Supporting information for:

Investigation of Antimony Adsorption on Zirconium-Porphyrin-Based Metal-Organic Framework

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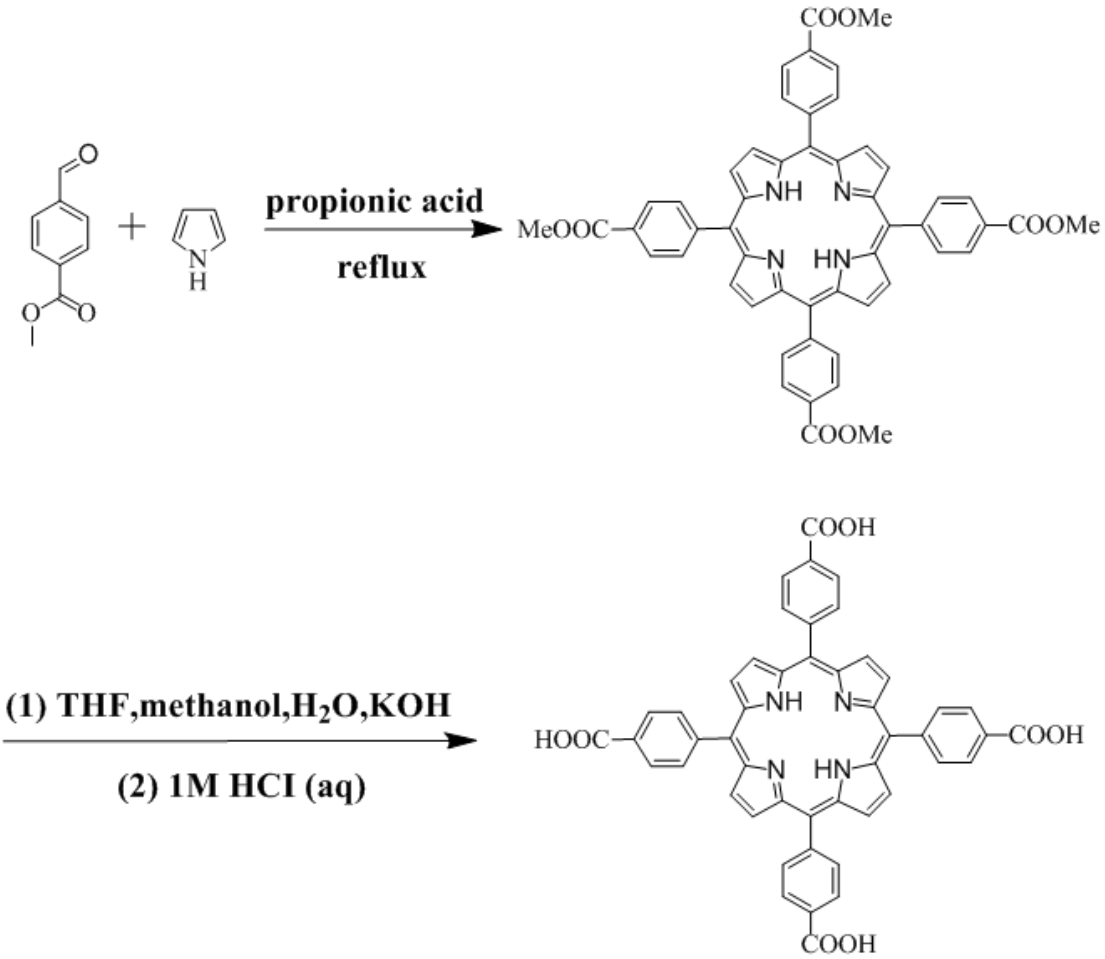

