Supporting Information

Hierarchical porous microspheres for Co(II) recovery

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Supplementary Tables

Table S1 Schemes and parameters adopted in the DFT calculations using DMol^3.

Electronic Hamiltonian	Scheme	Condition and Parameter
Exchange-correlation	GGA	BLYP
Integration accuracy	Grid	Fine
SCF	Tolerance	1.0×10^{-5} eV/atom
	Multipolar expansion	Hexadecapole
	Charge density mixing	Charge = 0.2, DIIS = 5
Core treatment	All electron	Basis file 3.5
Numerical basis set	DND	Fine
	Global	
Solvation mode	COSMO	Water

Table S2 Isotherm model parameters for Co^{2+} adsorption on EDTA@PSV.

Model	Parameter	EDTA@PSV	Unit
Langmuir	q_m	84.03	mg g^{-1}
	K_L	9.29x10^{-3}	L mg^{-1}
	R_L	0.264	
	R^2	0.991	
Freundlich	K_F	15.21	L mg^{-1}
	n	4.18	
	R^2	0.699	
Temkin	K_T	14.76	L mg^{-1}
	f	0.199	
	R^2	0.740	
Dubinin-Radushkevich	q_m	137.70	mg g^{-1}
	K_{DR}	2.71x10^{-3}	mol^2 kJ^{-2}
	E	13.58	kJ mol^{-1}
	R^2	0.735	

In Table S2, the mean adsorption energy (E) obtained by using the Dubinin-Radushkevich model for the adsorption isotherm fitting relates to K_{DR} according to Eq. (S1).

$$E = 1/\sqrt{2K_{DR}} \quad \text{(S1)}$$

Supplementary Figures

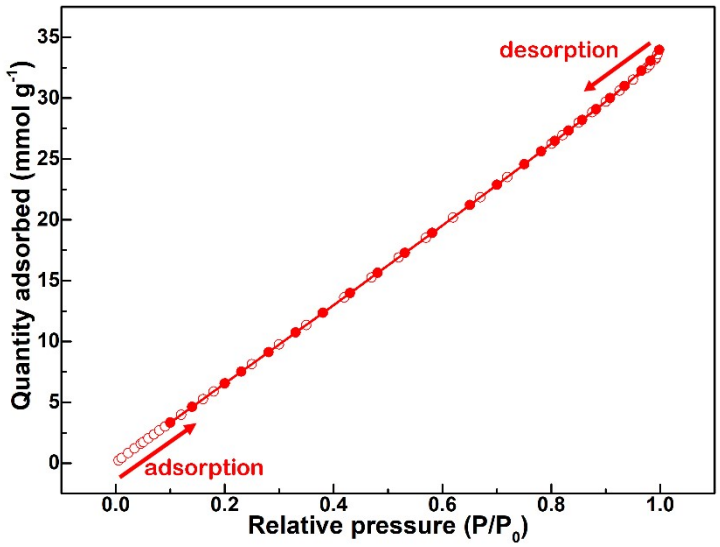

Figure S1 N_2 adsorption/desorption isotherms of @PSV.

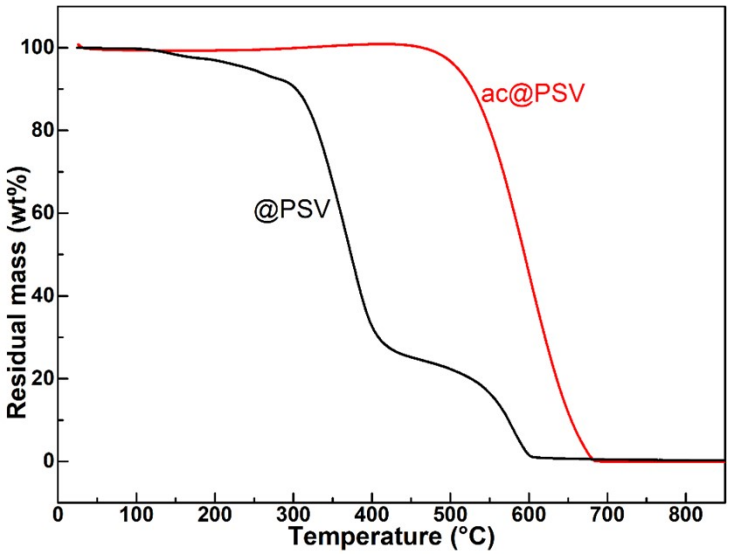

Figure S2 TGA curves of @PSV and ac@PSV.

After treatment with warm and concentrated $H_2SO_{4(aq)}$, the resulting ac@PSV shows improved thermal stability. It remains stable without degradation up to 500°C, whereas @PSV starts to degrade below 200°C.

