

Supporting Information (SI)

Novel pyridine-based covalent organic framework containing N, N, N-chelating sites for selective detection and effective removal of nickel

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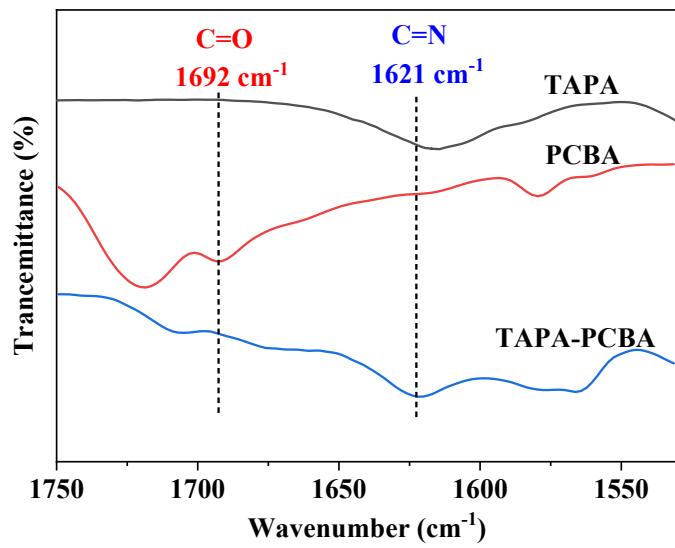


Fig. S1. Local details of the FT-IR spectra of TAPA, PCBA and TAPA-PCBA.

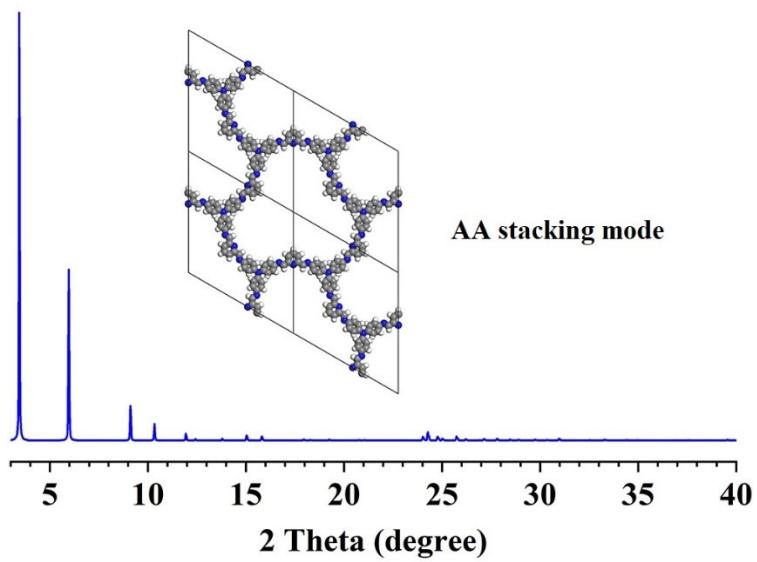


Fig. S2. AA stacking mode of TAPA-PCBA and the calculated PXRD pattern.

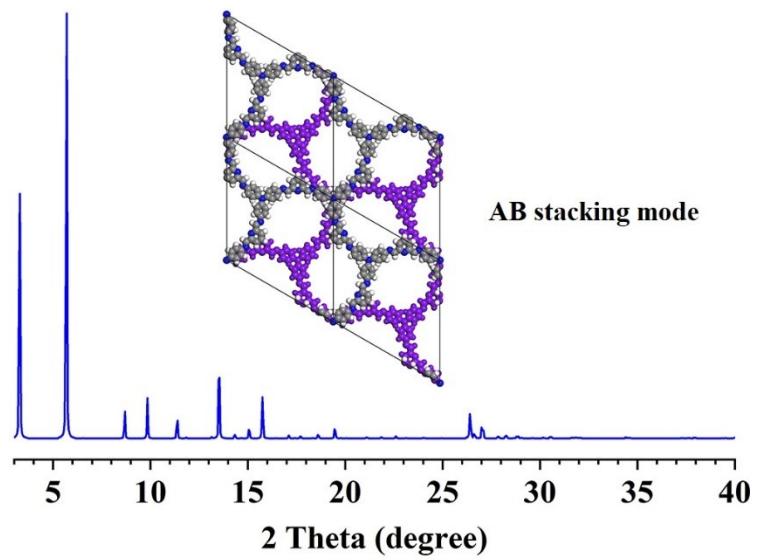


Fig. S3. AB stacking mode of TAPA-PCBA and the calculated PXRD pattern.

