

Supporting Information

Uncoordinated carbonyl groups of MOFs as anchoring sites for the preparation of highly active Pd nano-catalysts

Yingyi Pan,^a Deyun Ma,^{ab} Huimin Liu,^c Hao Wu,^c Dehua He^c and Yingwei Li*^a

^a *School of Chemistry and Chemical Engineering, South China University of Technology, Guangzhou 510640, China.*

^b *School of Chemistry and Chemical Engineering, Zhaoqing University, Zhaoqing 526061, China.*

^c *Department of Chemistry, Tsinghua University, Beijing 100084, China.*

E-mail: liyw@scut.edu.cn

Table S1. Crystal data and structure refinement for Tm-MOF.

Empirical formula	C ₉ H ₁₃ N ₃ O ₁₁ Tm		
Formula weight	508.15	<i>D_c</i> (mg/cm ³)	1.905
Crystal system	Triclinic	<i>F</i> (000)	490
Space group	<i>P</i> -1	<i>μ</i> (mm ⁻¹)	5.064
<i>a</i> / Å	6.0200(5)	Reflections collected	4623
<i>b</i> / Å	12.7722(11)	Independent reflections	3147 (<i>R</i> _{int} = 0.0279)
<i>c</i> / Å	13.1612(11)	Data/restraints/parameters	3147/5/212
<i>α</i> /°	118.8290(10)	GOF	1.047
<i>β</i> /°	90.6090(10)	<i>θ</i> range for data collection (°)	1.77 to 25.20
<i>γ</i> /°	91.6870(10)	Final <i>R</i> indices [<i>I</i> >2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0402 <i>ωR</i> ₂ = 0.0987
<i>V</i> (Å ³)	885.79(13)	<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0466 <i>ωR</i> ₂ = 0.1036
<i>Z</i>	2	Largest diff. peak and hole/eÅ ⁻³	1.98 and 0.99

$$R = \sum (|F_o| - |F_c|) / \sum |F_o|$$

$$wR = [\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)]^{1/2}$$

The Palladium contents of the samples were determined quantitatively by atomic absorption spectroscopy (AAS) on a HITACHI Z-2300 instrument. The calibration curve were obtained with a series of aqueous standard solutions of Pd(NO₃)₂. Approximately 0.0040 g of sample was weighed precisely and dissolved in 5 mL of aqua regia (HCl:HNO₃ = 3:1), and the solution was diluted with deionized water to reach a concentration of Pd approximately in the range from 0.5 to 1.5 mg L⁻¹.

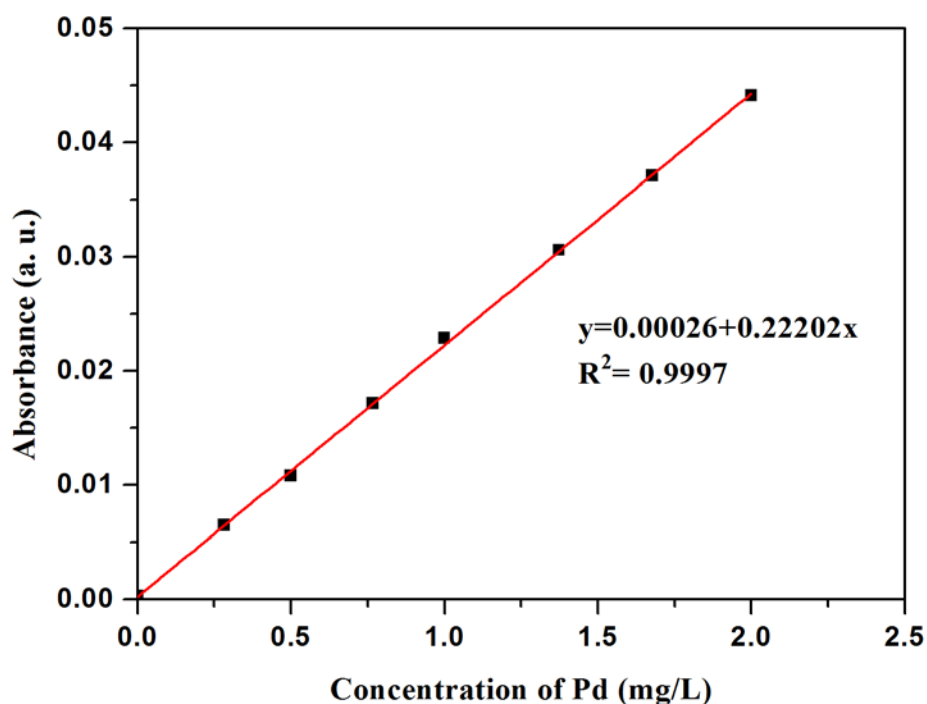


Figure S1. The AAS calibration curve for Pd using aqueous standard solution.

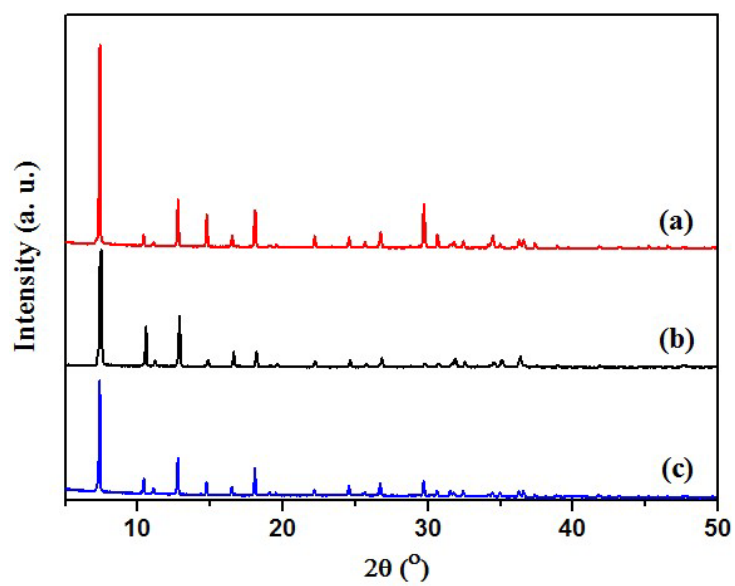


Figure S2. Powder X-ray diffraction patterns of ZIF-8: (a) stimulated, (b) as-synthesized, and (c) 1.0 wt% Pd/ZIF-8.