

Syntheses, structural diversity and photocatalytic properties of three coordination polymers assembled by different N-heterocyclic ligands

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Table S1 Selected bond lengths (\AA) and angles ($^\circ$) for **1-3**

| Complex 1 | | | |
|--------------------------------|-----------|--|-----------|
| Bond | Dist. | Bond | Dist. |
| Cu(1)-O(4) ^{#1} | 2.438(15) | Cu(1)-N(1) ^{#1} | 2.021(15) |
| Cu(1)-N(6) ^{#2} | 2.044(2) | Cu(1)-N(6) ^{#3} | 2.044(2) |
| Bond | Angle | Bond | Angle |
| O(4) ^{#1} -Cu(1)-O(1) | 180.0 | N(1) ^{#1} -Cu(1)-N(6) ^{#2} | 89.78(6) |
| N(1)-Cu(1)-O(1) | 87.07(10) | N(1) ^{#1} -Cu(1)-N(6) ^{#3} | 90.22(6) |
| N(1)-Cu(1)-O(1) | 92.93(6) | N(6) ^{#2} -Cu(1)-O(1) | 88.18(5) |
| N(1)-Cu(1)-O(1) ^{#1} | 87.07(6) | N(6) ^{#3} -Cu(1)-O(1) | 91.82(5) |
| | | N(6) ^{#2} -Cu(1)-N(6) ^{#3} | 180.0 |

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

| Complex 2 | | | |
|-------------------------------|------------|--|-------------|
| Bond | Dist. | Bond | Dist. |
| Cu(1)-O(2) ^{#1} | 2.372(4) | Cu(1)-N(4) ^{#2} | 2.033(3) |
| Cu(1)-O(3) | 1.973(4) | Cu(1)-O(1) | 1.978(3) |
| Cu(1)-N(1) | 2.020(3) | N(4)-Cu(1) ^{#4} | 2.020(4) |
| Bond | Angle | Bond | Angle |
| O(1)-Cu(1)-O(2) | 85.80(11) | O(3)-Cu(1)-N(1) | 90.60(11) |
| O(1)-Cu(1)-O(3) | 170.77(11) | O(3)-Cu(1)-N(4) ^{#2} | 91.17(18) |
| O(1)-Cu(1)-N(1) | 87.89(12) | N(1)-Cu(1)-O(2) ^{#1} | 90.40(12) |
| O(1)-Cu(1)-N(4) ^{#2} | 93.24(12) | N(4) ^{#2} -Cu(1)-O(2) ^{#1} | 88.75(12) |
| O(3)-Cu(1)-O(2) ^{#1} | 85.14(10) | N(4) ^{#2} -Cu(1)-N(1) | 177.796(12) |

Symmetry codes: #1: -x+1, y-1/2, -z+3/2; #2: -x+3/2, -y+1, z+1/2; #3: -x+1, y+1/2, -z+3/2; #4: -x+3/2, -y+1, z-1/2.

| Complex 3 | | | |
|---------------------------------|-----------|--|-----------|
| Bond | Dist. | Bond | Dist. |
| Cd(1)-O(1) ^{#1} | 2.301(11) | Cd(1)-O(3) ^{#3} | 2.273(15) |
| Cd(1)-O(2) ^{#2} | 2.281(14) | Cd(1)-N(1) ^{#5} | 2.298(11) |
| Bond | Angle | Bond | Angle |
| O(1) ^{#1} -Cd(1))-O(1) | 71.7(4) | O(3) ^{#5} -Cd(1)-N(1) ^{#3} | 76.9(5) |

| | | | |
|--|----------|--|----------|
| O(2) ^{#2} -Cd(1)-O(1) | 117.0(4) | O(3) ^{#4} -Cd(1)-O(3) ^{#5} | 40.0(7) |
| O(2) ^{#2} -Cd(1)-O(1) ^{#1} | 171.3(5) | O(3) ^{#5} -Cd(1)-N(1) ^{#3} | 76.9(5) |
| O(2) ^{#2} -Cd(1)-N(1) ^{#3} | 89.4(3) | O(3) ^{#4} -Cd(1)-N(1) ^{#3} | 116.9(5) |
| O(3) ^{#5} -Cd(1)-O(1) | 154.3(4) | N(1)-Cd(1)-O(1) | 83.9(3) |
| O(3) ^{#5} -Cd(1)-O(1) ^{#1} | 80.1(5) | N(1)-Cd(1)-O(1) ^{#1} | 91.6(3) |
| O(3) ^{#5} -Cd(1)-O(2) ^{#2} | 171.3(5) | N(1)-Cd(1)-N(1) ^{#3} | 165.7(5) |