Fig. S1 Scheme for the synthesis of TCPP

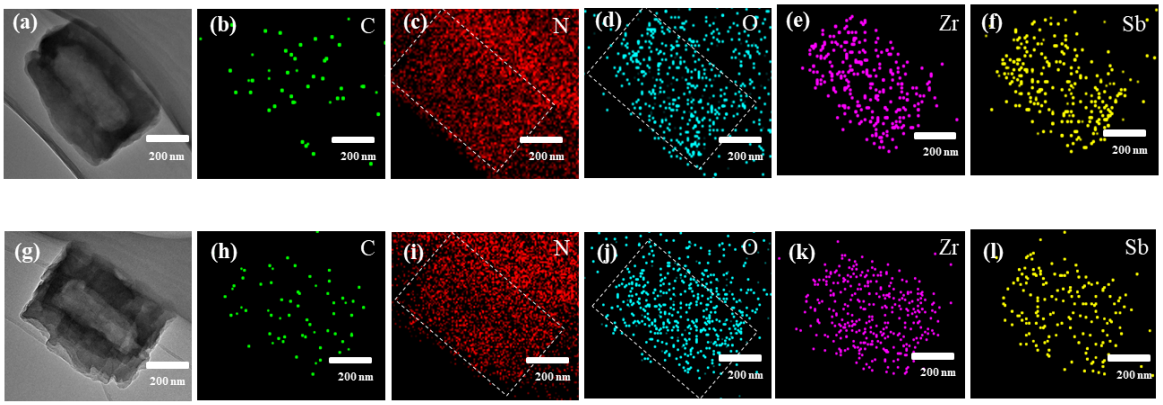

Fig. S2 (a) HRTEM image of PCN-222 after antimony adsorption at pH=5; (b-f) EDS elemental mappings of PCN-222 after antimony adsorption at pH=5. (g) HRTEM image of PCN-222 after antimony adsorption at pH=8; (h-l) EDS elemental mappings of PCN-222 after antimony adsorption at pH=8.

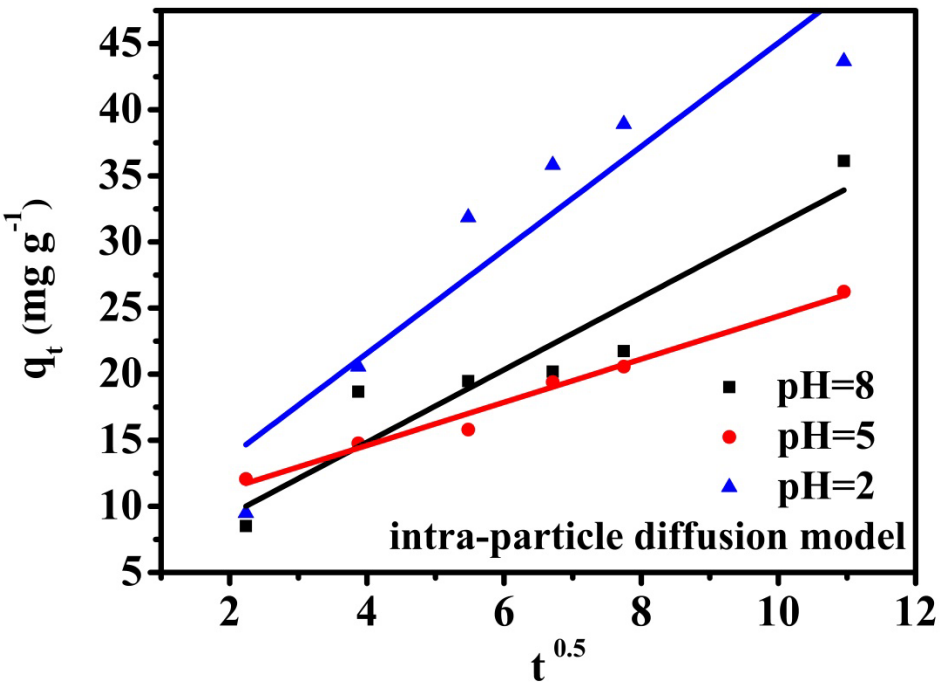

Fig. S3 Intra-particle diffusion kinetic model simulation.

Table S1. Adsorption kinetic constants of Sb(III) adsorption.

Models	pH		
	2	5	8
	$q_{e,exp}$=49.78 mg g^{-1}	$q_{e,exp}$=44.01 mg g^{-1}	$q_{e,exp}$=48.27 mg g^{-1}
Pseudo-first-order model	$q_{m,cal}$=49.80 mg g^{-1}	$q_{m,cal}$=46.84 mg g^{-1}	$q_{m,cal}$= 48.44 mg g^{-1}
	K_1=0.00446 min^{-1}	K_1=0.00156 min^{-1}	K_1=0.00313 min^{-1}
	R^2=0.834	R^2=0.872	R^2=0.870
Pseudo-second-order model	$q_{m,cal}$=50.30 mg g^{-1}	$q_{m,cal}$=43.66 mg g^{-1}	$q_{m,cal}$=49.21 mg g^{-1}
	K_2=0.0199 g $(mg \cdot min)^{-1}$	K_2=0.0229 g $(mg \cdot min)^{-1}$	K_2=0.0203 g $(mg \cdot min)^{-1}$
	R^2=0.999	R^2=0.980	R^2=0.998
Elovich model	α= 17.00	α= 5.41	α= 4.44
	β= 0.146	β= 0.187	β= 0.133
	R^2= 0.872	R^2= 0.959	R^2= 0.94
Intra-particle diffusion model	α_i= 5.90	α_i= 8.08	α_i= 3.87
	k_i= 3.91	k_i= 1.63	k_i= 2.74
	R^2= 0.855	R^2= 0.981	R^2= 0.871

