Electronic supplementary information (ESI)

Hybrid material based on coordination complex modified polyoxometalate nanorod (CC/POMNR) and PPy: A new visible light active and high efficient photocatalyst

Xinxin Xu[a], Xin Gao[a], Tingting Lu[a], Xiaoxia Liu*[a] and Xiuli Wang*[b]

[a]*Department of Chemistry, College of Science, Northeast University, Shenyang, Liaoning, 110819, People's Republic of China*

[b]*Department of Chemistry, Bohai University, Jinzhou, Liaoning, 121013, People's Republic of China*

Table S1. Crystal data and structure refinement results for **ZnP_2Mo_5**

Empirical formula	$C_{48}H_{52}N_{12}O_{29}ZnP_2Mo_5$
Formula weight	1868.03
Crystal system	Monoclinic
Space group	$P\ 2_1/c$
a/Å	10.1704(6)
b/Å	21.3474(12)
c/Å	29.3979(16)
α/°	90
β/°	90.5890(10)
γ/°	90
V/Å^3	6382.3(6)
Z	4
D_{calcd}/(g cm^{-3})	1.944
Reflections collected	35473
Reflections unique	11070
R(int)	0.0415
Goodness - of - fit on F^2	1.108
R_1 [$I > 2\sigma(I)$]	0.0523
wR_2 [$I > 2\sigma(I)$]	0.1465
R_1 (all data)	0.0637
wR_2 (all data)	0.1564

Note. $R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$; $wR_2 = \Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]^{1/2}$

Table S2. Selected bond lengths of **ZnP_2Mo_5**

Mo(1)-O(2)	2.307(5)	Mo(1)-O(9)	1.863(5)
Mo(1)-O(10)	1.721(5)	Mo(1)-O(13)	1.715(5)
Mo(1)-O(11)	1.970(5)	Mo(1)-O(16)	2.256(5)
Mo(2)-O(2)	2.210(5)	Mo(2)-O(4)	1.698(5)
Mo(2)-O(7)	2.309(4)	Mo(2)-O(8)	1.718(5)
Mo(2)-O(11)	1.940(5)	Mo(2)-O(23)	1.961(5)
Mo(3)-O(6)	1.723(5)	Mo(3)-O(7)	2.293(5)
Mo(3)-O(15)	1.723(5)	Mo(3)-O(17)	2.293(5)
Mo(3)-O(18)	1.908(5)	Mo(3)-O(23)	1.929(5)
Mo(4)-O(3)	1.721(5)	Mo(4)-O(17)	2.385(5)
Mo(4)-O(18)	1.943(5)	Mo(4)-O(19)	1.961(5)
Mo(4)-O(20)	1.704(5)	Mo(4)-O(21)	2.182(5)
Mo(5)-O(5)	1.731(6)	Mo(5)-O(9)	1.939(5)
Mo(5)-O(12)	1.702(5)	Mo(5)-O(14)	2.230(5)
Mo(5)-O(19)	1.919(5)	Mo(5)-O(21)	2.425(5)
Zn(1)-O(1)#1	1.980(5)	Zn(1)-O(22)	1.982(5)
Zn(1)-O(24)	2.139(6)	Zn(1)-N(1)	2.161(6)
Zn(1)-N(4)	2.205(6)	P(1)-O(1)	1.521(5)
P(1)-O(7)	1.555(5)	P(1)-O(16)	1.531(5)
P(1)-O(21)	1.564(5)	P(2)-O(2)	1.568(5)
P(2)-O(14)	1.528(5)	P(2)-O(17)	1.549(5)
P(2)-O(22)	1.522(5)		

