

A Porous π -Stacked Self-Assembly of Cup-Shaped Palladium Complex for Iodine Capture

Lin-Lin Li^{1,4,5}, Min Huang^{3,4,5}, Ting Chen^{3,4,5}, Xiao-Feng Xu^{4,5}, Zhu Zhuo^{4,5},

Wei Wang^{4,5}, You-Gui Huang^{2,4,5*}

¹ College of Chemistry, Fuzhou University, Fuzhou, 350108, China

² Fujian Science & Technology Innovation Laboratory for Optoelectronic Information of China, Fuzhou, Fujian, 350108, China

³ College of Chemistry and Materials Science, Fujian Normal University, Fuzhou, Fujian, 350002, P. R. China

⁴ CAS Key Laboratory of Design and Assembly of Functional Nanostructures, and Fujian Provincial Key Laboratory of Nanomaterials, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, China

⁵ Xiamen Institute of Rare Earth Materials, Haixi Institute, Chinese Academy of Science, Xiamen 361021, China

Table S1. Crystallographic data of compound **1**.

Compound	1
Formula	Pd ₃ C ₆₆ H ₄₈ N ₁₃
Formula weight	1342.37
Temp. (K)	200
Crystal System	Cubic
Space group	I-43m
<i>a</i> (Å)	26.0030(2)
<i>V</i> (Å ³)	17582.1(4)
<i>Z</i>	8
$\rho_{cal.}$ (g cm ⁻³)	1.014
μ	0.643
<i>F</i> (000)	5384
θ range (°)	4.43–67.346
Reflections (<i>I</i> > 2 σ)	5662
<i>R</i> ₁ (<i>I</i> > 2 σ)	0.0459
<i>wR</i> ₂ (<i>all</i>)	0.1342
<i>GOF</i> on <i>F</i> ²	1.083
CCDC#	2245193

^[a] $R_1 = \Sigma||F_o| - |F|| / \Sigma|F_o|$ and $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2 / \Sigma wF_o^4]^{1/2}$ for $F_o^2 > 2\sigma(F_o^2)$

Table S2. Fitting the iodine adsorption kinetics of compound **1**.

adsorbate	I ₂ vapor			Dissolved I ₂		
model	pseudo first-order			pseudo second-order		
parameter	<i>k</i> ₁ (g g ⁻¹ min ⁻¹)	<i>Q</i> _e (g g ⁻¹)	<i>R</i> ²	<i>k</i> ₂ (g g ⁻¹ min ⁻¹)	<i>Q</i> _e (g g ⁻¹)	<i>R</i> ²
	1.0×10 ⁻⁴	1.81	0.996	3.0×10 ⁻³	0.603	0.977

Table S3. The comparison of I₂ adsorption capacities for various adsorbents.

Adsorbents	I ₂ vapor (g g ⁻¹)	Adsorption of I ₂ in solution (g g ⁻¹)	Ref.
Cu-BTC@PES	0.639	0.260	41
DUT-68	1.08	/	42
P-TzTz	/	0.494	43
ZIF-8@PU	/	0.33	44
1	1.81	0.60	This work

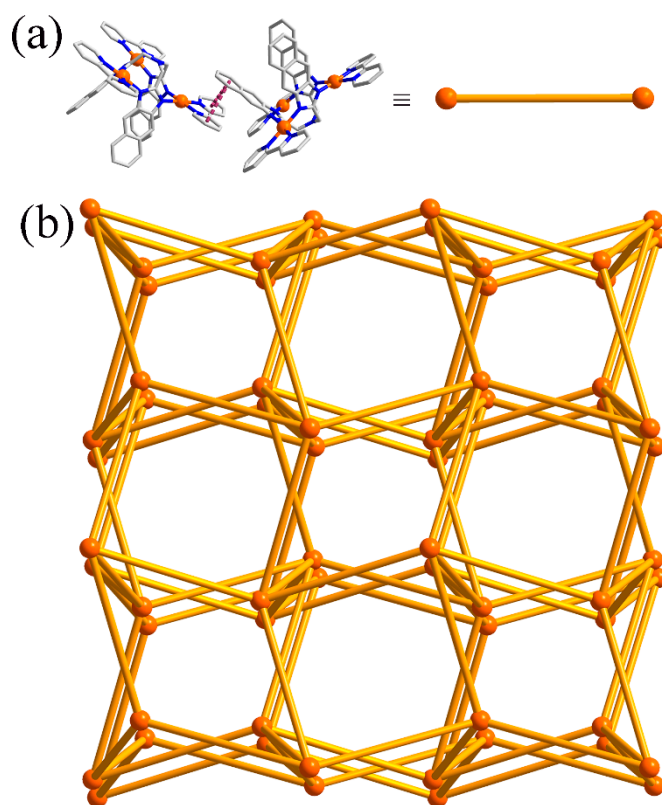


Figure S1. (a) The simplification of the network of compound **1**. (b) The simplified **pcu** network of the supramolecular framework of compound **1**.

