

## Supporting Information

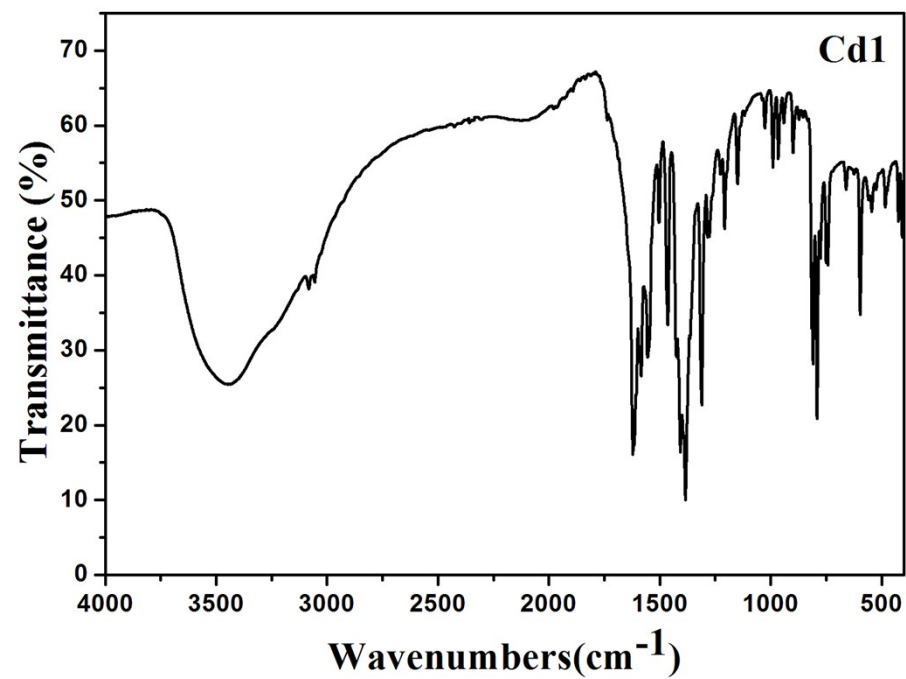
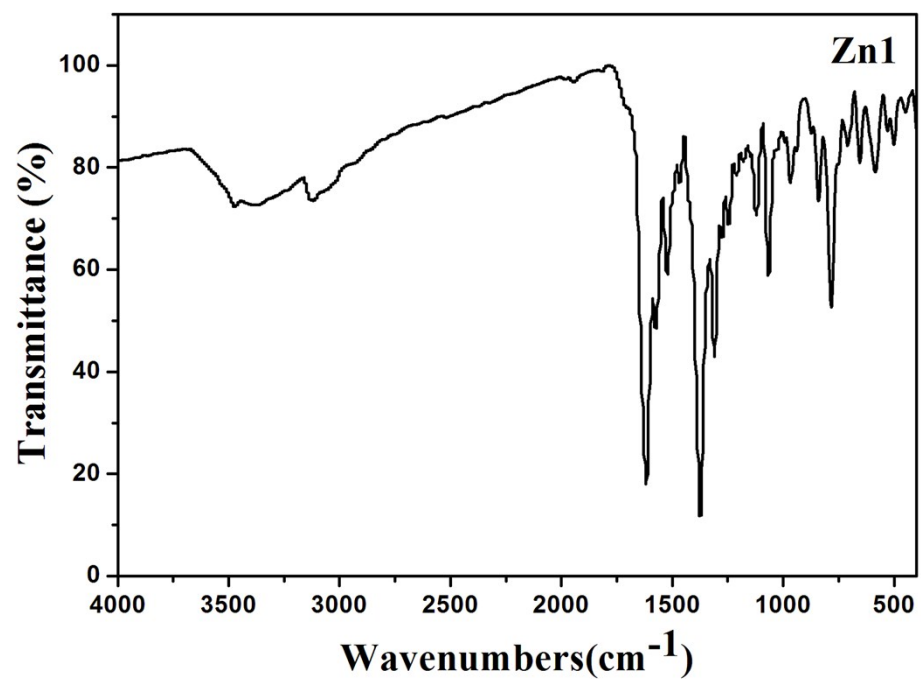
### **Multifunctional Zn(II)/Cd(II) Metal Complexes for Tunable Luminescence Properties and High Efficient Dye-Sensitized Solar Cells**

