K)	-	26
Cd(m-BDC)(BIM)		Cd^{2+}		755 (293K)	-	27
				554		27
Cd(m-BDC)(H_2O)	BDC	Cd^{2+}	H_2O/benzimidazole(BIM)	698(RT)	-	27
				404(RT)		27

Cd(m-BDC)(BIM)		Cd^{2+}	4-methylumbelliferone, Fluorescent Green B, Fluorescent Green B, Rhodamine 123, Rhodamine 6G, Rhodamine B	293(RT)	-	28
RhB@coronene@PCN-921		Zn^{2+}	 and Rhodamine B	0.0625 (RT)	White (93.6%)	This work

References

[1] Z. Wei, W. Lu, H. L. Jiang, H. C. Zhou, *Inorg. Chem.* **2013**, *52*, 1164.

[2] J. Cepeda, E. S. Sebastian, D. Padro, A. Rodriguez-Dieguez, J. A. Garcia, J. M. Ugalde and J. M. Seco, Chemical Communications. 2016, 52, 8671-8674.

[3] Y. S. Yang, K. Z. Wang and D. P. Yan, ACS Appl. Mater. Interfaces. 2017, 9, 17400-17408.

[4] X. S. Xing, Z. W. Chen, L. Z. Cai, C. Sun, L. R. Cai, M. S. Wang and G. C. Guo, RSC Adv. 2016, 6, 24190-24194.

[5] T. O. Knedel, S. Buss, I. Maisuls, C. G. Daniliuc, C. Schlusener, P. Brandt, O. Weingart, A. Vollrath, C. Janiak and C. A. Strassert, Inorg. Chem. 2020, 59, 7252-7264.

[6] S. Z. Zhan, M. Li, S. W. Ng and D. Li, Chem.-Eur. J. 2013, 19, 10217-10225.

[7] Y. Ling, Z. X. Chen, Y. M. Zhou, L. H. Weng and D. Y. Zhao, Crystengcomm, 2011, 13, 1504-1508.

[8] F. Luo, G. M. Sun, A. M. Zheng, S. X. Lian, Y. L. Liu, X. F. Feng and Y. Y. Chu, Dalton Transactions. 2012, 41, 13280-13283.

[9] A. J. Calahorro, A. Salinas-Castillo, D. Fairen-Jimenez, J. M. Seco, C. Mendicute-Fierro, S. Gomez-Ruiz, M. E. Lopez-Viseras and A. Rodriguez-Dieguez, Inorganica Chimica Acta. 2015, 427, 131-137.

[10] X. G. Yang and D. P. Yan, Chemical Communications. 2017, 53, 1801-1804.

[11] L. Chen, J. Ma, Q. H. Chen, R. Feng, F. L. Jiang and M. C. Hong, Inorganic Chemistry Communications. 2012, 15, 208-211.

[12] M. S. Wang, S. P. Guo, Y. Li, L. Z. Cai, J. P. Zou, G. Xu, W. W. Zhou, F. K. Zheng and G. C. Guo, Journal of the American Chemical Society. 2009, 131, 13572-+.

[13] J. P. Zhang, Y. Y. Lin, X. C. Huang and X. M. Chen, Journal of the American Chemical Society. 2005, 127, 5495-5506.

[14] X. G. Yang and D. P. Yan, Journal of Materials Chemistry C. 2017, 5, 7898-7903.

[15] A. A. Garcia-Valdivia, J. M. Seco, J. Cepeda and A. Rodriguez-Dieguez, Inorg. Chem. 2017, 56, 13897-13912.

[16] J. M. Seco, S. Perez-Yanez, D. Briones, J. A. Garcia, J. Cepeda and A. Rodriguez-Dieguez, Crystal Growth & Design. 2017, 17, 3893-3906.

[17] J. M. Seco, A. Rodriguez-Dieguez, D. Padro, J. A. Garcia, J. M. Ugalde, E. S. Sebastian and J. Cepeda, Inorg. Chem. 2017, 56, 3149-3152.

[18] X. Liu, L. Zhai, W. W. Zhang, J. L. Zuo, Z. X. Yang and X. M. Ren, Dalton Transactions. 2017, 46, 7953-7959.

[19] X. G. Yang and D. P. Yan, Advanced Optical Materials. 2016, 4, 897-905.

[20] X. G. Yang and D. P. Yan, Chem. Sci. 2016, 7, 4519-4526.

[21] Y. S. Yang, K. Z. Wang and D. P. Yan, Chemical Communications. 2017, 53, 7752-7755.

[22] X. G. Yang, X. M. Lu, Z. M. Zhai, Y. Zhao, X. Y. Liu, L. F. Ma and S. Q. Zang, Chemical Communications. 2019, 55, 11099-11102.

[23] Z. C. Cheng, H. F. Shi, H. L. Ma, L. F. Bian, Q. Wu, L. Gu, S. Z. Cai, X. Wang, W. W. Xiong, Z. F. An and W. Huang, Angew. Chem.-Int. Edit. 2018, 57, 678-682.

[24] H. R. Fu, N. Wang, X. X. Wu, F. F. Li, Y. Zhao, L. F. Ma and M. Du, Advanced Optical Materials. 2020, 8, 10.

[25] S. Yuan, Y. K. Deng and D. Sun, Chem.-Eur. J. 2014, 20, 10093-10098.

[26] H. Mieno, R. Kabe, N. Notsuka, M. D. Allendorf and C. Adachi, Advanced Optical Materials. 2016, 4, 1015-1021.

[27] Y. S. Yang, K. Z. Wang and D. P. Yan, ACS Appl. Mater. Interfaces. 2016, 8, 15489-15496.

[28] J. B. Liu, Y. X. Zhuang, L. Wang, T. L. Zhou, N. Hirosaki and R. J. Xie, ACS Appl. Mater. Interfaces. 2018, 10, 1802-1809.