Table S1. Unit cell parameters and fractional atomic coordinates of TAPA-PCBA with eclipsed arrangement.

Space group		P-6 (No. 174)	
Unit cell		$a = b = 30.2577 \text{ \AA}$, $c = 4.2507 \text{ \AA}$, $\alpha = \beta = 90^\circ$, $\gamma = 120^\circ$	
Pawley refinement		$R_{wp} = 4.84\%$, $R_p = 3.91\%$	
Atom	x/a	y/b	z/c
C1	0.04518	0.61041	0.5
C2	0.04572	0.65706	0.5
C3	0.0925	0.60812	0.5
C4	0.71744	0.37827	0.5
C5	0.72754	0.42365	0.5
C6	0.77594	0.46729	0.5
C7	0.81559	0.46656	0.5
C8	0.80606	0.42156	0.5
C9	0.75762	0.37803	0.5
N10	0.86396	0.51284	0.5
C11	0.6104	0.04518	0.5
C12	0.65706	0.04572	0.5
C13	0.6081	0.09249	0.5
C14	0.37827	0.71744	0.5
C15	0.42365	0.72754	0.5
C16	0.46729	0.77593	0.5
C17	0.46657	0.81558	0.5
C18	0.42156	0.80605	0.5
C19	0.37804	0.75761	0.5
N20	0.51285	0.86395	0.5
C21	1	0.65737	0.5

N22	1	0.56609	0.5
H23	0.08123	0.69272	0.5
H24	0.08965	0.57119	0.5
H25	0.69773	0.42572	0.5
H26	0.78286	0.50194	0.5
H27	0.83528	0.42024	0.5
H28	0.75147	0.34421	0.5
H29	0.69271	0.08123	0.5
H30	0.57117	0.08963	0.5
H31	0.42572	0.69773	0.5
H32	0.50195	0.78286	0.5
H33	0.42024	0.83527	0.5
H34	0.34421	0.75147	0.5
H35	0.99999	0.69316	0.5
N36	0.66667	0.33333	0.5
N37	0.33333	0.66667	0.5

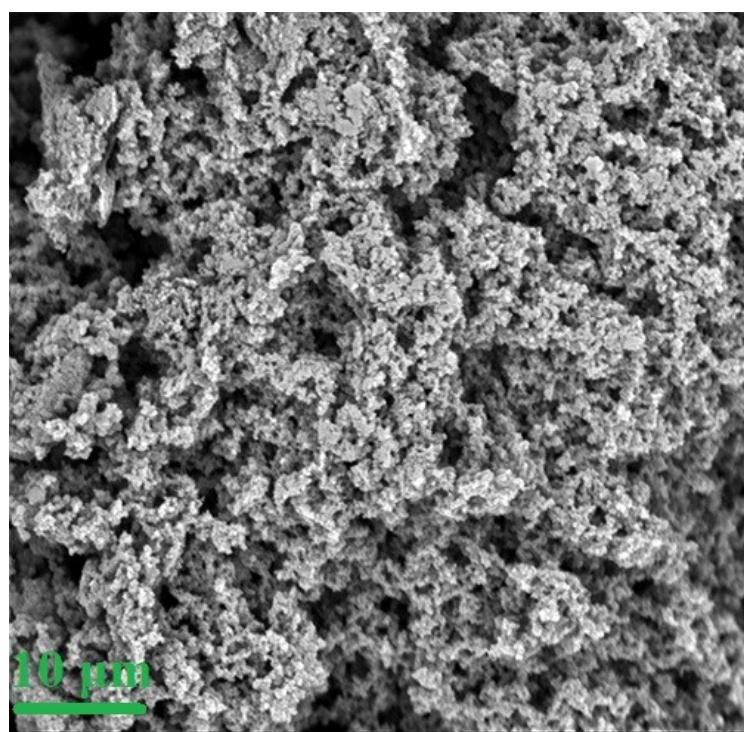
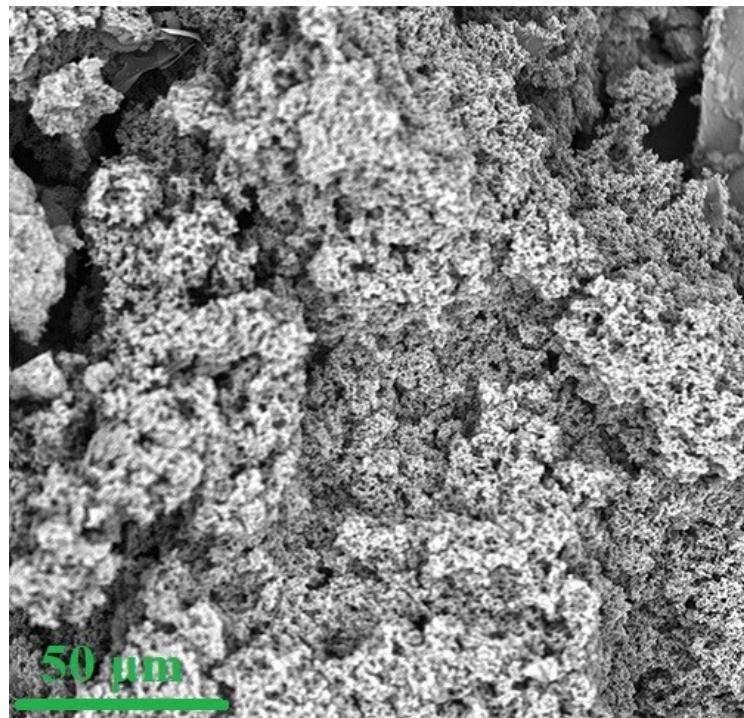


