## Supporting information for

Solvent-controlled formation of four Ni(II) coordination polymers based on flexible bis(imidazole) ligand: syntheses, structural diversification, properties

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1. Table S1 The selected bond distances (Å) and angles (°) for 1-4.

- 2. Fig.S1 PXRD patterns of 1.
- 3. Fig.S2 PXRD patterns of 2.
- 4. Fig.S3 PXRD patterns of 3.
- 5. Fig.S4 PXRD patterns of 4.
- 6. **Fig.S5** TGA curves of **1**.
- 7. Fig.S6 TGA curves of 2.
- 8. Fig.S7 TGA curves of 3.
- 9. Fig.S8 TGA curves of 4.

| 1                   |           |                     |            |
|---------------------|-----------|---------------------|------------|
| Ni(1)-N(4)#1        | 2.044(6)  | Ni(1)-O(4)          | 2.052(4)   |
| Ni(1)-N(1)          | 2.085(6)  | Ni(1)-O(5)          | 2.129(5)   |
| Ni(1)-O(1)#2        | 2.130(4)  | Ni(1)-O(2)#2        | 2.137(5)   |
| N(4)#1-Ni(1)-O(4)   | 92.5(2)   | N(4)#1-Ni(1)-N(1)   | 93.5(2)    |
| O(4)-Ni(1)-N(1)     | 92.57(19) | N(4)#1-Ni(1)-O(5)   | 89.7(2)    |
| O(4)-Ni(1)-O(5)     | 91.11(17) | N(1)-Ni(1)-O(5)     | 175.0(2)   |
| N(4)#1-Ni(1)-O(1)#2 | 106.2(2)  | O(4)-Ni(1)-O(1)#2   | 160.34(18) |
| N(1)-Ni(1)-O(1)#2   | 92.19(19) | O(5)-Ni(1)-O(1)#2   | 83.22(17)  |
| N(4)#1-Ni(1)-O(2)#2 | 166.4(2)  | O(4)-Ni(1)-O(2)#2   | 99.20(17)  |
| N(1)-Ni(1)-O(2)#2   | 92.7(2)   | O(5)-Ni(1)-O(2)#2   | 83.3(2)    |
| O(1)#2-Ni(1)-O(2)#2 | 61.51(17) |                     |            |
| 2                   |           |                     |            |
| Ni(1)-N(1)          | 2.002(6)  | Ni(1)-N(4)          | 2.019(7)   |
| Ni(1)-O(1)          | 2.090(5)  | Ni(1)-O(3)#1        | 2.100(6)   |
| Ni(1)-O(4)#1        | 2.154(6)  | Ni(1)-O(2)          | 2.189(6)   |
| N(1)-Ni(1)-N(4)     | 92.8(3)   | N(1)-Ni(1)-O(1)     | 96.1(3)    |
| N(4)-Ni(1)-O(1)     | 96.5(2)   | N(1)-Ni(1)-O(3)#1   | 100.5(3)   |
| N(4)-Ni(1)-O(3)#1   | 107.0(2)  | O(1)-Ni(1)-O(3)#1   | 150.3(2)   |
| N(1)-Ni(1)-O(4)#1   | 92.2(3)   | N(4)-Ni(1)-O(4)#1   | 168.4(2)   |
| O(1)-Ni(1)-O(4)#1   | 93.3(2)   | O(3)#1-Ni(1)-O(4)#1 | 61.8(2)    |
| N(1)-Ni(1)-O(2)     | 158.2(3)  | N(4)-Ni(1)-O(2)     | 92.0(2)    |
| O(1)-Ni(1)-O(2)     | 62.2(2)   | O(3)#1-Ni(1)-O(2)   | 98.4(2)    |
| O(4)#1-Ni(1)-O(2)   | 87.1(2)   |                     |            |
| 3                   |           |                     |            |
| Ni(1)-O(1)          | 2.010(3)  | Ni(1)-O(5)          | 2.081(3)   |
| Ni(1)-N(1)          | 2.098(4)  | Ni(1)-O(3)#1        | 2.100(3)   |
| Ni(1)-O(7)#2        | 2.106(3)  | Ni(1)-O(4)#1        | 2.111(3)   |