Symmetry codes: #1: 1-x,-y,1-z; #2: -1/2+x,1/2-y,1-z; #3: -1+x,+y,+z; #4: -1+x,+y,1-z; #5: +x,+y,1-z;

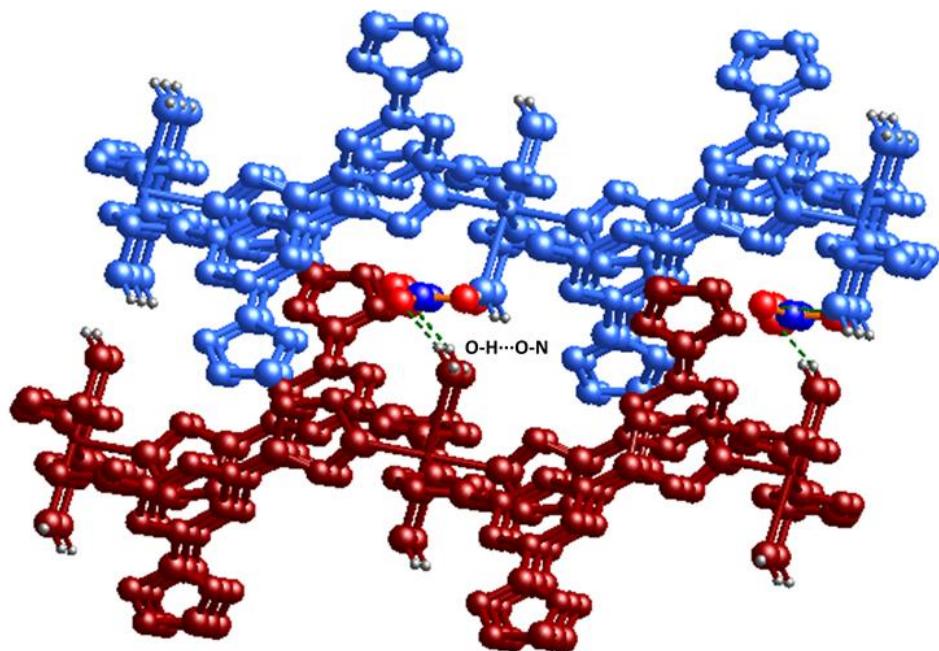


Fig. S1 The H-bonds(O-H \cdots O-N) which interacted two neighbouring 2D layers

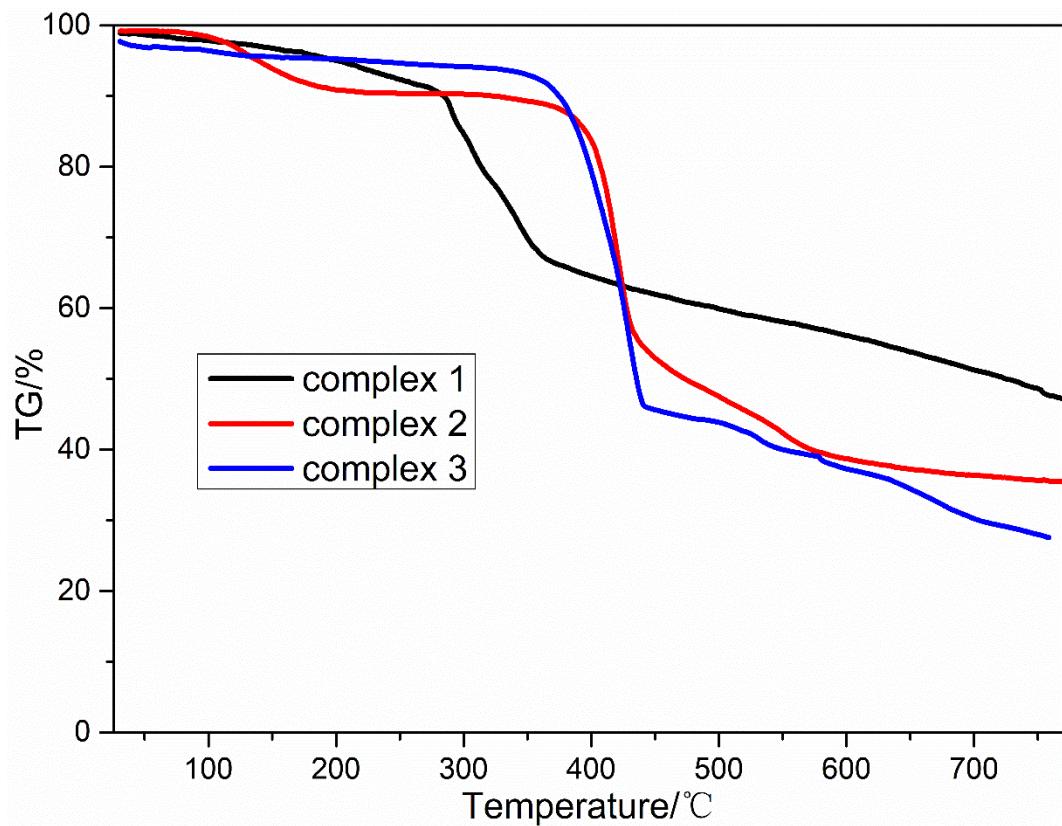


Fig S2. The TG curves of 1- 3.