Table S3. Selected bond angles of ZnP_2Mo_5

O(9)-Mo(1)-O(2)	87.66(19)	O(9)-Mo(1)-O(11)	148.0(2)
O(9)-Mo(1)-O(16)	79.85(19)	O(10)-Mo(1)-O(2)	165.5(2)
O(10)-Mo(1)-O(9)	102.6(2)	O(10)-Mo(1)-O(11)	96.8(2)
O(10)-Mo(1)-O(16)	85.2(2)	O(11)-Mo(1)-O(2)	69.60(18)
O(11)-Mo(1)-O(16)	76.62(18)	O(13)-Mo(1)-O(2)	87.1(2)
O(13)-Mo(1)-O(9)	100.3(2)	O(13)-Mo(1)-O(10)	100.9(2)
O(13)-Mo(1)-O(11)	100.7(2)	O(13)-Mo(1)-O(16)	173.6(2)
O(16)-Mo(1)-O(2)	86.55(16)	O(2)-Mo(2)-O(7)	72.97(17)
O(4)-Mo(2)-O(2)	156.9(2)	O(4)-Mo(2)-O(7)	86.8(2)
O(4)-Mo(2)-O(8)	103.6(3)	O(4)-Mo(2)-O(11)	97.4(2)
O(4)-Mo(2)-O(23)	100.7(2)	O(8)-Mo(2)-O(2)	98.7(2)
O(8)-Mo(2)-O(7)	164.1(2)	O(8)-Mo(2)-O(11)	100.0(2)
O(8)-Mo(2)-O(23)	93.4(2)	O(11)-Mo(2)-O(2)	72.26(18)
O(11)-Mo(2)-O(7)	90.46(18)	O(11)-Mo(2)-O(23)	154.3(2)
O(23)-Mo(2)-O(2)	84.14(19)	O(23)-Mo(2)-O(7)	72.57(18)
O(6)-Mo(3)-O(7)	167.9(2)	O(6)-Mo(3)-O(17)	90.5(2)
O(6)-Mo(3)-O(18)	101.1(2)	O(6)-Mo(3)-O(23)	99.1(2)
O(15)-Mo(3)-O(6)	102.4(2)	O(15)-Mo(3)-O(7)	88.6(2)
O(15)-Mo(3)-O(17)	166.5(2)	O(15)-Mo(3)-O(18)	98.6(2)
O(15)-Mo(3)-O(23)	100.5(2)	O(17)-Mo(3)-O(7)	79.05(16)
O(18)-Mo(3)-O(7)	82.09(18)	O(18)-Mo(3)-O(17)	74.51(18)
O(18)-Mo(3)-O(23)	148.38(19)	O(23)-Mo(3)-O(7)	73.47(18)
O(23)-Mo(3)-O(17)	81.29(19)	O(3)-Mo(4)-O(17)	87.8(2)
O(3)-Mo(4)-O(18)	102.7(2)	O(3)-Mo(4)-O(19)	93.9(2)
O(3)-Mo(4)-O(21)	158.1(2)	O(18)-Mo(4)-O(17)	71.73(17)
O(18)-Mo(4)-O(19)	154.7(2)	O(18)-Mo(4)-O(21)	83.03(18)
O(19)-Mo(4)-O(17)	90.26(19)	O(19)-Mo(4)-O(21)	74.78(19)
O(20)-Mo(4)-O(3)	104.0(3)	O(20)-Mo(4)-O(17)	164.0(2)
O(20)-Mo(4)-O(18)	94.8(2)	O(20)-Mo(4)-O(19)	99.6(2)
O(20)-Mo(4)-O(21)	96.5(2)	O(21)-Mo(4)-O(17)	73.82(17)
O(5)-Mo(5)-O(9)	97.7(2)	O(5)-Mo(5)-O(14)	170.5(2)
O(5)-Mo(5)-O(19)	98.8(3)	O(5)-Mo(5)-O(21)	83.9(2)
O(9)-Mo(5)-O(14)	79.62(19)	O(9)-Mo(5)-O(21)	83.85(18)
O(12)-Mo(5)-O(5)	102.6(3)	O(12)-Mo(5)-O(9)	103.8(2)
O(12)-Mo(5)-O(14)	86.9(2)	O(12)-Mo(5)-O(19)	100.1(2)
O(12)-Mo(5)-O(21)	169.0(2)	O(14)-Mo(5)-O(21)	86.70(17)
O(19)-Mo(5)-O(14)	79.4(2)	O(19)-Mo(5)-O(9)	147.1(2)
O(19)-Mo(5)-O(21)	69.87(18)	O(1)-P(1)-O(7)	109.0(3)
O(1)-P(1)-O(16)	112.2(3)	O(1)-P(1)-O(21)	111.3(3)
O(7)-P(1)-O(21)	109.3(3)	O(16)-P(1)-O(7)	108.6(3)
O(16)-P(1)-O(21)	106.4(3)	O(14)-P(2)-O(2)	106.4(3)
O(14)-P(2)-O(17)	109.3(3)	O(17)-P(2)-O(2)	108.6(3)

