Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Thermally-induced single-crystal-to-single-crystal transformations from 2D two-fold interpenetrating square lattice layer to 3D four-fold interpenetrating diamond framework and its application in dye-sensitized solar cells

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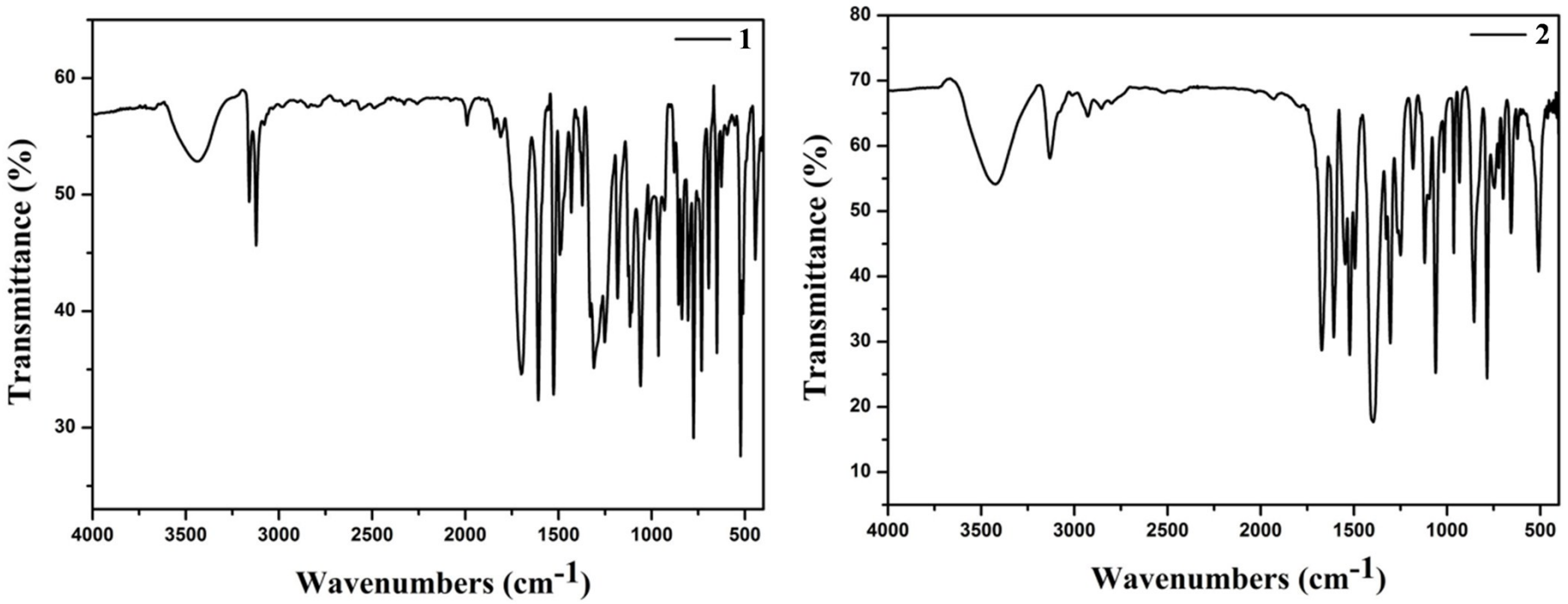

Fig. S1 Infrared spectra of complexes **1** and **2** recorded from a KBr pellet.