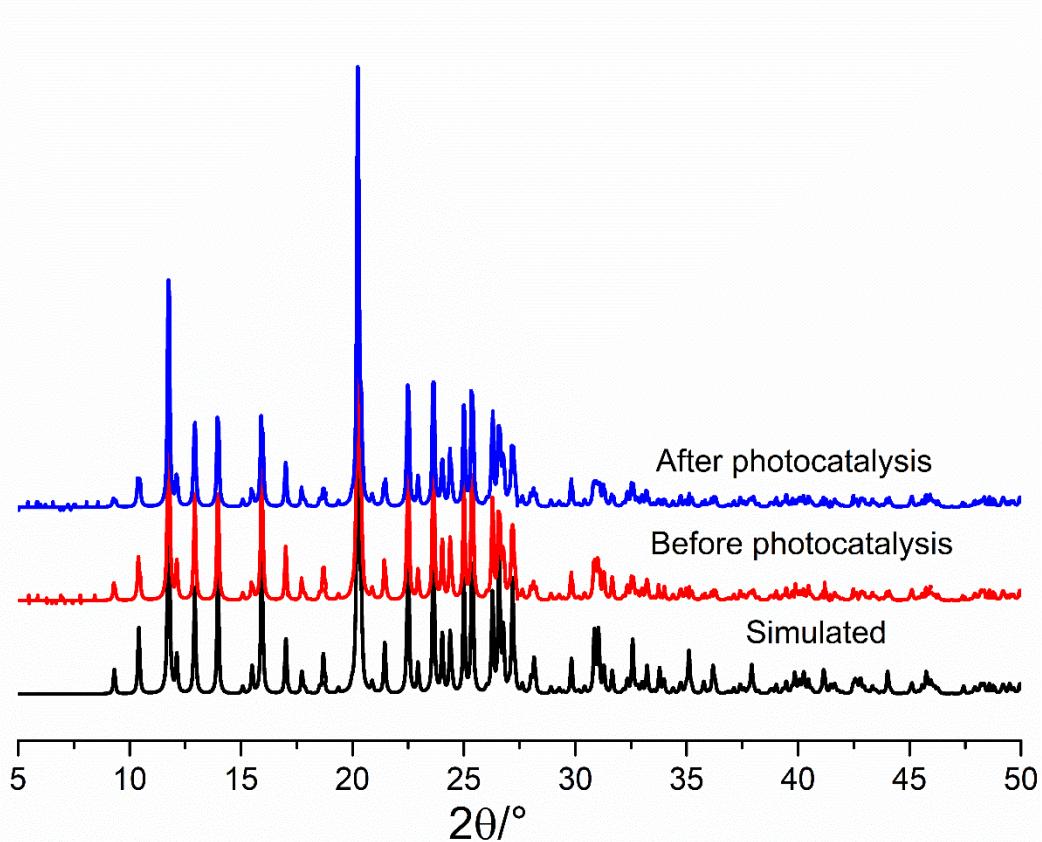


Fig. S3 PXRD patterns of the complex 1 before and after photocatalysis process

