The Effect of Metal Ions on Photocatalytic Performance Based on

Isostructural Framework

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Fig. S1 (a) Coordination environment around Mn^{II} in 1. (b) View of connection between 1D chains. (c) View of hydrogen bond in **5**.



Fig. S2 Simulated and experimental PXRD data for 1 (up) and 5 (down).



Fig. S3 Thermogravimetric analyses of 1 and 5.



Fig. S4 Simulated and experimental PXRD data of 1-5 after refluxing in water system.



Fig.S5 Photocatalytic decomposition of four kinds of dyes in the presence of complexes 1, 5 and the control experiment without any catalyst under the same conditions (a: 1, b: without catalyst, c: 5).



Fig.S6 Absorption spectra of six kinds of dyes during the decomposition reaction under visible light irradiation in the presence of complex **5**.



Fig.S7 MS spectrum before (up) and after (down) the reaction of photocatalytic decomposition of MB solution.



Fig.S8 Photocatalytic decomposition of six kinds of dyes solution under visible light irradiation in the presence of complex **5**.



Fig.S9 The PXRD patterns of 1 (up) and 5 (down) at the end of final repeated bleaching experiment.





Fig.S11 Kubelka-Munk-transformed diffuse reflectance of complexes 1 and 5.

| desemption. | | | | | | |
|---------------------|------------------------|-------------------------|--------------|--|--|--|
| Complex 1 | | | | | | |
| O(1)-Mn(1) | 2.2201(19) | Mn(1)-O(3)#2 | 2.169(2) | | | |
| O(1)-Mn(2)#1 | 2.255(2) | Mn(1)-O(7)#2 | 2.173(3) | | | |
| O(7)-Mn(1) | 2.173(3) | Mn(1)-O(1)#2 | 2.2201(19) | | | |
| O(8)-Mn(2) | 2.109(2) | Mn(2)-O(6)#3 | 2.114(2) | | | |
| O(5)-Mn(2)#1 | 2.156(2) | Mn(2)-O(5)#4 | 2.156(2) | | | |
| O(9)-Mn(2) | 2.224(2) | Mn(2)-O(1)#4 | 2.255(2) | | | |
| O(3)-Mn(1) | 2.169(2) | Mn(2)-N(1) | 2.316(2) | | | |
| O(6)-Mn(2)#3 | 2.114(2) | O(6)#3-Mn(2)-O(1)#4 | 174.52(7) | | | |
| O(3)#2-Mn(1)-O(3) | 180.000(1) | O(5)#4-Mn(2)-O(1)#4 | 82.36(7) | | | |
| O(3)#2-Mn(1)-O(7)#2 | 90.06(11) | O(9)-Mn(2)-O(1)#4 | 86.37(8) | | | |
| O(3)-Mn(1)-O(7)#2 | 89.94(11) | O(8)-Mn(2)-N(1) | 96.86(11) | | | |
| O(3)#2-Mn(1)-O(7) | 89.94(11) | O(6)#3-Mn(2)-N(1) | 91.40(9) | | | |
| O(3)-Mn(1)-O(7) | 90.06(11) | O(5)#4-Mn(2)-N(1) | 81.60(8) | | | |
| O(7)#2-Mn(1)-O(7) | 180.0 | O(9)-Mn(2)-N(1) | 168.20(8) | | | |
| O(3)#2-Mn(1)-O(1)#2 | 83.98(7) | O(1)#4-Mn(2)-N(1) | 84.47(8) | | | |
| Symmetry codes: | #1 x,y-1,z #2 -x,-y,-z | +2 #3 -x+1,-y+1,-z+1 | #4 x,y+1,z | | | |
| | Com | plex 5 | | | | |
| Co(1)-O(5) | 2.069(3) | Co(2)-O(2) | 2.020(3) | | | |
| Co(1)-O(5)#1 | 2.069(3) | Co(2)-O(9)#2 | 2.054(2) | | | |
| Co(1)-O(4)#1 | 2.115(2) | Co(2)-O(8)#3 | 2.107(2) | | | |
| Co(1)-O(4) | 2.115(2) | Co(2)-O(1) | 2.134(3) | | | |
| Co(1)-O(6)#1 | 2.162(2) | Co(2)-O(6)#3 | 2.168(2) | | | |
| Co(1)-O(6) | 2.162(2) | Co(2)-N(1) | 2.176(3) | | | |
| O(5)-Co(1)-O(5)#1 | 180.0 | O(2)-Co(2)-O(9)#2 | 88.21(11) | | | |
| O(5)-Co(1)-O(4)#1 | 90.37(11) | O(2)-Co(2)-O(8)#3 | 175.30(10) | | | |
| O(5)#1-Co(1)-O(4)#1 | 89.63(11) | O(9)#2-Co(2)-O(8)#3 | 96.07(9) | | | |
| O(5)-Co(1)-O(4) | 89.63(11) | O(2)-Co(2)-O(1) | 91.64(12) | | | |
| O(5)#1-Co(1)-O(4) | 90.37(11) | O(9)#2-Co(2)-O(1) | 92.39(10) | | | |
| O(4)#1-Co(1)-O(4) | 180.00(12) | O(8)#3-Co(2)-O(1) | 90.12(10) | | | |
| O(5)-Co(1)-O(6)#1 | 88.45(10) | O(2)-Co(2)-O(6)#3 | 89.99(10) | | | |
| O(5)#1-Co(1)-O(6)#1 | 91.55(10) | O(9)#2-Co(2)-O(6)#3 | 178.06(8) | | | |
| O(4)#1-Co(1)-O(6)#1 | 86.53(9) | O(8)#3-Co(2)-O(6)#3 | 85.70(8) | | | |
| O(4)-Co(1)-O(6)#1 | 93.47(9) | O(1)-Co(2)-O(6)#3 | 88.39(10) | | | |
| O(5)-Co(1)-O(6) | 91.55(10) | O(2)-Co(2)-N(1) | 95.40(12) | | | |
| O(5)#1-Co(1)-O(6) | 88.45(10) | O(9)#2-Co(2)-N(1) | 91.89(10) | | | |
| O(4)#1-Co(1)-O(6) | 93.47(9) | O(8)#3-Co(2)-N(1) | 82.56(9) | | | |
| O(4)-Co(1)-O(6) | 86.53(9) | O(1)-Co(2)-N(1) | 171.87(10) | | | |
| O(6)#1-Co(1)-O(6) | 180.0 | O(6)#3-Co(2)-N(1) | 87.54(9) | | | |
| Symmetry codes: | #1 -x+2,-y+2,-z #2 -x | +1,-y+1,-z+1 #3 x,y-1,z | z #4 x,y+1,z | | | |