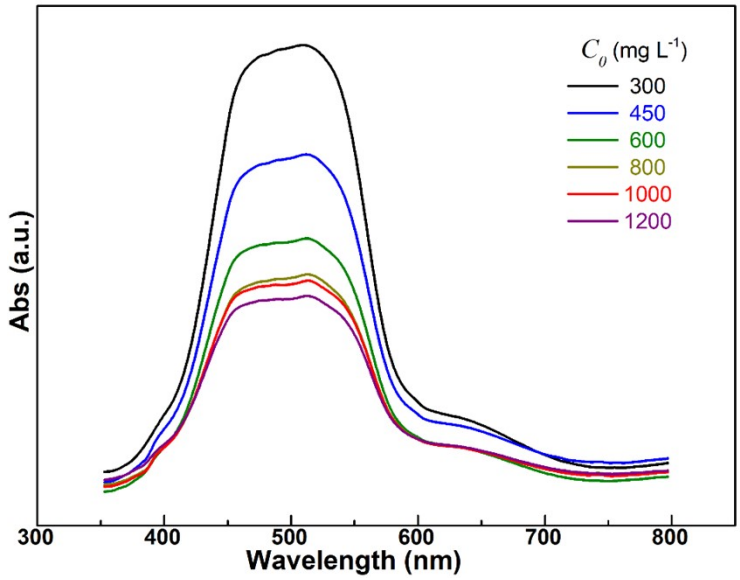

Figure S3 The UV-Vis absorption spectra of Co^{2+} in aqueous solutions with varying initial concentrations (C_0) at pH 6 and a temperature of 25°C.

Figure S4 A solubility test for Co^{2+} in aqueous solutions at 25°C with varying pH values.

Figure S4 demonstrates that the Co^{2+} solution remains clear until the pH reaches 8, where a precipitate forms (circled) due to the precipitation reaction below:

$$Co^{2+}_{(aq)} + 2OH^{-}_{(aq)} \rightarrow Co(OH)_{2(s)}\downarrow \quad \text{(S2)}$$