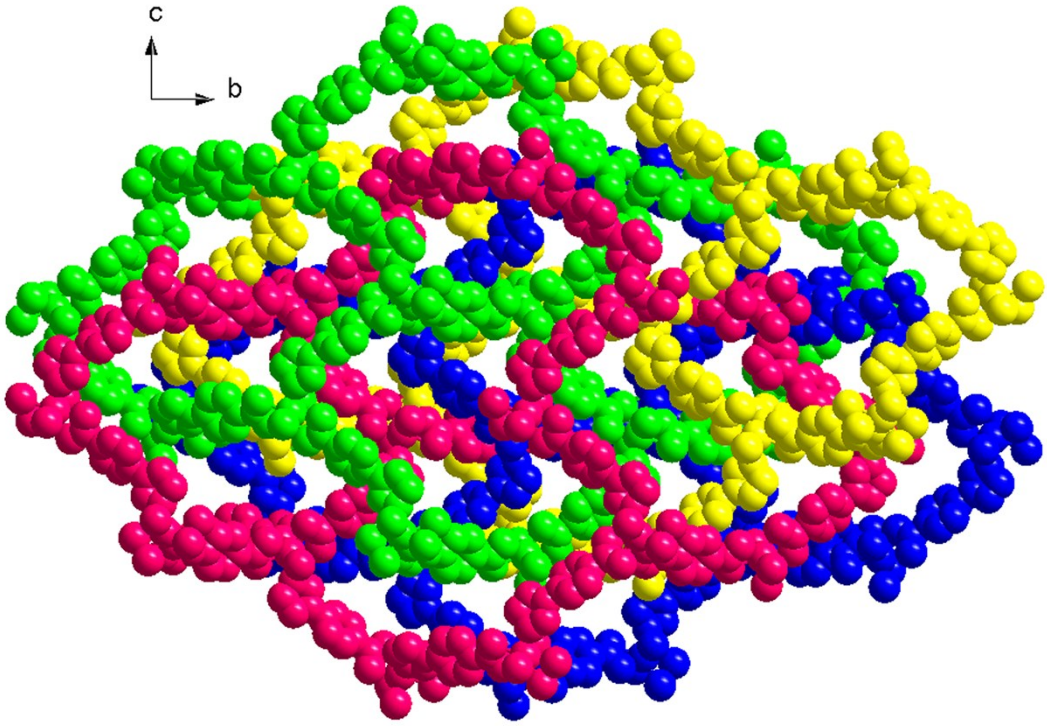

Fig. S2 Space filling diagram of the four-fold interpenetrating framework of **2**.

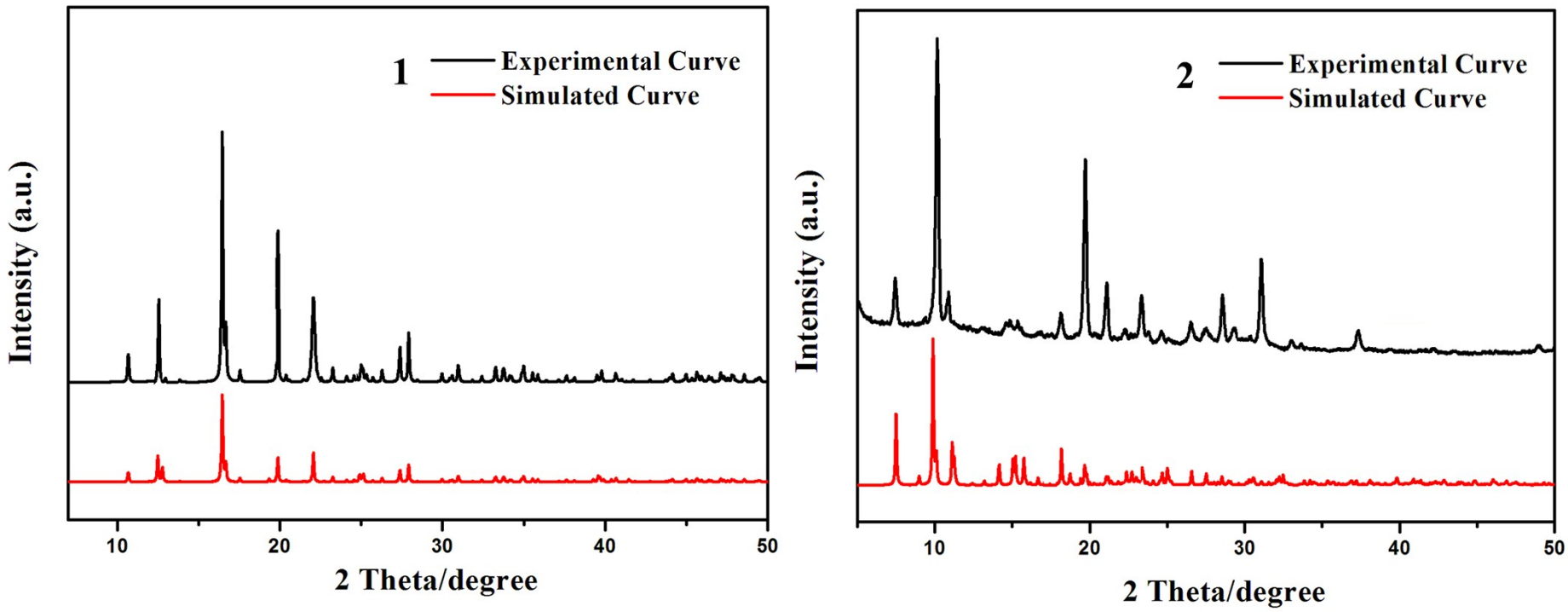

Fig. S3 The PXRD contrast curves of complexes **1** and **2**.