Table S1 Selected bond lengths (Å) and bond angles (deg) for 1 and 5 crystal structure description.

| Complex | D-H···A | d(D-H) (Å) | d(H····A) | d(D…A) | <(D-H…A) | |
|----------------------------|-------------------|------------|------------|----------|----------|--|
| | | | (Å) | (Å) | (deg) | |
| 5 | O(2)-H(2W1)O(3)#1 | 0.852(19) | 1.86(2) | 2.701(4) | 167(4) | |
| Symmetry codes: #1 x-1,y,z | | | | | | |

Table S3. Hydrogen Bonds of complexes 5.

| Complex | 2 | 3 | 4 |
|---------|------------|------------|------------|
| a/Å | 7.4267(15) | 7.4136(14) | 7.4158(11) |
| b/Å | 8.5085(17) | 8.5154(11) | 8.4779(12) |
| c/Å | 10.381(2) | 10.279(3) | 10.165(9) |
| a/u | 82.69(4) | 82.64(2) | 82.67(4) |
| b/u | 83.44(6) | 83.45(9) | 83.36(8) |
| c/u | 79.82(8) | 79.72(3) | 79.89(6) |
| V/Å3 | 632.7(2) | 629.2(4) | 625.6(7) |

Table S2 Crystallographic parameters of 2-4.