**Song Gao,<sup>a</sup> Rui Qing Fan,<sup>\*a</sup> Xin Ming Wang,<sup>a</sup> Liang Sheng Qiang,<sup>a</sup> Li Guo Wei,<sup>a</sup> Ping Wang,<sup>a</sup> Yu Lin Yang,<sup>\*a</sup> Yu Lei Wang,<sup>b</sup> Tian Zhu Luan<sup>c</sup>**

*<sup>a</sup> Department of Chemistry, Harbin Institute of Technology, Harbin 150001, P. R. China*

*<sup>b</sup> National Key Laboratory of Science and Technology on Tunable Laser, Harbin Institute of Technology, Harbin 150080, P. R. China*

*<sup>c</sup> The First Affiliated Hospital of Harbin Medical University, Harbin, 150001, P. R. China*



**Fig. S1** Infrared spectra of complexes **Zn1** and **Cd1** recorded from a KBr pellet.

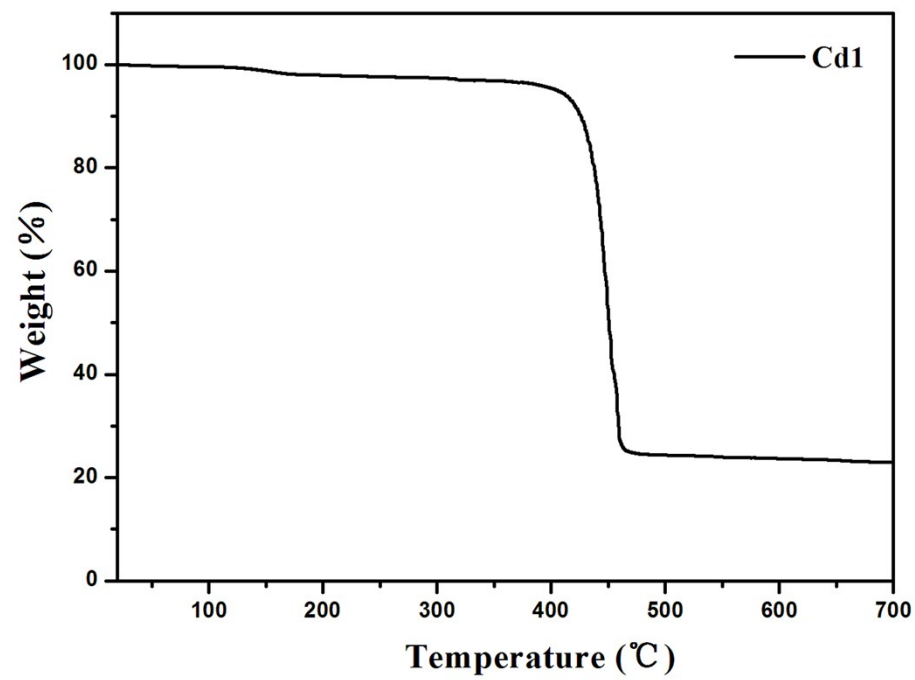
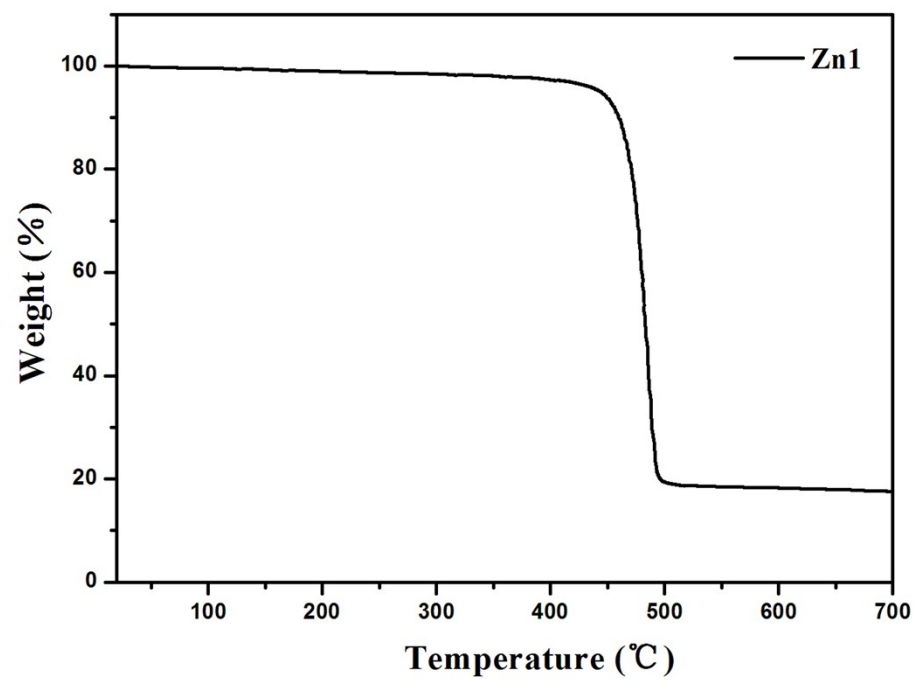


