

Supplementary Information

Self-assembly of Dawson-type

$\text{H}_6\text{P}_2\text{W}_{18}\text{O}_{62}@\text{[Cu}_6\text{O(TZI)}_3(\text{H}_2\text{O})_6\text{]}_4$ towards high performance of aerobic oxidation desulfurization of fuel

Wenjia Qu, Pengpeng Wei, Jingfang Li*, Liye Liang, Liqiang Ma, Guangming Li*

Key Laboratory of Functional Inorganic Material Chemistry (MOE), School of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, Heilongjiang, China.

E-mail: fjlaaa.ok@163.com (J. Li); gmlj@hlju.edu.cn (G. Li)

Table S1. Crystal data and structure refinements for $\text{D-P}_2\text{W}_{18}@\text{rht-MOF-1}$

Parameters	$\text{D-P}_2\text{W}_{18}@\text{rht-MOF-1}$
Empirical formula	$\text{C}_{36}\text{H}_{84}\text{Cu}_8\text{N}_{16}\text{O}_{113}\text{P}_2\text{W}_{18}$
CCDC No.	2005522
Formula weight	6428.75
Crystal system	cubic
Space group	<i>Fmm</i>
Unit cell	$a=b=c=44.4562(1)\text{Å}$ $\alpha=\beta=\gamma=90^\circ$
Volume	$87861.2(6)\text{Å}^3$
<i>Z</i>	24
Density (calcd)	2.916 g/cm^3
Temperature	100.00 (2) K
Wavelength	0.71073 Å
Reflections collected	77508
μ	15.338 mm^{-1}
<i>F</i> (000)	69840.0
Final R_1^a , wR_2^b [$I > 2\sigma(I)$]	0.0753, 0.2121
Final R_1^a , wR_2^b (all data)	0.0807, 0.2172
GOF on F^2	1.087

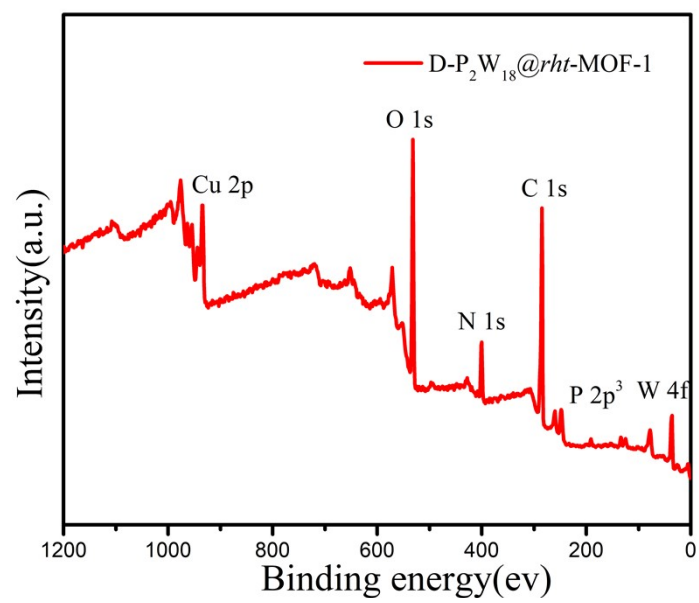


Fig. S1. XPS fully spectrum for D-P₂W₁₈@rht-MOF-1.