A zinc metal-organic framework for concurrent adsorption and detection of uranium

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Table S1. Crystal data and structure refinement parameters for **HNU-50**.

Crystal data	HNU-50
Empirical formula	$Zn_2C_{21}N_3O_{15}H_{23}$
Formula weight	688.20
Crystal system	monoclinic
Space group	*Cc*
a (Å)	16.5622
b (Å)	9.4906
c (Å)	15.8484
α (°)	90
β (°)	95.957
γ (°)	90
Volume (Å^3)	2477.68
Z	4
D_{calcd} (g/cm^3)	1.845
F(000)	1400.0
μ Mo Kα (mm^{-1})	2.009
Temperature (K)	150
Range of *h*, *k*, *l*	20,11,19
θ min/max	5.37/74.728
Reflections collected/unique/	0.1021(4844)
Data/restraints/parameters	1.95/0.98
R indices (all data)	0.0331

Table S2. The kinetic parameters for the U(VI) sorption on **HNU-50**.

Pseudo-first kinetics model			Pseudo-second kinetics model		
K_1 (min^{-1})	q_e (mg/g)	R^2	K_2 (min^{-1})	q_e (mg/g)	R^2
0.0083	400	0.9568	2.7627	452	0.9969

Table S3. Adsorption constants for Langmuir and Freundlich isotherm models.

Langmuir adsorption isotherm			Freundlich adsorption isotherm		
Q_m (mg/g)	k_l (L/mg)	R^2	k_f (mg/g)	n	R^2
632	0.265	0.9983	126	0.9708	0.9139

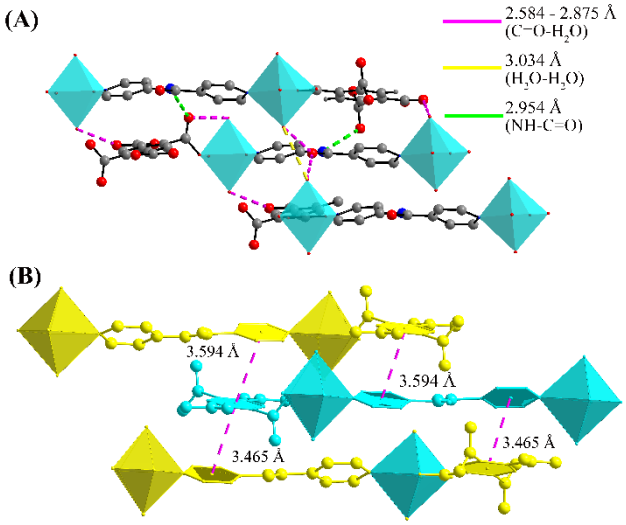

Figure S1. (A) Schematic diagram of H-bond between two-dimensional layers of **HNU-50**; (B) Diagram of π - π stacking between two layers of **HNU-50**.

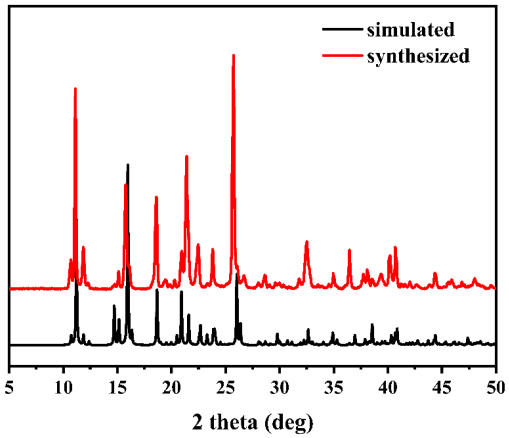

Figure S2. Simulated and experimental powder X-ray diffraction patterns (PXRD) of **HNU-50**.

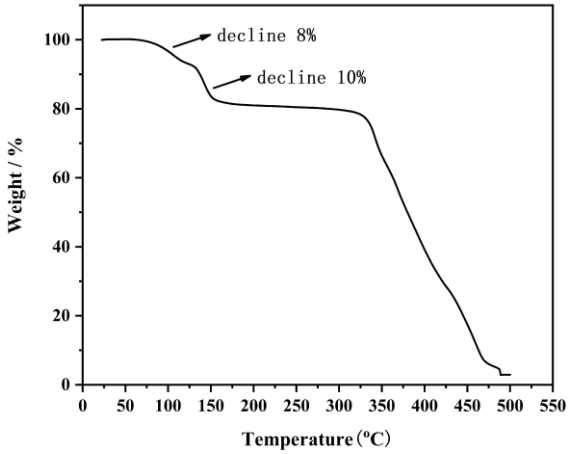

Figure S3. TGA curve of **HNU-50**.

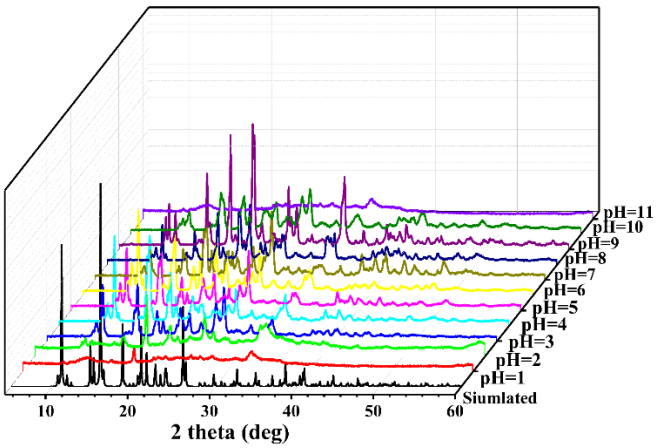

Figure S4. PXRD of **HNU-50** in aqueous solution with different pH for 12 hours.