Fig. S2 The TGA curves of complexes **Zn1** and **Cd1**.

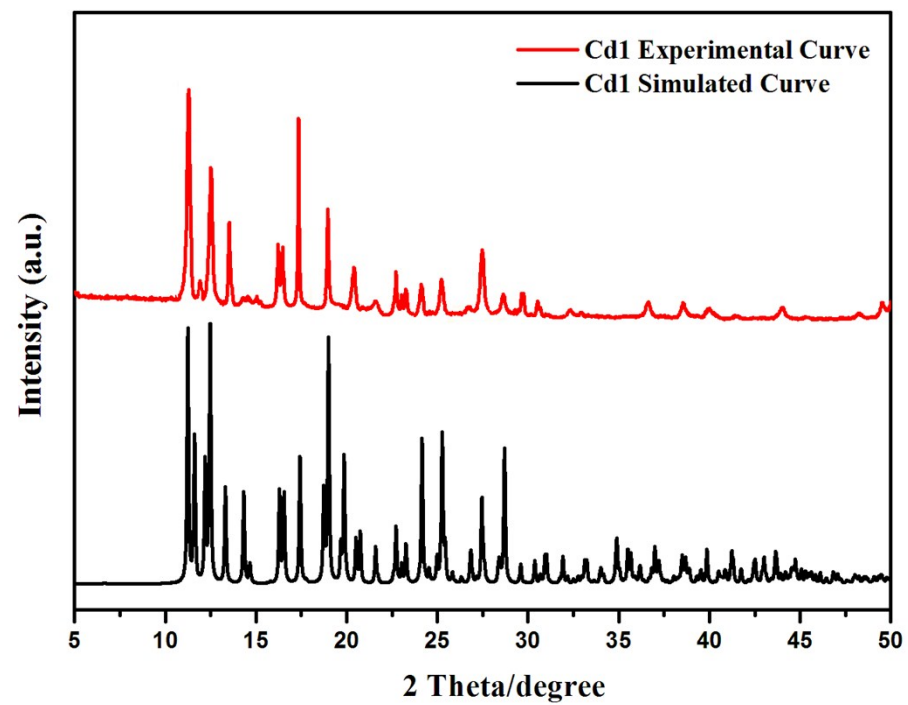
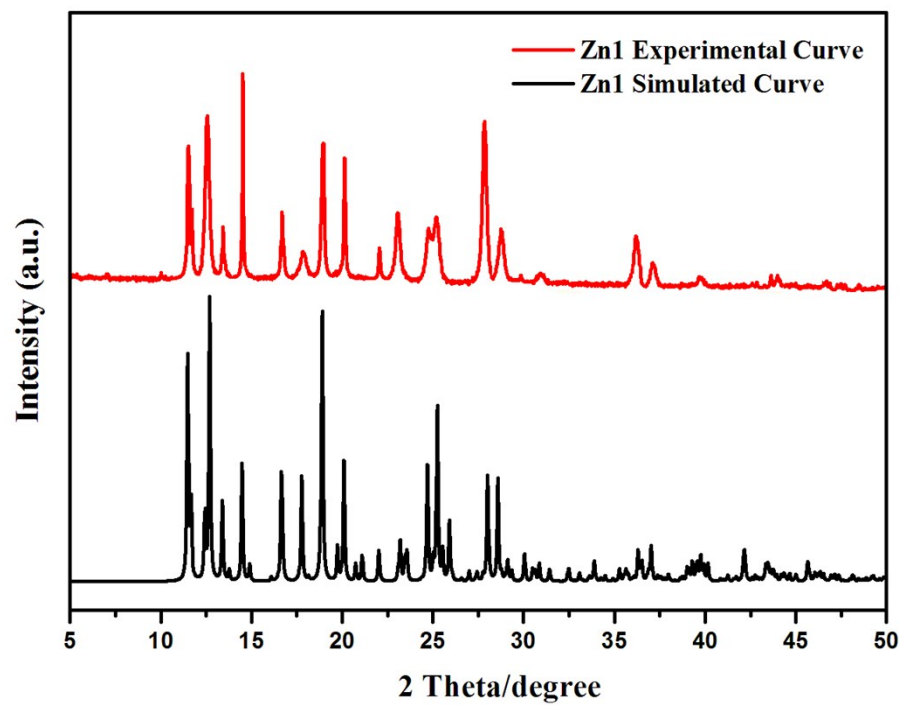
