

Supporting Information

Zeolitic Imidazolate Framework $[\text{Zn}_2(\text{IM})_4 \cdot (\text{DMF})]$ for UV-white Light-emitting Diodes[†]

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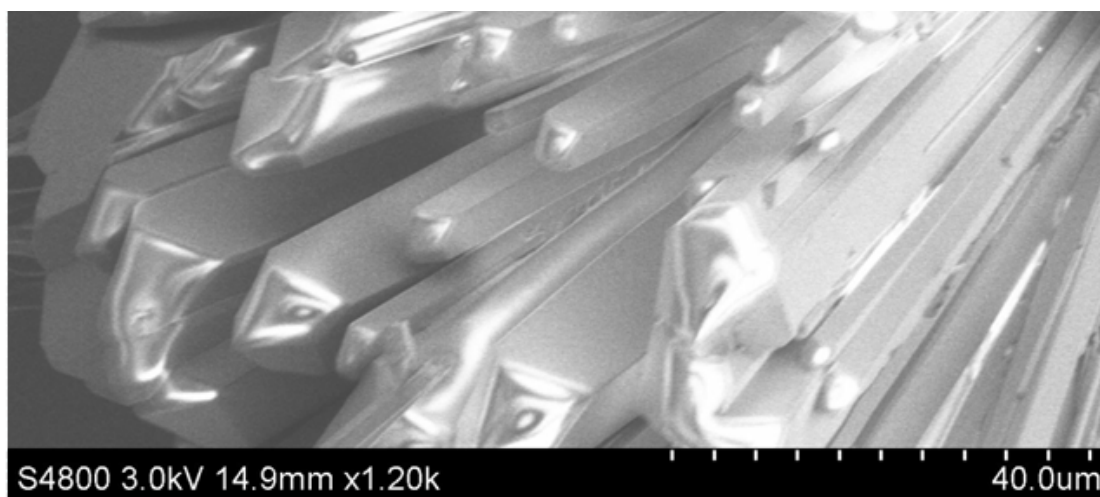


Fig. S1 SEM image of $[\text{Zn}_2(\text{IM})_4 \cdot (\text{DMF})]$.

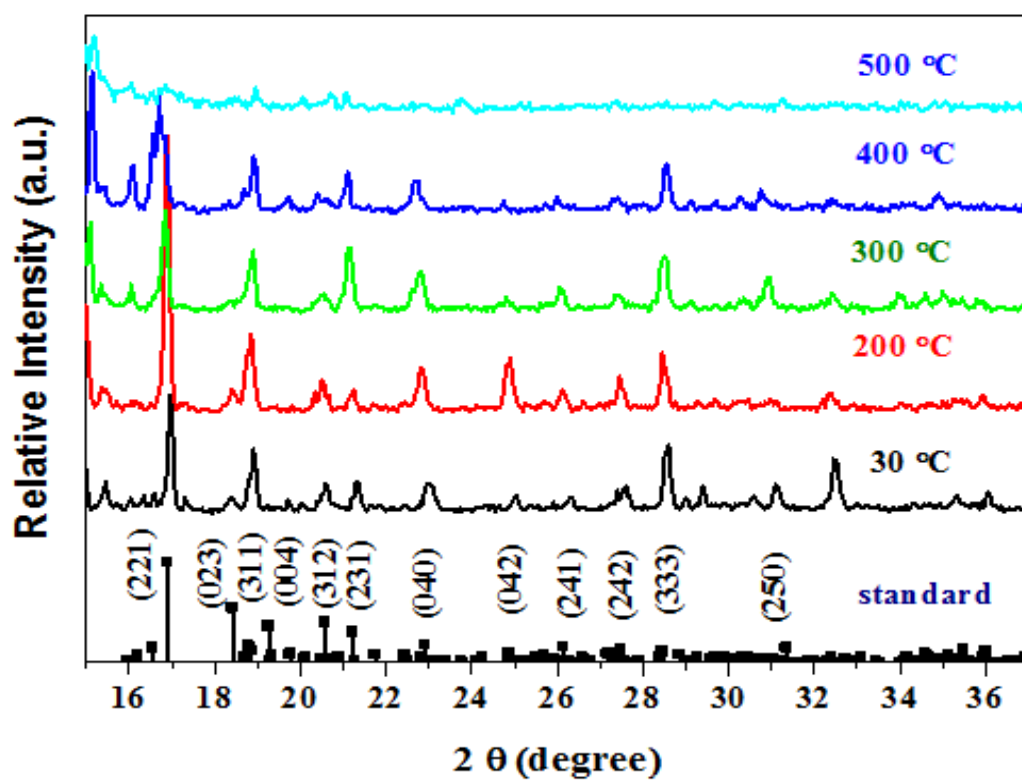


Fig. S2 *In situ* temperature-variant XRD patterns of $[\text{Zn}_2(\text{IM})_4 \cdot (\text{DMF})]$.

