Electronic Supplementary Material (ESI) for RSC Advances.

Mixed–solvothermal synthesis, structures, surface photovoltage, luminescence and molecular recognition properties of three new transition metal phosphonates with 3D framework and supramolecular structures

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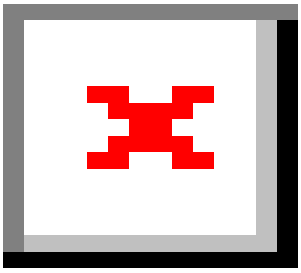

Fig. S1. The simulated XRD pattern of compound **1** (black line) and experimental powder XRD patterns of compounds **1** (red line) and **2** (green line).

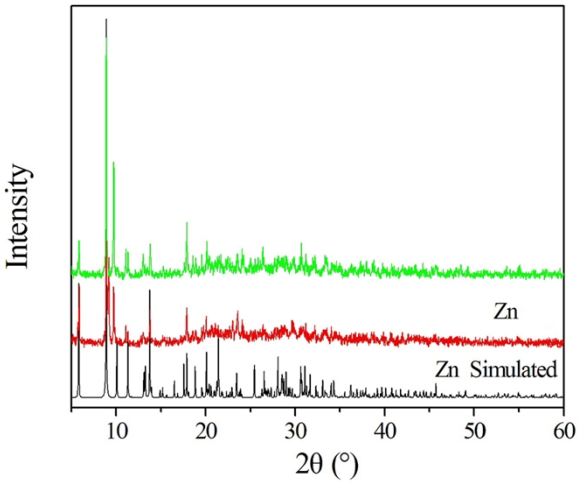

Fig. S2. The simulated XRD pattern (black line), the experimental powder XRD pattern (red line) and the XRD pattern of compound **3** into DMF solvent after aging (green line).

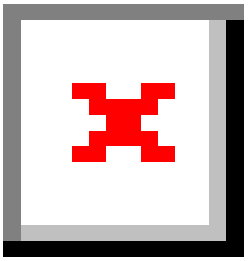

Fig. S3 IR spectra of compounds **1** and **2**.

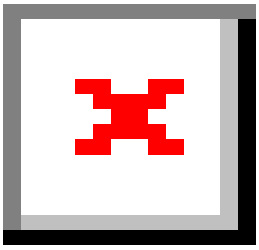

Fig. S4 The IR spectrum of compound **3**.

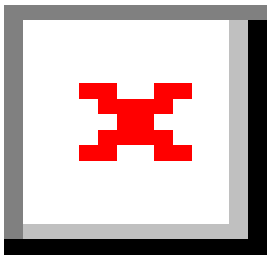

Fig. S5 TG curve of compound **1**.

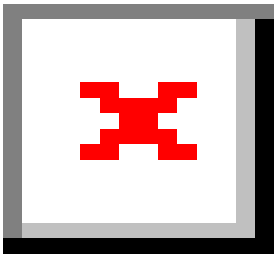

Fig. S6 TG curve of compound **2**.

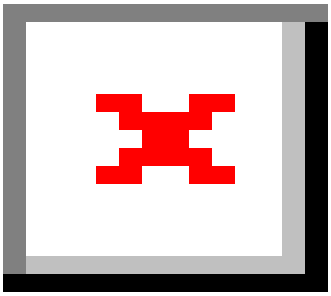

Fig. S7 The TG curve of compound **3**.

Table S1 Selected bond lengths (Å) and angles (º) for compound **1**[a]

Ni(1)–O(1)#1	2.051(5)	Ni(2)–O(2)	2.007(5)
Ni(1)–O(4)#2	2.056(5)	Ni(2)–O(2)#4	2.007(5)
Ni(1)–O(5)	2.057(5)	Ni(2)–O(6)	2.061(5)
Ni(1)–N(1)#3	2.098(2)	Ni(2)–O(6)#4	2.061(5)
Ni(1)–O(3)	2.147(5)	Ni(2)–O(8)	2.153(2)
Ni(1)–O(7)	2.164(2)	Ni(2)–O(8)#4	2.153(2)
O(1)#1–Ni(1)–O(4)#2	89.5(2)	O(2)–Ni(2)–O(2)#4	180.0(2)
O(1)#1–Ni(1)–O(5)	91.5(2)	O(2)–Ni(2)–O(6)	89.3(2)
O(4)#2–Ni(1)–O(5)	177.27(19)	O(2)#4–Ni(2)–O(6)	90.7(2)
O(1)#1–Ni(1)–N(1)#3	92.27(16)	O(2)–Ni(2)–O(6)#4	90.7(2)
O(4)#2–Ni(1)–N(1)#3	92.59(15)	O(2)#4–Ni(2)–O(6)#4	89.3(2)
O(5)–Ni(1)–N(1)#3	89.92(15)	O(6)–Ni(2)–O(6)#4	180.000(1)
O(1)#1–Ni(1)–O(3)	171.11(19)	O(2)–Ni(2)–O(8)	89.13(15)
O(4)#2–Ni(1)–O(3)	92.36(19)	O(2)#4–Ni(2)–O(8)	90.87(15)
O(5)–Ni(1)–O(3)	86.30(19)	O(6)–Ni(2)–O(8)	96.11(15)
N(1)#3–Ni(1)–O(3)	96.33(14)	O(6)#4–Ni(2)–O(8)	83.89(15)
O(1)#1–Ni(1)–O(7)	90.07(15)	O(2)–Ni(2)–O(8)#4	90.87(15)
O(4)#2–Ni(1)–O(7)	95.49(15)	O(2)#4–Ni(2)–O(8)#4	89.13(15)
O(5)–Ni(1)–O(7)	81.96(15)	O(6)–Ni(2)–O(8)#4	83.89(15)
N(1)#3–Ni(1)–O(7)	171.61(8)	O(6)#4–Ni(2)–O(8)#4	96.11(15)
O(3)−Ni(1)−O(7)	81.09(14)	O(8)–Ni(2)–O(8)#4	180.0

[a] Symmetry transformations used to generate equivalent atoms: #1 –x + 2, y + 1/2, –z + 1/2; #2 –x + 2, y – 1/2, –z + 1/2; #3 x + 1/2, y, –z + 1/2; #4 –x + 2, –y, –z + 1.

Table S2 Selected bond lengths (Å) and angles (º) for compound **3**[a]

Zn(1)–O(3)#1	1.926(5)	Zn(2)–O(8)#2	1.926(6)
Zn(1)–O(7)	1.929(6)	Zn(2)–O(2)	1.945(5)
Zn(1)–O(4)	1.939(5)	Zn(2)–O(6)	1.945(6)
Zn(1)–O(1)	1.990(5)	Zn(2)–O(10)#2	1.9635(16)
O(3)#1–Zn(1)–O(7)	115.5(2)	O(8)#2–Zn(2)–O(2)	121.3(3)
O(3)#1–Zn(1)–O(4)	107.9(2)	O(8)#2–Zn(2)–O(6)	113.3(2)
O(7)–Zn(1)–O(4)	111.5(2)	O(2)–Zn(2)–O(6)	103.3(2)
O(3)#1–Zn(1)–O(1)	107.6(2)	O(8)#2–Zn(2)–O(10)#2	101.51(17)
O(7)–Zn(1)–O(1)	110.4(2)	O(2)–Zn(2)–O(10)#2	105.15(17)
O(4)–Zn(1)–O(1)	103.2(2)	O(6)–Zn(2)–O(10)#2	112.26(18)

[a] Symmetry transformations used to generate equivalent atoms: #1 –x + 2, y – 1/2, –z + 1/2; #2 x, y + 1, z.