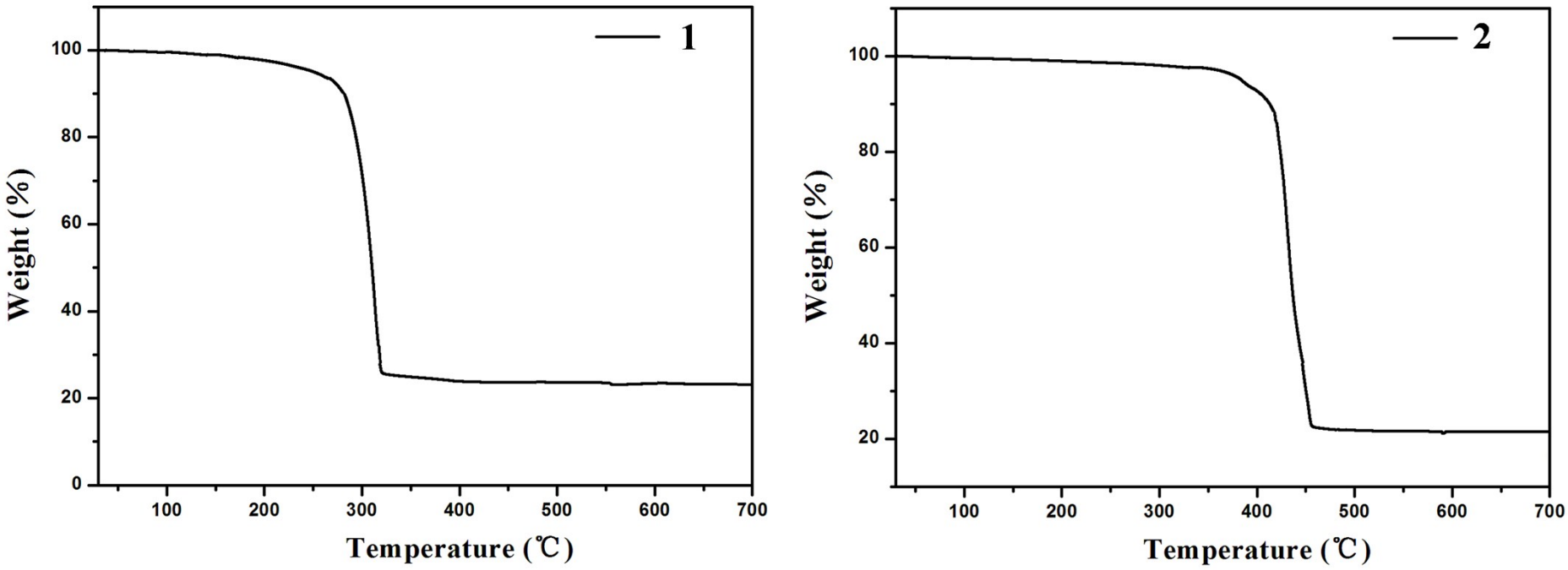

Fig. S4 The TGA curves of complexes **1** and **2**.