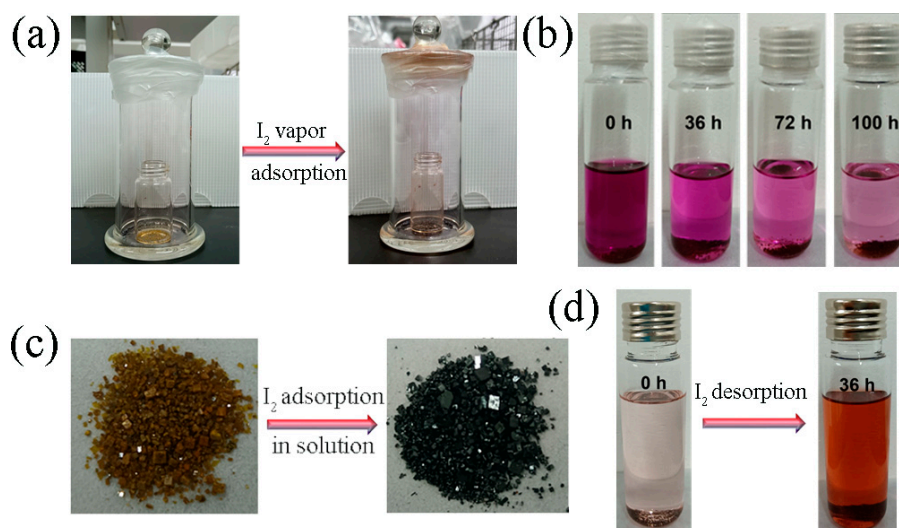


Figure S2. (a) The setup for I₂ vapor adsorption. (b) Photographs showing color changes of the I₂/cyclohexane solution as a function of time when 0.050 g compound **1** was immersed in the solution. (c) Photographs showing the color change of the crystals of compound **1** before and after dissolved I₂ adsorption. (d) Photographs showing the release of I₂ from I₂@**1** in CH₂Cl₂.

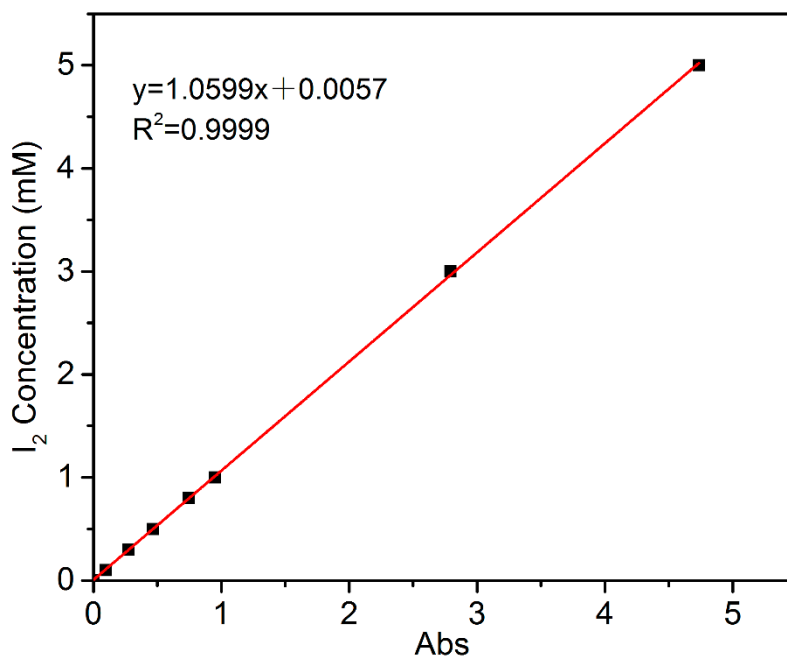


Figure S3. Standard plot between absorbance ($\lambda = 523$ nm) and I₂ concentration of the solution of I₂ in cyclohexane.