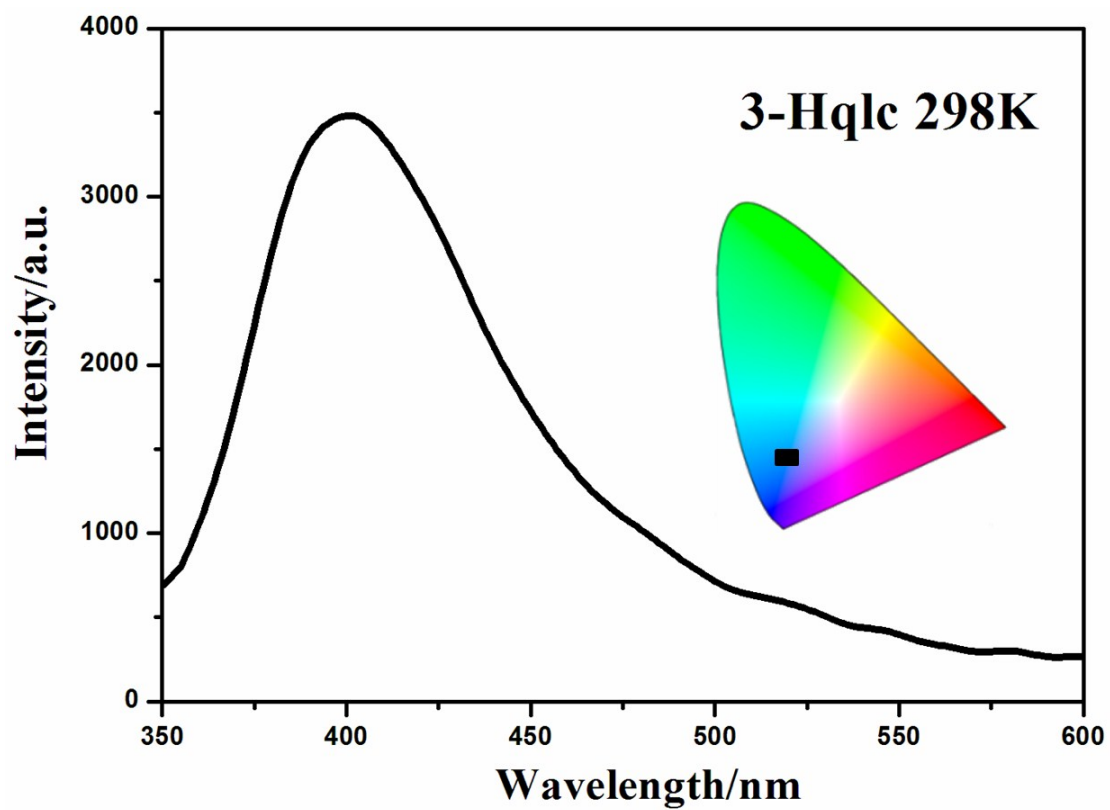


Fig. S3 The PXR contrast curves of complexes **Zn1** and **Cd1**.