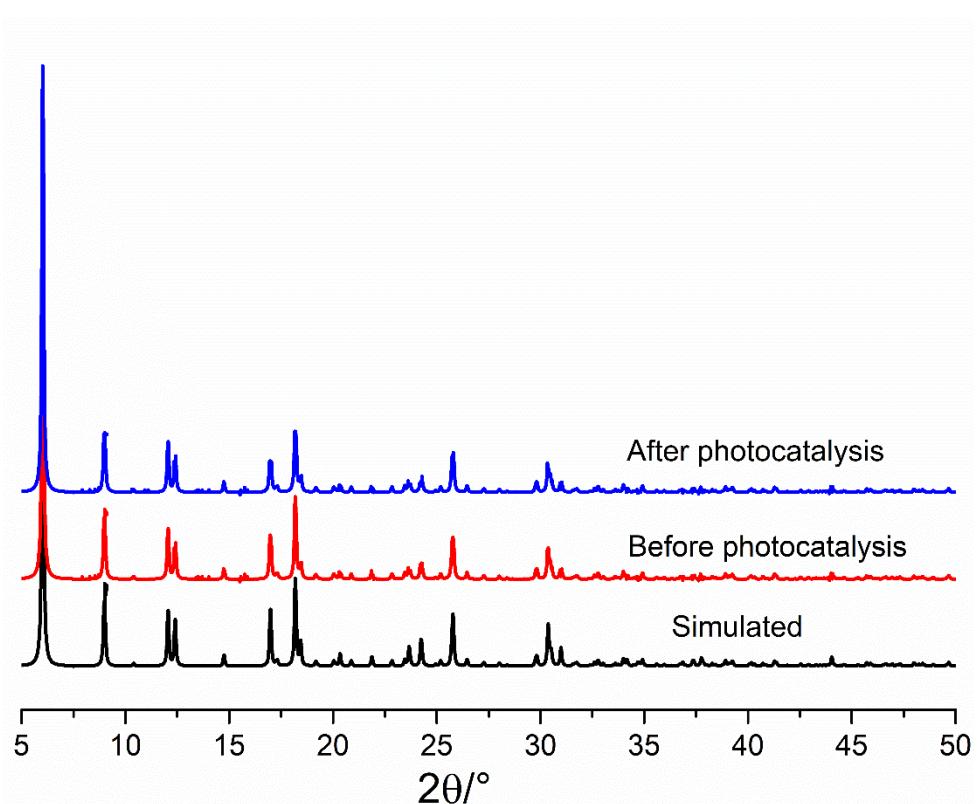


Fig. S4 PXRD patterns of the complex **2** before and after photocatalysis process