Table S2. Adsorption isotherm constants of Sb(III) adsorption

T(K)	Langmuir constants			Freundlich constants			Temkin constants		
	q_m (mg g^{-1})	K_L (L mg^{-1})	R^2	K_F	n	R^2	B	K_T	R^2
293	161.61	6.16×10^{-3}	0.9	13.49	1.75	0.901	63.1	0.519	0.895
298	175.17	6.27×10^{-3}	0.9	14.98	1.73	0.898	59.4	0.555	0.889
303	204.61	7.11×10^{-3}	0.9	15.8	1.61	0.912	54.4	0.618	0.871

Nitrogen adsorption and desorption analysis

Nitrogen adsorption and desorption analysis is an important means of material characterization, and information such as material specific surface area and pore size distribution can be obtained. Firstly, the sample was placed in the instrument and treated at 120 °C under vacuum for 12 hours. Test temperature was 77 K. The specific surface area was determined using Brunauer-Emmett-Teller (BET) method. The pore size distribution was obtained by the density functional theory (DFT) analysis.

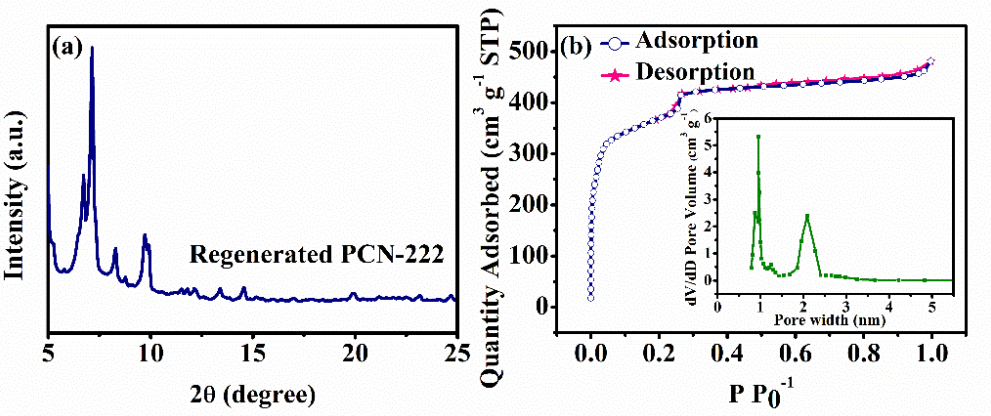

Fig. S4 (a) XRD spectrum of regenerated PCN-222; (b) N_2 adsorption-desorption measurement of regenerated PCN-222; Inset shows DFT pore size distribution for regenerated PCN-222 using data measured with N_2 at 77 K.

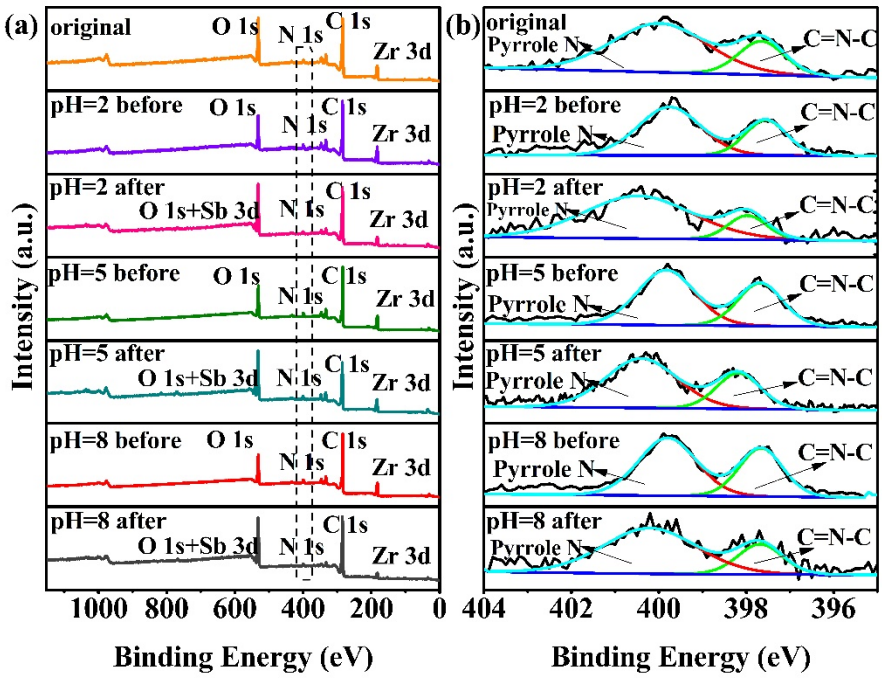

Fig. S5 XPS spectra of PCN-222 before and after Sb(III) adsorption at pH=2,5,8: (a) XPS survey spectrum; (b) N 1s spectra.