O(22)-P(2)-O(2)	109.1(3)	O(22)-P(2)-O(14)	112.6(3)
O(22)-P(2)-O(17)	110.6(3)	O(1)#1-Zn(1)-O(22)	131.4(2)
O(1)#1-Zn(1)-O(24)	93.7(2)	O(22)-Zn(1)-O(24)	86.8(2)
O(1)#1-Zn(1)-N(1)	114.4(2)	O(1)#1-Zn(1)-N(4)	97.6(2)
O(22)-Zn(1)-N(1)	114.2(2)	O(22)-Zn(1)-N(4)	87.3(2)
O(24)-Zn(1)-N(1)	89.2(2)	O(24)-Zn(1)-N(4)	168.6(2)
N(1)-Zn(1)-N(4)	84.4(2)		

Symmetry transformations used to generate equivalent atoms for **ZnP_2Mo_5**: #1 x-1, y, z.

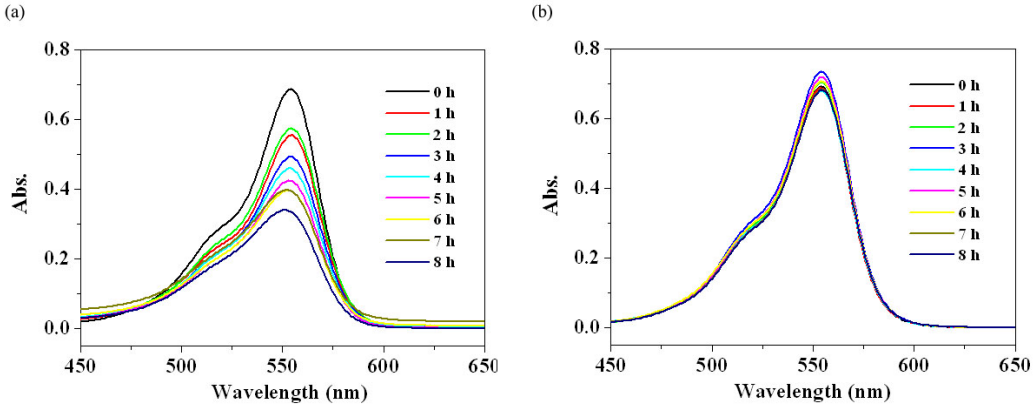

Figure S1. Absorption spectra of RhB degraded by **ZnP_2Mo_5NR** under ultraviolet and visible light irradiation