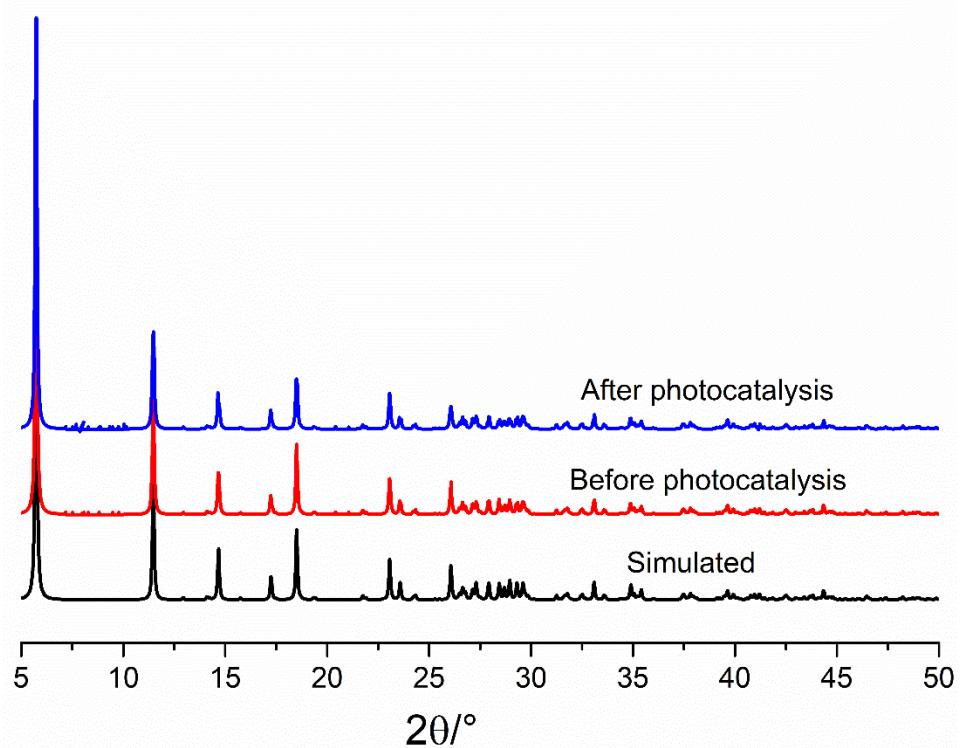


Fig. S5 PXRD patterns of the complex **3** before and after photocatalysis process

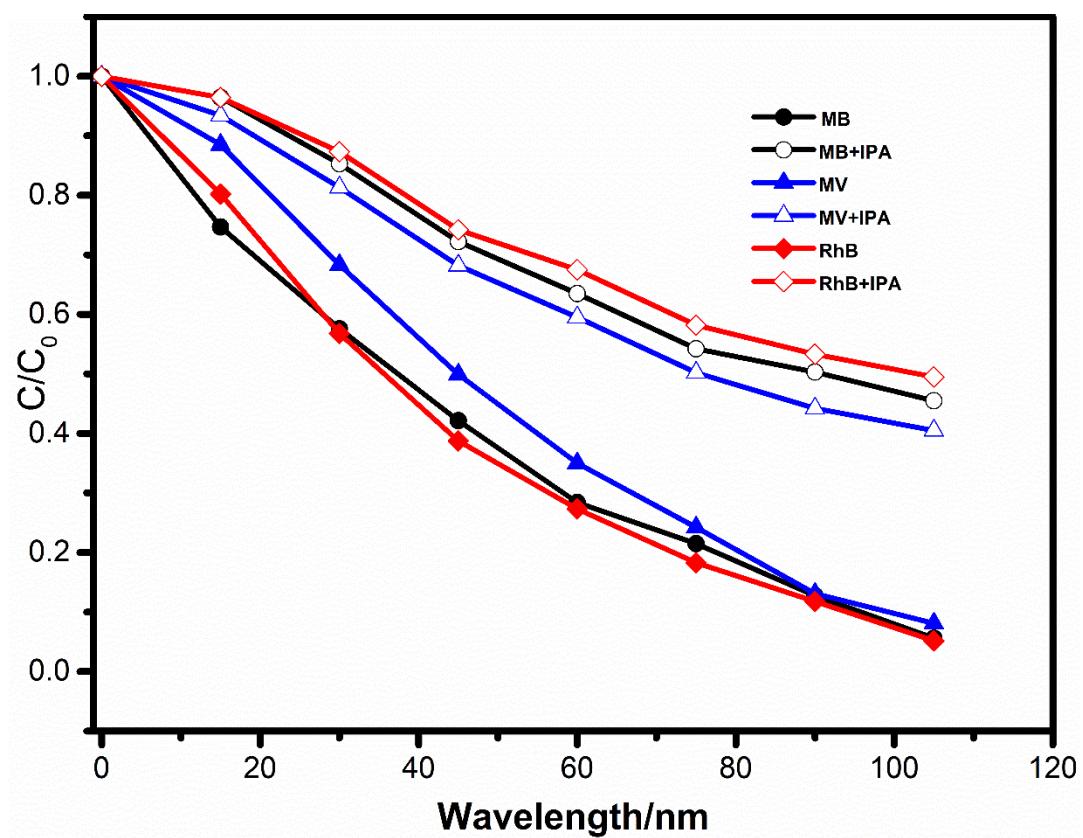


Fig. S6 Change in the three dyes solution with UV light irradiation time in the presence of the complex **1** and different active species scavengers