Supporting information for

Metal ions impact on the isostructurality and properties of 2D coordination polymers

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Details of isostructurality calculation

Due to the space group, the coordinates of **1-7** are orthogonalized, the special Fortran code was written to calculate the geometric descriptors – the indexes of cell similarity (π) and isostructurality (*Is*). The cell parameters were reoriented to have the same order for all compounds and the indexes of cell similarity were calculated using the formula presented in the manuscript (Table S1). To calculate the *Is*, the atoms were renamed and sorted into one-to-one correspondence. The origin of coordinates for all compounds was chosen on the metal. Then coordinate systems **1-7** were transformed so that one of the coordinate planes coincided with the plane of three Me atoms and coordinated nitrogen atoms, and the z axis was aligned with the Me-N bond (Table S3). The ΔRi was calculated as distance differences between the corresponding atoms for each pair of compounds. Table S1 and table S2 show all these calculations based on compounds **1** and **2**.

Table S1. Reoriented cell parameters and index π for **1** and **2**

Cell parameters	Cell similarity (π) for **1** and **2**
12.377 9.4953 10.2036	1 2 0.0040
12.2124 9.47 10.267	
12.9449 9.5117 9.9745	
12.4717 9.4383 10.1540	
13.6165 9.4836 9.7867	
12.6536 9.4825 10.0787	
13.3860 9.4973 9.8617	

Table S2. Transformed coordinates (Å) of non-hydrogen atoms in asymmetric unit cells for **1** and **2**

Atom	Compound **1**	Compound **2**
Me	0.0000 0.0000 0.0000	0.0000 0.0000 0.0000
C	-0.0967 2.6078 -1.3576	-0.1033 2.5775 -1.3743
C	-0.3849 3.6138 -2.4035	-0.3760 3.5732 -2.4585
C	0.2013 4.8669 -2.4188	0.2068 4.8274 -2.4729
C	-0.8598 5.4794 -4.3115	-0.8625 5.4256 -4.3795
C	-1.5263 4.2684 -4.3677	-1.5124 4.2221 -4.4421
C	-1.2600 3.3125 -3.4289	-1.2514 3.2688 -3.4822
C	0.1307 2.3456 2.0310	0.1194 2.3450 1.9994
C	0.0776 1.1463 2.9116	0.0629 1.1659 2.8700
C	0.0875 1.1658 4.3013	0.0633 1.1885 4.2715

C	0.2629	3.7289	2.6147	0.2371	3.7316	2.5713
C	0.0000	0.0000	5.0064	0.0000	0.0000	4.9583
N	0.0000	5.7850	-3.3442	0.0000	5.7494	-3.4164
N	0.0144	3.1139	-0.1240	-0.0044	3.1064	-0.1536
N	0.0479	2.0691	0.7852	0.0470	2.0643	0.7530
N	0.0000	0.0000	2.2320	0.0000	0.0000	2.2078
O	-0.0753	1.3731	-1.6576	-0.0622	1.3534	-1.6834

Table S3. Combined crystallographic data for compounds **1** - **7**

Compound	**1**	**2**	**3**	**4**	**5**	**6**	**7**
Metal(s)	Fe	Co	Mn	Zn	Cd	MnZn	$Cd_{1.25}Zn_{0.75}$
Crystal system	Orthorhombic						
Space group	$P2_12_12$						
a (Å)	12.377(3)	12.2124(5)	12.9449(4)	12.4717(3)	13.6165(4)	12.6536(8)	13.3860(6)
b (Å)	9.4953(13)	9.4700(4)	9.5117(4)	9.4383(3)	9.4836(4)	9.4825(6)	9.4973(4)
c (Å)	10.2036(15)	10.2670(6)	9.9745(4)	10.1540(3)	9.7867(3)	10.0787(8)	9.8617(4)
V (Å^3)	1199.2(4)	1187.39(10)	1228.14(8)	1195.24(6)	1263.79(8)	1209.32(14)	1253.71(9)
Z	2	2	2	2	2	1	1
ρ_{calc} (g cm^{-3})	1.412	1.486	1.426	1.474	1.488	1. 437	1.418