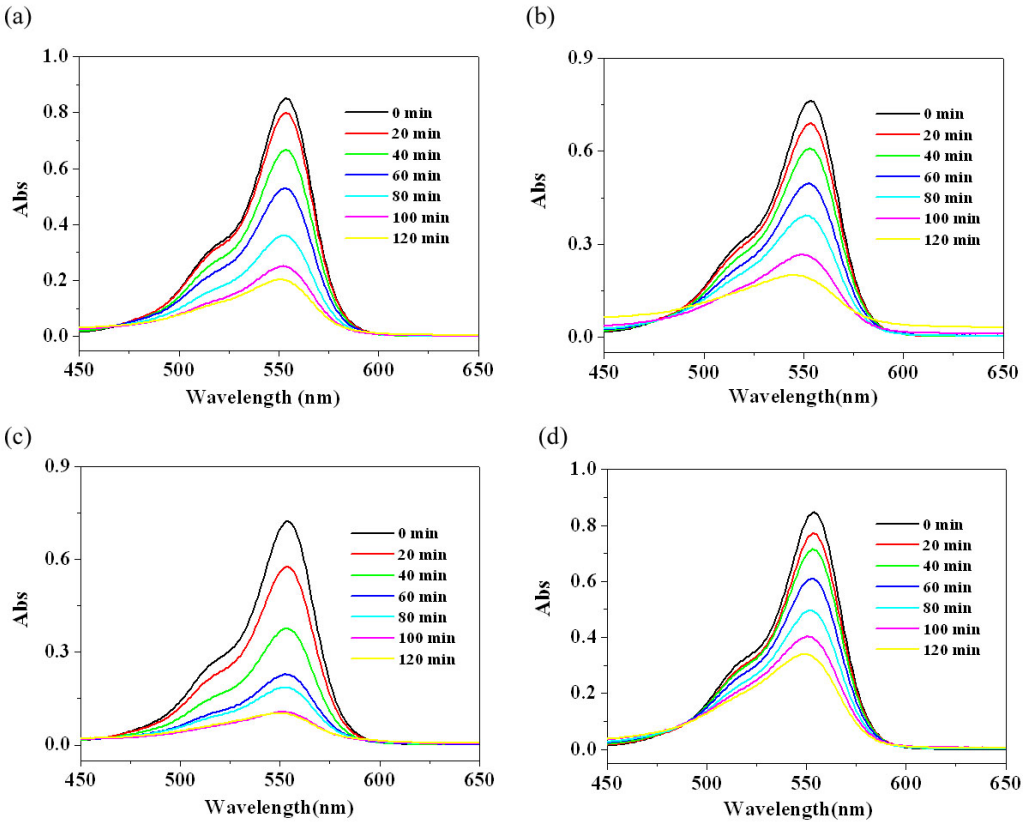

Figure S2. Absorption spectra of RhB degraded by: (a) **PPy(A)/ZnP$_2$Mo$_5$NR**; (b) **PPy(B)/ZnP$_2$Mo$_5$NR**; (c) **PPy(C)/ZnP$_2$Mo$_5$NR**; (d) **PPy(D)/ZnP$_2$Mo$_5$NR** by visible light irradiation.