Fig. S4. SEM images of TAPA-PCBA.

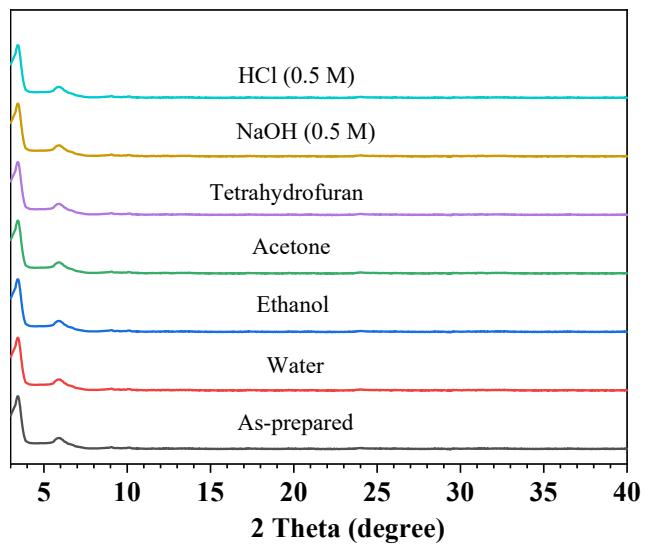


Fig. S5. PXRD patterns of TAPA-PCBA upon 12 h treatment in different solvents.

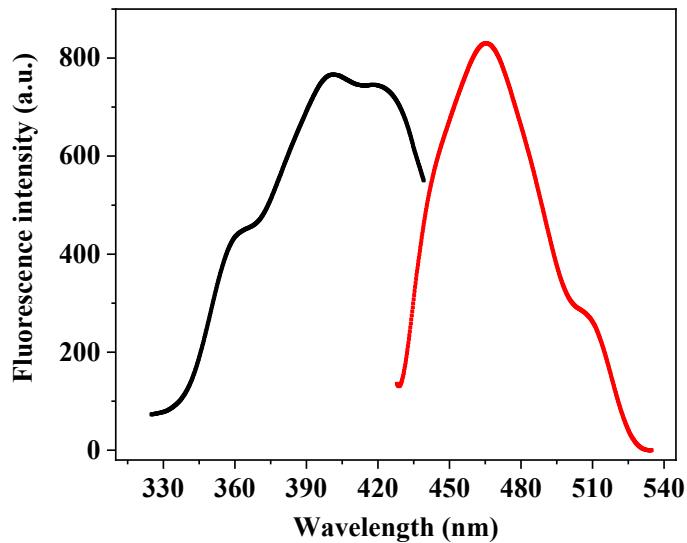


Fig. S6. Fluorescence excitation (black) and emission (red) spectra of TAPA-PCBA in water suspension.