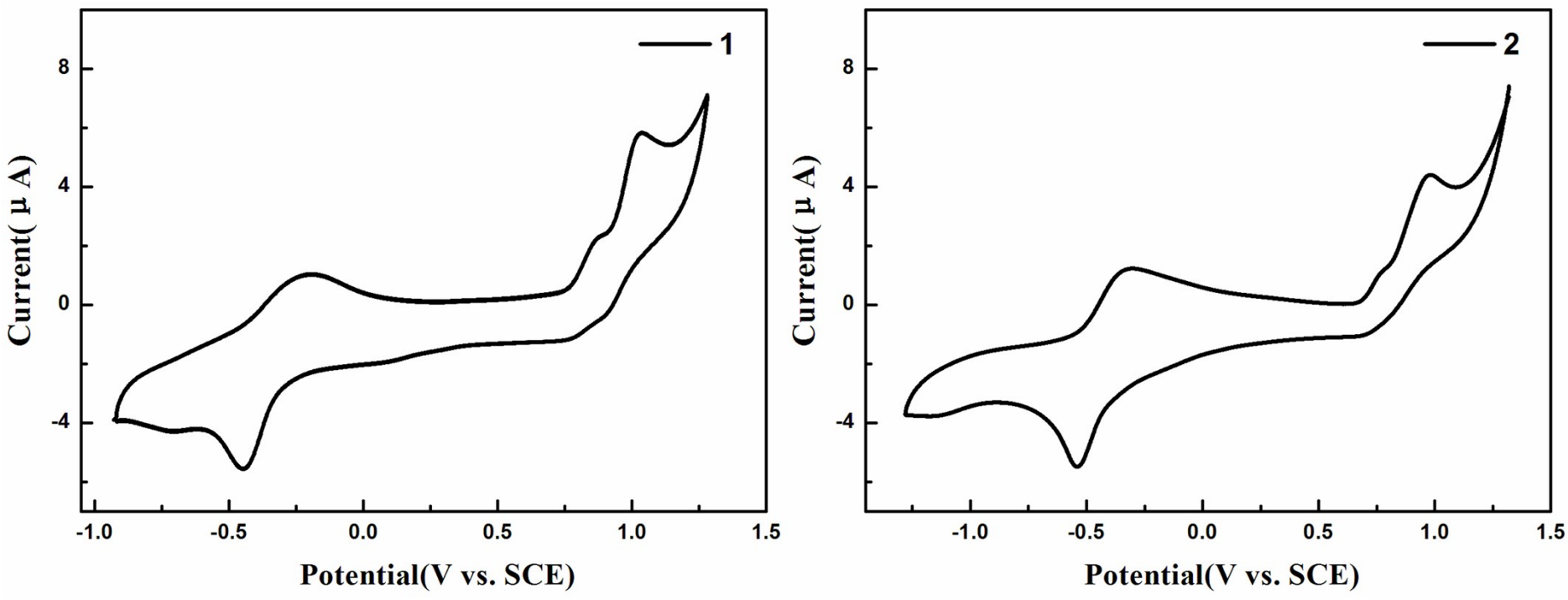

Fig. S5 Cyclic voltammograms of complexes **1** and **2** in ethanol solution containing 0.1 M $TBAPF_6$ solution.

Table S1 Selected bond lengths (Å) and bond angles (°) for complexes **1** and **2**

1			
Cd(1)-N(1)#1	2.269(2)	Cd(1)-O(1)#1	2.279(2)
Cd(1)-N(1)	2.269(2)	Cd(1)-O(2)#1	2.463(3)
Cd(1)-O(1)	2.279(2)	Cd(1)-O(2)	2.463(3)
N(1)#1-Cd(1)-N(1)	90.2(1)	N(1)-Cd(1)-O(2)#1	85.6(9)
N(1)#1-Cd(1)-O(1)	125.8(1)	O(1)-Cd(1)-O(2)#1	100.6(9)
N(1)-Cd(1)-O(1)	93.2(1)	O(1)#1-Cd(1)-O(2)#1	54.8(1)
N(1)#1-Cd(1)-O(1)#1	93.2(1)	N(1)#1-Cd(1)-O(2)	85.6(9)
N(1)-Cd(1)-O(1)#1	125.8(1)	N(1)-Cd(1)-O(2)	133.6(9)
O(1)-Cd(1)-O(1)#1	126.1(2)	O(1)-Cd(1)-O(2)	54.8 (1)
N(1)#1-Cd(1)-O(2)#1	133.6(9)	O(1)#1-Cd(1)-O(2)	100.6(9)
O(2)#1-Cd(1)-O(2)	128.5(1)		
2			
Cd(1)-N(3)	2.275(8)	Cd(1)-O(5)	2.388(7)
Cd(1)-O(1)	2.323(7)	Cd(1)-O(3)	2.486(7)
Cd(1)-N(1)#1	2.323(7)	Cd(1)-O(2)	2.642(7)
Cd(1)-O(4)	2.392(7)	N(3)-Cd(1)-O(1)	126.7(3)
N(3)-Cd(1)-N(1)#1	98.3(3)	N(1)#1-Cd(1)-O(5)	176.2(3)
O(1)-Cd(1)-N(1)#1	102.2(3)	O(4)-Cd(1)-O(5)	89.7(2)
N(3)-Cd(1)-O(4)	88.7(3)	N(3)-Cd(1)-O(3)	141.2(3)
O(1)-Cd(1)-O(4)	140.7(2)	O(1)-Cd(1)-O(3)	87.6(2)
N(1)#1-Cd(1)-O(4)	86.5(3)	N(1)#1-Cd(1)-O(3)	90.0(3)
N(3)-Cd(1)-O(5)	81.5(3)	O(4)-Cd(1)-O(3)	53.8(2)
O(1)-Cd(1)-O(5)	80.7(2)	O(5)-Cd(1)-O(3)	87.8(2)
N(3)-Cd(1)-O(2)	80.6(3)	O(4)-Cd(1)-O(2)	166.2(2)
O(1)-Cd(1)-O(2)	52.7(2)	O(5)-Cd(1)-O(2)	97.2(2)
N(1)#1-Cd(1)-O(2)	86.5(2)	O(3)-Cd(1)-O(2)	138.0(2)

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