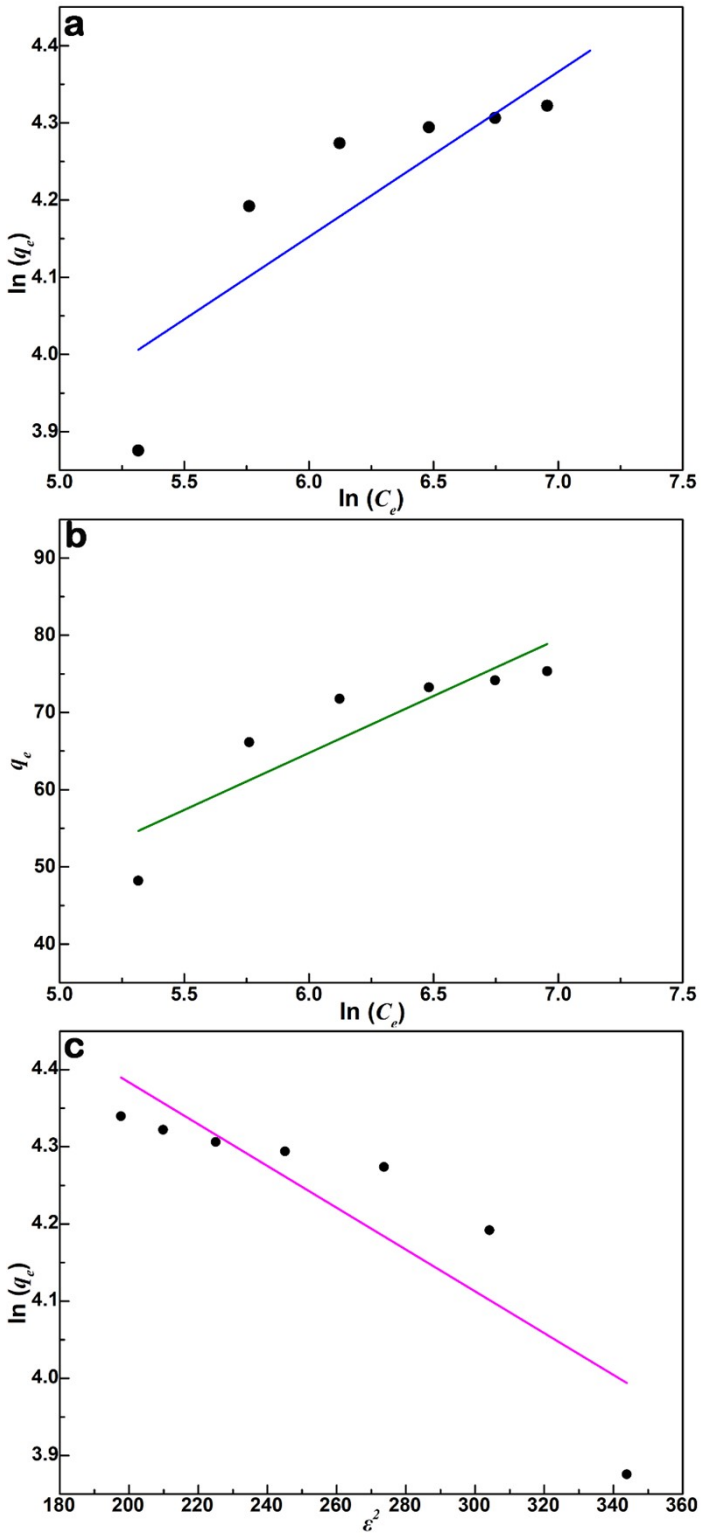

Figure S5 (a) Freundlich, (b) Temkin, and (c) Dubinin-Radushkevich isotherm linear plots for Co^{2+} adsorption on EDTA@PSV.

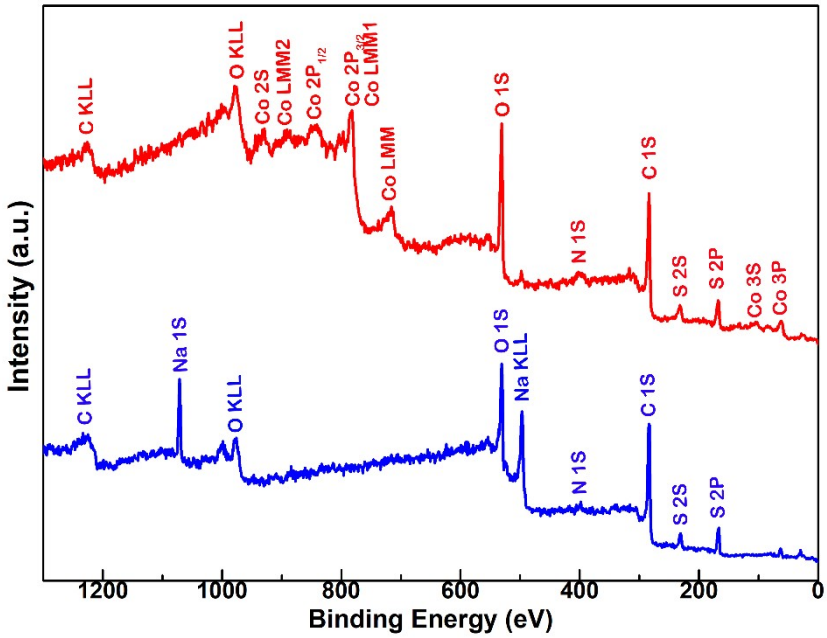

Figure S6 XPS spectra of EDTA@PSV before (blue) and after (red) Co^{2+} adsorption.

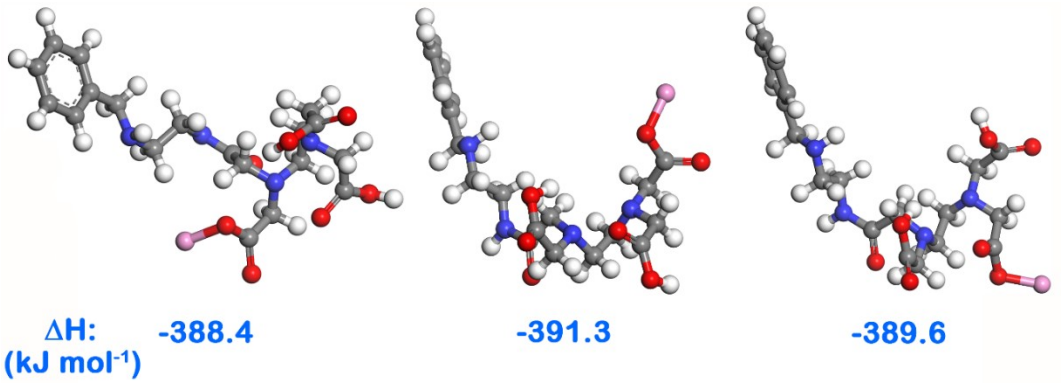

Figure S7 Optimized structures of the complexes formed from Co^{2+} interacting with three different -COOH groups of EDTA on EDTA@PSV, along with their corresponding formation energies indicated.