For compounds **6** and **7** - Z = 1. In our opinion, the formula has mainly chemical meaning, but not only a crystallographic one. These compounds contain two different metal atoms, Mn and Zn in **6**, and Zn and Cd in **7**, so two different complexes are involved in the coordination polymers (different metal atoms and different metal-ligand distances). The assumption that the structure of these compounds can be ordered (for example, due to different crystallisation conditions) obviously led to Z = 1 and to the presented formula. The fact that the positions of metal atoms or polymer chains are disordered in a crystal does not change the chemical meaning of these compounds, it will remain chemically the same. In the case when Z = 2, we get formulas that really do not exist and do not reflect the composition of the compounds. It is impossible for two different atoms to occupy the same place locally; this is only a formal crystallographic description of the fact of disorder in the case of $Mn_{0.5}Zn_{0.5}$ when Z=2, and, in our opinion, unacceptable for the formula unit.
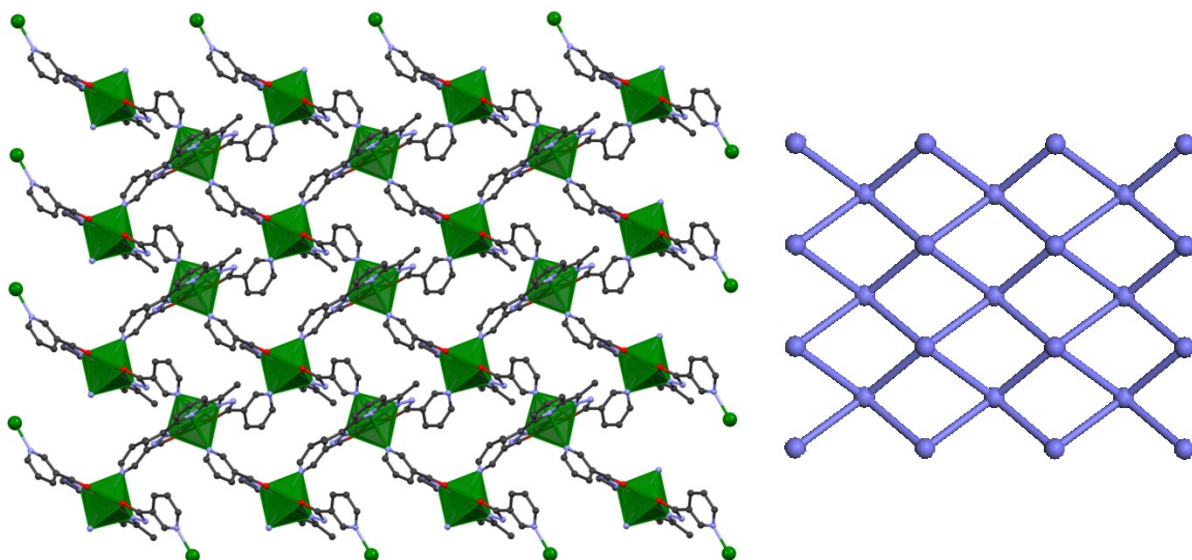
Fig. S1 Fragment of polymeric wave-like layer with 4,4-net topology in compounds **1**-**7**.

Photoluminescence measurements

The energy gap (*Eg*) can be estimated from observed photoluminescence spectra as follows:
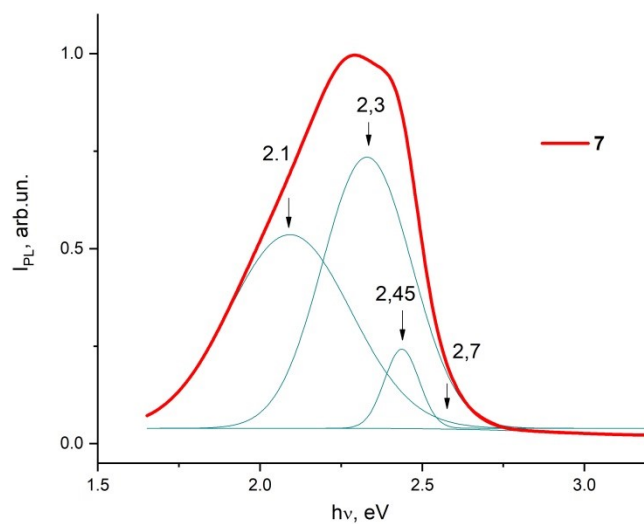
$$Eg \sim \frac{hc}{\lambda_m}$$

where *h* is Planck's constant, *c* is the light speed, λ_m is the wavelength of maximal PL intensity.

The error of *Eg* estimation can be calculated using the half-width of the spectral line:

$$\Delta(Eg) = \frac{hc}{2(\frac{1}{\lambda_1} - \frac{1}{\lambda_2})}$$

where the width of the spectral line is the distance between the points λ_1 and λ_2 corresponding to the intensity equal to half of maximum.
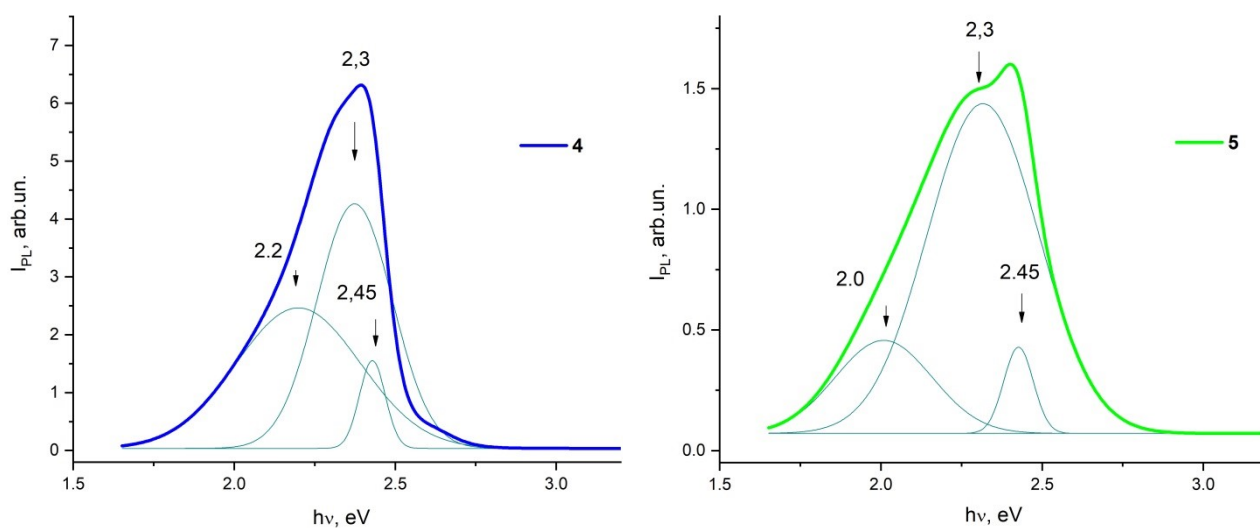
Fig. S2 Solid-state PL emission spectra for compounds **4**, **5** and **7**. The deconvolution of Gaussian resolution functions are shown by thin dash lines with the presentation of the maximum peaks in eV.