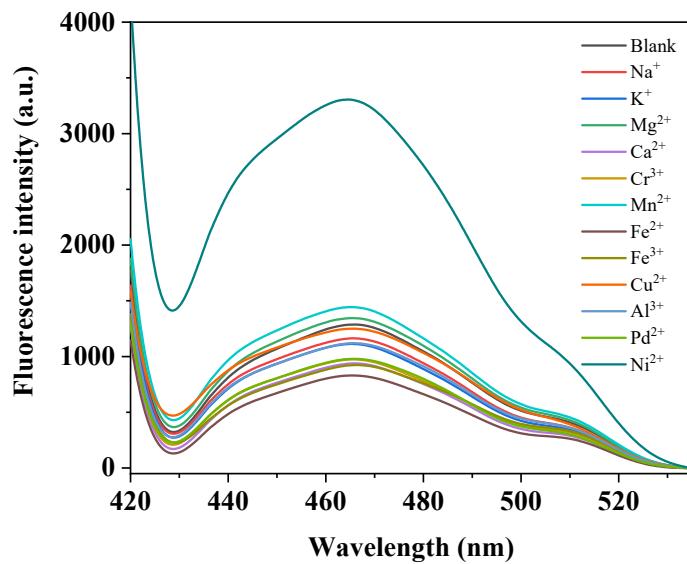


Fig. S7. Fluorescence spectra of TAPA-PCBA in the presence of various metal ions.

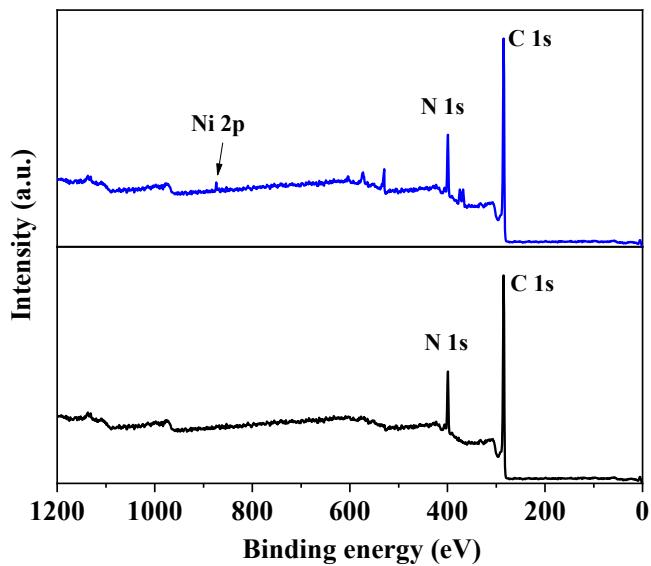


Fig. S8. Low-resolution XPS spectra of TAPA-PCBA before (black) and after (blue) Ni²⁺ adsorption.

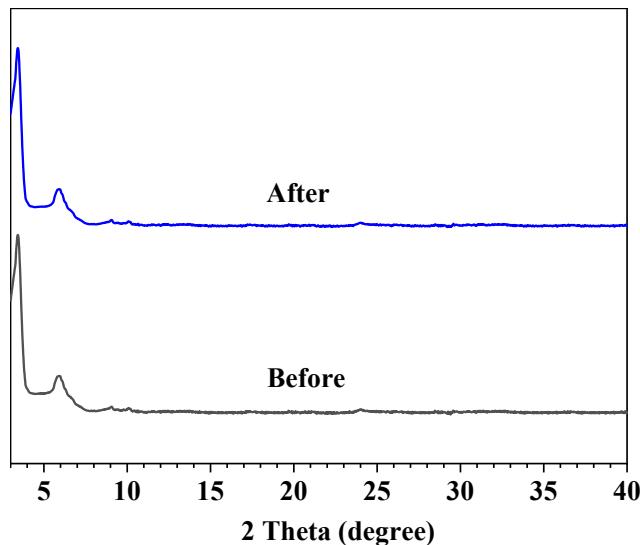


Fig. S9. Comparison of PXRD pattern of TAPA-PCBA before and after Ni^{2+} adsorption.