1. Table S1 The selected bond distances (Å) and angles (°) for 1-4.

| Ni(2)-O(2)          | 2.014(3)   | Ni(2)-O(6)          | 2.018(3)   |
|---------------------|------------|---------------------|------------|
| Ni(2)-O(7)#2        | 2.045(3)   | Ni(2)-N(4)          | 2.050(4)   |
| Ni(2)-O(1W)         | 2.127(4)   | Ni(2)-O(8)#2        | 2.380(4)   |
| O(1)-Ni(1)-O(5)     | 88.16(15)  | O(1)-Ni(1)-N(1)     | 90.08(15)  |
| O(5)-Ni(1)-N(1)     | 172.76(15) | O(1)-Ni(1)-O(3)#1   | 157.79(14) |
| O(5)-Ni(1)-O(3)#1   | 84.88(14)  | N(1)-Ni(1)-O(3)#1   | 99.25(15)  |
| O(1)-Ni(1)-O(7)#2   | 102.86(13) | O(5)-Ni(1)-O(7)#2   | 883.61(13) |
| N(1)-Ni(1)-O(7)#2   | 89.93(15)  | O(3)#1-Ni(1)-O(7)#2 | 97.31(13)  |
| O(1)-Ni(1)-O(4)#1   | 96.32(14)  | O(5)-Ni(1)-O(4)#1   | 91.16(15)  |
| N(1)-Ni(1)-O(4)#1   | 96.02(16)  | O(3)#1-Ni(1)-O(4)#1 | 62.84(13)  |
| O(7)#2-Ni(1)-O(4)#1 | 159.92(13) | O(2)-Ni(2)-O(6)     | 95.74(15)  |
| O(2)-Ni(2)-O(7)#2   | 92.61(14)  | O(6)-Ni(2)-O(7)#2   | 97.59(13)  |
| O(2)-Ni(2)-N(4)     | 86.75(16)  | O(6)-Ni(2)-N(4)     | 97.18(16)  |
| O(7)#2-Ni(2)-N(4)   | 165.21(15) | O(2)-Ni(2)-O(1W)    | 176.22(15) |
| O(6)-Ni(2)-O(1W)    | 87.75(15)  | O(7)#2-Ni(2)-O(1W)  | 88.35(15)  |
| N(4)-Ni(2)-O(1W)    | 91.39(17)  | O(2)-Ni(2)-O(8)#2   | 96.81(14)  |
| O(6)-Ni(2)-O(8)#2   | 153.54(14) | O(7)#2-Ni(2)-O(8)#2 | 58.68(12)  |
| N(4)-Ni(2)-O(8)#2   | 106.70(15) | O(1W)-Ni(2)-O(8)#2  | 80.57(14)  |
| 4                   |            |                     |            |
| Ni(1)-N(4)          | 2.034(6)   | Ni(1)-N(1)          | 2.040(6)   |
| Ni(1)-O(4)          | 2.058(5)   | Ni(1)-O(1)          | 2.060(5)   |
| Ni(1)-O(3)          | 2.243(5)   | Ni(1)-O(2)          | 2.248(5)   |
| N(4)-Ni(1)-N(1)     | 91.5(2)    | N(4)-Ni(1)-O(4)     | 102.3(2)   |
| N(1)-Ni(1)-O(4)     | 98.6(2)    | N(4)-Ni(1)-O(1)     | 92.8(2)    |
| N(1)-Ni(1)-O(1)     | 96.5(2)    | O(4)-Ni(1)-O(1)     | 158.3(2)   |
| N(4)-Ni(1)-O(3)     | 95.2(2)    | N(1)-Ni(1)-O(3)     | 159.0(2)   |
| O(4)-Ni(1)-O(3)     | 60.58(19)  | O(1)-Ni(1)-O(3)     | 103.1(2)   |
| N(4)-Ni(1)-O(2)     | 154.0(2)   | N(1)-Ni(1)-O(2)     | 93.8(2)    |
| O(4)-Ni(1)-O(2)     | 102.05(19) | O(1)-Ni(1)-O(2)     | 61.3(2)    |
|                     |            |                     |            |

symmetrical codes: 1: #1 x, -y+3/2, z-1/2; #2 x+1, -y+1/2, z+1/2. 2: #1 -x+1, y-1/2, - z+3/2. 3: #1 x, y-1, z; #2 x-1, y, z.

2. Fig.S1 PXRD patterns of 1.



3. Fig.S2 PXRD patterns of 2.



4. Fig.S3 PXRD patterns of 3.



5. Fig.S4 PXRD patterns of 4.



6. Fig.S5 TGA curves of 1.



7. Fig.S6 TGA curves of 2.



8. Fig.S7 TGA curves of 3.



9. Fig.S8 TGA curves of 4.