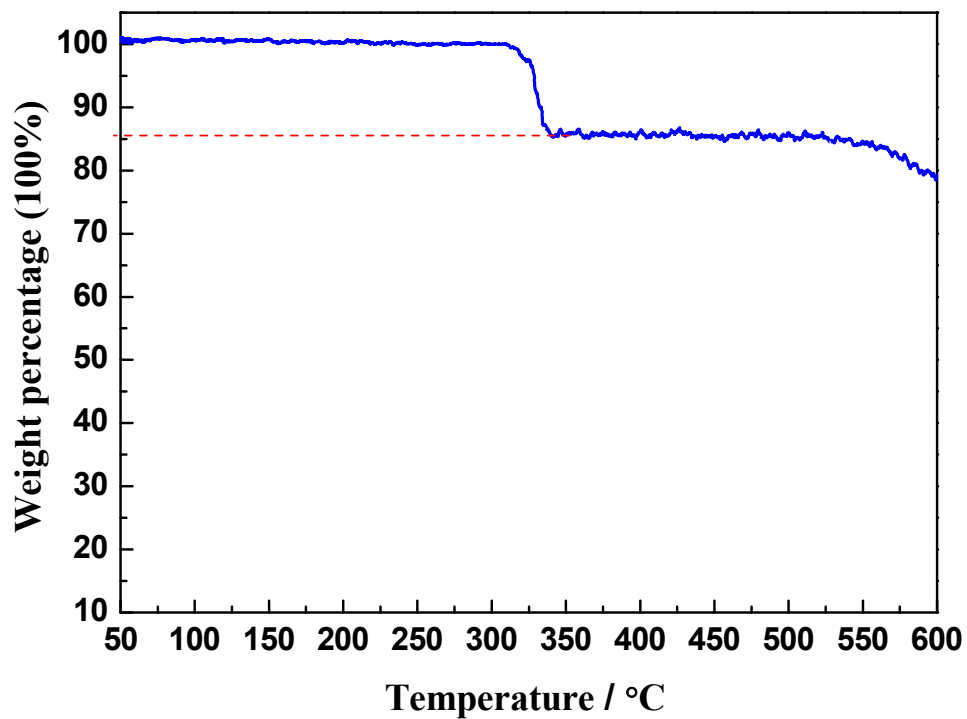


Fig. S3 TGA curves of $[\text{Zn}_2(\text{IM})_4 \cdot (\text{DMF})]$ in flowing N_2 with heating at a rate of $10 \text{ }^\circ\text{C min}^{-1}$.

Table S1 (a) Crystallographic Structure Data of $[\text{Zn}_2(\text{IM})_4\cdot(\text{DMF})]$ at 295 K. (b) Atomic Coordinates. (c) Selected Interatomic Distances (Å) and angles ($^\circ$) of $[\text{Zn}_2(\text{IM})_4\cdot(\text{DMF})]$.

(a)

$\text{C}_{15}\text{H}_{19}\text{N}_9\text{OZn}_2$	$[\text{Zn}_2(\text{IM})_4\cdot(\text{DMF})]$
Crystal system	Orthorhombic
Space group	$Pbca(61)$
Z	8
Cell Parameters:	$a = 15.4109(2) \text{ \AA}$ $\alpha = 90^\circ$ $b = 15.5132(2) \text{ \AA}$ $\beta = 90^\circ$ $c = 18.4120(2) \text{ \AA}$ $\gamma = 90^\circ$
Cell volume:	$4401.8(1) \text{ \AA}^3$
Reliability Factor:	GOF = 1.406 $R_p = 5.14\%$ $R_{wp} = 17.11\%$

(b)

Atom	Wyck.	x	y	z	Frac	Uiso(Å ²)
Zn1	8c	0.20030	0.14090	0.0938	1.00	0.053(1)
Zn2	8c	0.0082	0.1627	-0.185	1.00	0.053(1)
N(1)	8c	0.1724(2)	0.1244(3)	-0.0095(2)	1.00	0.059(1)
N(2)	8c	0.0997(2)	0.1318(2)	-0.1135(2)	1.00	0.058(1)
N(3)	8c	0.1334(2)	0.2400(2)	0.1349(2)	1.00	0.056(1)
N(4)	8c	0.0609(2)	0.3131(2)	0.2196(2)	1.00	0.059(1)
N(5)	8c	0.1621(2)	0.0389(2)	0.1514(2)	1.00	0.062(1)
N(6)	8c	0.0769(2)	-0.0663(2)	0.1915(2)	1.00	0.060(1)
N(7)	8c	0.3255(2)	0.1629(2)	0.1126(2)	1.00	0.059(1)
N(8)	8c	0.4418(2)	0.2374(2)	0.1464(2)	1.00	0.057(1)

(c)

[Zn ₂ (IM) ₄ ·(DMF)]			
Distances/Å			
Zn1-N1	1.9667 x3	Zn2-N2	1.9878 x3
Zn1-N3	1.9998x3	Zn2-N4	1.9713x3
Zn1-N5	1.9938x3	Zn2-N6	1.9927x3
Zn1-N7	1.9897x3	Zn2-N8	1.9885x3
Angles /°			
N1_Zn1_N3	110.689	N2_Zn2_N4	110.108
N1_Zn1_N5	105.278	N2_Zn2_N6	109.006
N1_Zn1_N7	113.739	N2_Zn2_N8	108.439
N3_Zn1_N5	104.870	N4_Zn2_N6	111.135
N3_Zn1_N7	107.592	N4_Zn2_N8	112.462
N5_Zn1_N7	109.264	N6_Zn2_N8	105.527