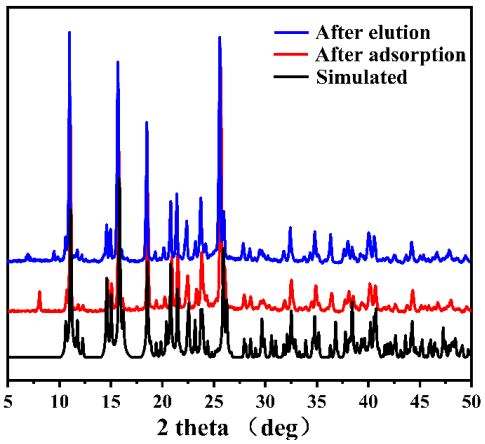

Figure S5. PXRD of simulated, after adsorption and after elution of **HNU-50**.

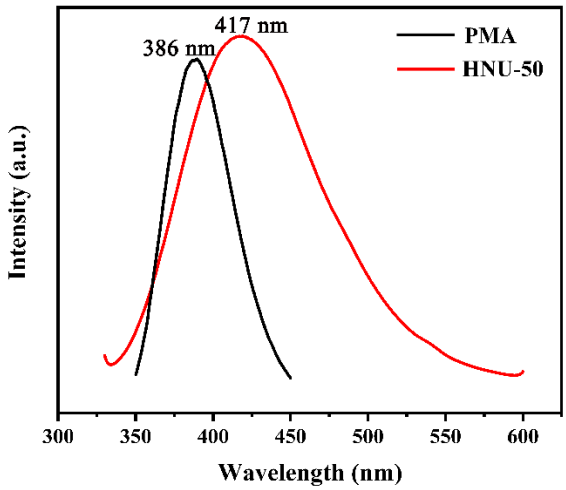

Figure S6. Emission spectra of PMA (black, λ_{ex} =345 nm) and **HNU-50** (red, λ_{ex} = 312 nm).

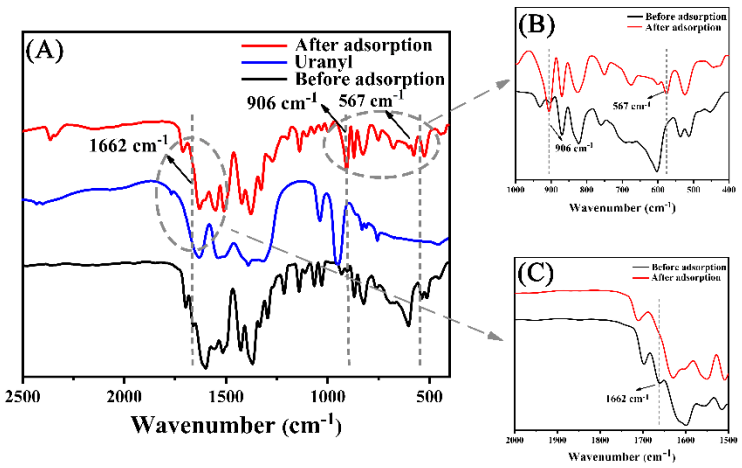

Figure S7. The IR spectra of uranyl nitrate, as-synthesized and U(VI) loaded **HNU-50**.

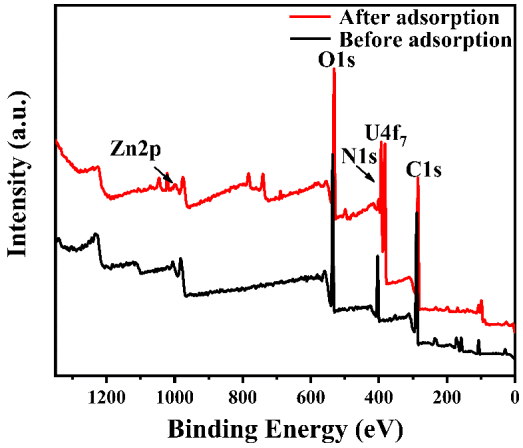

Figure S8. XPS survey spectra of **HNU-50** before and after U(VI) adsorption.

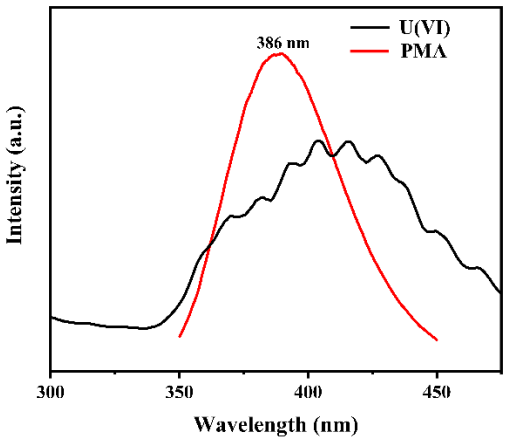

Figure S9. Emission spectrum of PMA (red, λ_{ex} =345 nm) and absorption spectrum of uranyl nitrate (black, λ_{em} = 513 nm).