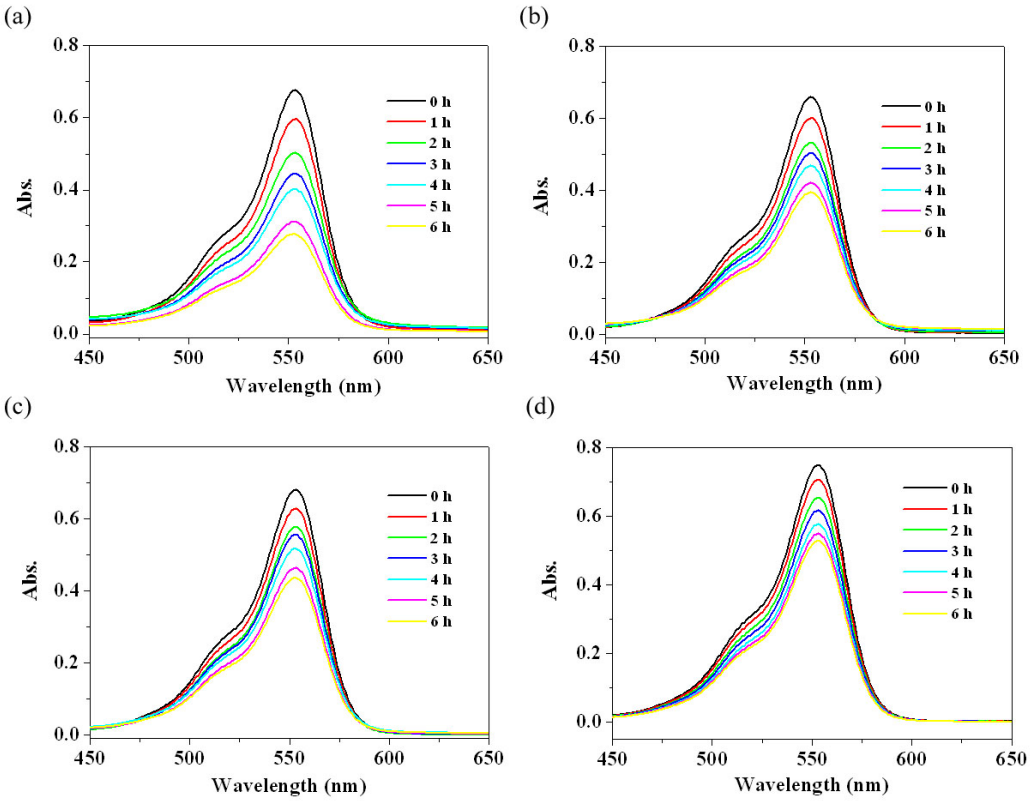

Figure S3. Absorption spectra of RhB degraded by: (a) PPy(A); (b) PPy(B); (c) PPy(C); (d) PPy(D) under visible light irradiation.

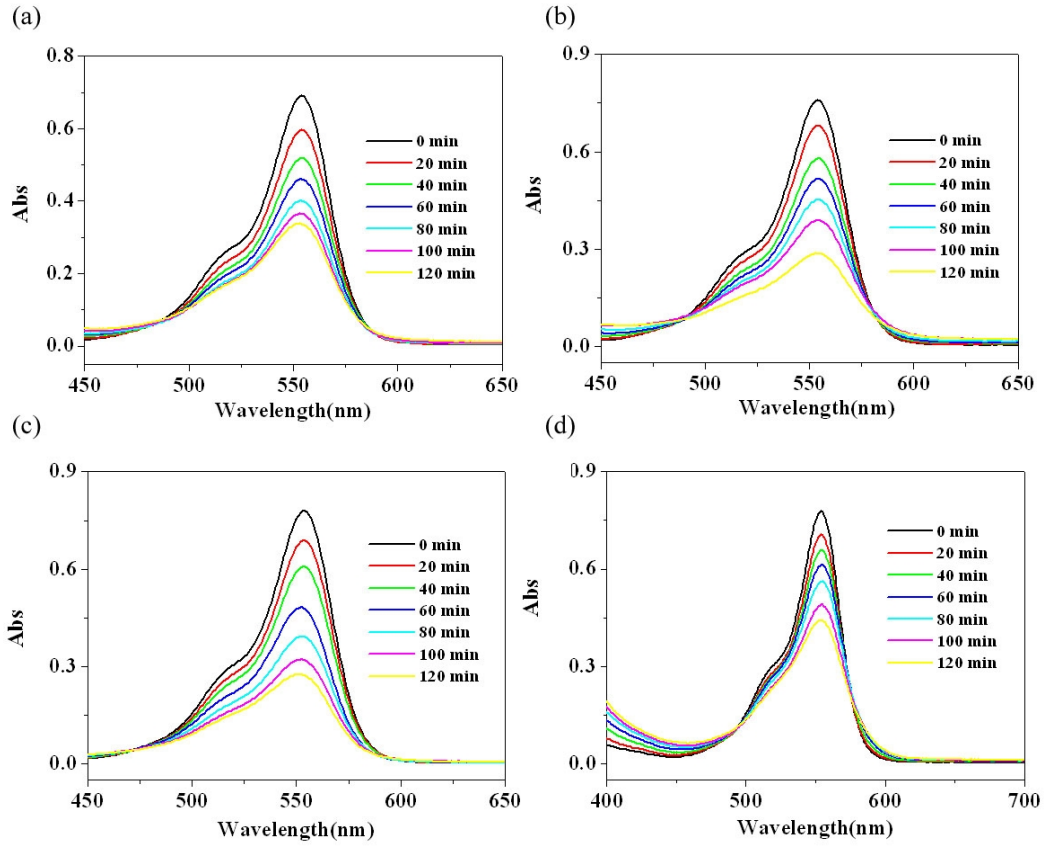

Figure S4. Absorption spectra of RhB degraded by: (a) **PPy(A)/ZnP$_2$Mo$_5$NR(M)**; (b) **PPy(B)/ZnP$_2$Mo$_5$NR(M)**; (c) **PPy(C)/ZnP$_2$Mo$_5$NR(M)**; (d) **PPy(D)/ZnP$_2$Mo$_5$NR(M)** by visible light irradiation.