**Fig. S4** Emission spectra of ligand 3-Hqlc in the solid state at 298 K and the corresponding color coordinate diagram of emission.

**Table S1** Selected bond lengths (Å) and bond angles (°) for complexes **Zn1** and **Cd1**.

---

<b>Zn1</b>			
Zn(1)-O(1)	1.968(3)	Zn(1)-O(3)	1.927(2)
Zn(1)-N(1)	2.106(3)	Zn(1)-N(2)	2.097(3)
O(3)-Zn(1)-O(1)	138.4(1)	O(3)-Zn(1)-N(2)	110.2(1)
O(1)-Zn(1)-N(2)	100.8(1)	O(3)-Zn(1)-N(1)	100.3(1)
O(1)-Zn(1)-N(1)	100.5(1)	N(2)-Zn(1)-N(1)	100.9(1)
<b>Cd1</b>			
Cd(1)-O(1)	2.276(2)	Cd(1)-O(2)	2.164(2)
Cd(1)-O(4)#1	2.406(2)	Cd(1)-O(3)	2.765(2)
Cd(1)-N(1)	2.332(2)	Cd(1)-N(2)	2.348(2)
O(2)-Cd(1)-O(1)	158.9 (9)	O(2)-Cd(1)-O(4)#1	110.3(9)
O(1)-Cd(1)-O(4)#1	56.1(7)	O(1)-Cd(1)-O(3)	110.1(1)
O(4)-Cd(1)-O(3)	93.2(9)	N(2)-Cd(1)-O(3)	152.6(9)
N(1)-Cd(1)-O(4)#1	145.7(8)	N(2)-Cd(1)-O(4)#1	96.5(8)
N(1)-Cd(1)-N(2)	97.3(8)		

---

Symmetry transformations used to generate equivalent atoms: #1 x,-y,z+1/2.

**Table S2** Luminescence data for complexes **Zn1**, **Cd1** and 3-Hqlc ligand.

Complexes	Excitation ( $\lambda$ , nm)	Emission ( $\lambda_{\text{max}}$ , nm)	CIE (x, y)	Lifetime ( $\mu\text{s}$ )					Conditions <sup>a</sup>
				$\tau_1$ ( $\mu\text{s}$ )	$A_1\%$	$\tau_2$ ( $\mu\text{s}$ )	$A_2\%$	$\langle\tau\rangle$ ( $\mu\text{s}$ )	
<b>Zn1</b>	330	424	0.19, 0.20	—	—	—	—	—	DMSO, 298K
	330	418	0.19, 0.19	—	—	—	—	—	CH <sub>3</sub> OH, 298K
	330	412	0.20, 0.21	—	—	—	—	—	CHCl <sub>3</sub> , 298K
	330	409	0.20, 0.20	—	—	—	—	—	THF, 298K
	330	468	0.24, 0.28	1.00	52.36%	8.62	47.64%	7.76	Solid State, 298K
	330	483 <sup>sh</sup> , 510, 571 <sup>sh</sup>	0.29, 0.42	1.30	37.67%	11.41	62.33%	10.76	Solid State, 77K
<b>Cd1</b>	330	418	0.19, 0.16	—	—	—	—	—	DMSO, 298K
	330	412	0.20, 0.13	—	—	—	—	—	CH <sub>3</sub> OH, 298K
	330	407	0.20, 0.16	—	—	—	—	—	CHCl <sub>3</sub> , 298K
	330	405	0.18, 0.14	—	—	—	—	—	THF, 298K
	330	450	0.23, 0.25	1.06	65.46%	8.95	34.54%	7.50	Solid State, 298K
	330	449 <sup>sh</sup> , 485, 542 <sup>sh</sup>	0.25, 0.33	1.50	45.14%	10.87	54.86%	9.91	Solid State, 77K
3-Hqlc	330	400	0.18, 0.15	—	—	—	—	—	Solid State, 298K

<sup>a</sup> Concentration in DMSO, CH<sub>3</sub>OH, CHCl<sub>3</sub> and THF solutions: (M) =  $1 \times 10^{-5}$  M.