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Supplementary Material

Selective removal and recovery of Ni(II) using a sulfonic-based magnetic rattle-type ion-imprinted polymer: Adsorption performance and mechanisms

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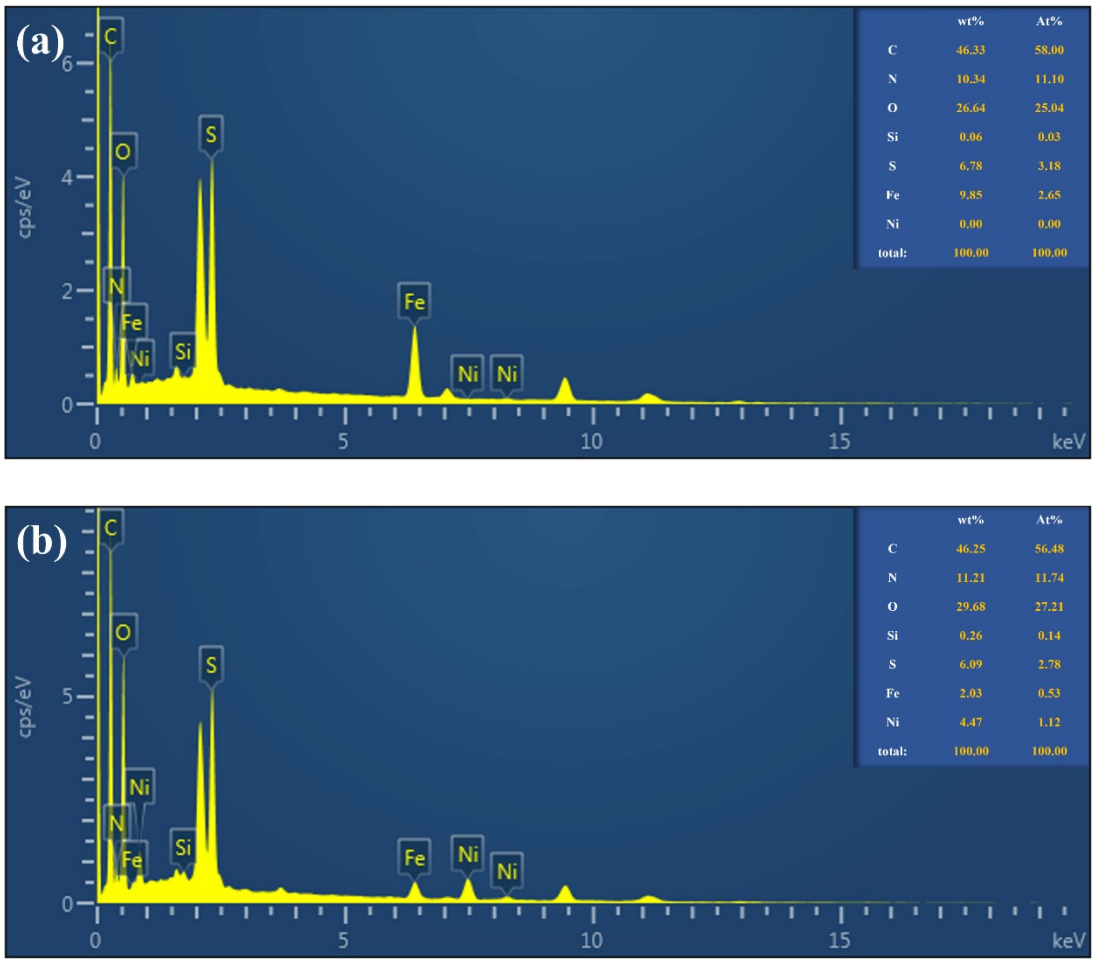

Fig. S1. EDS spectra of (a) Fe_3O_4@void@IIP-Ni(II) before adsorption, (b) Fe_3O_4@void@IIP-Ni(II) after adsorption

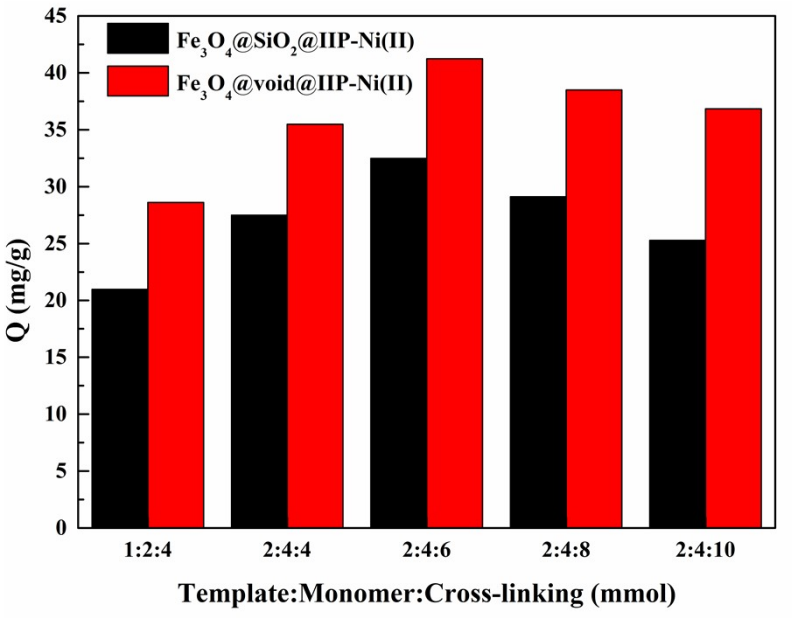

Fig. S2. Effect of the dosage of template, monomer, and cross-linking on the adsorption performance.

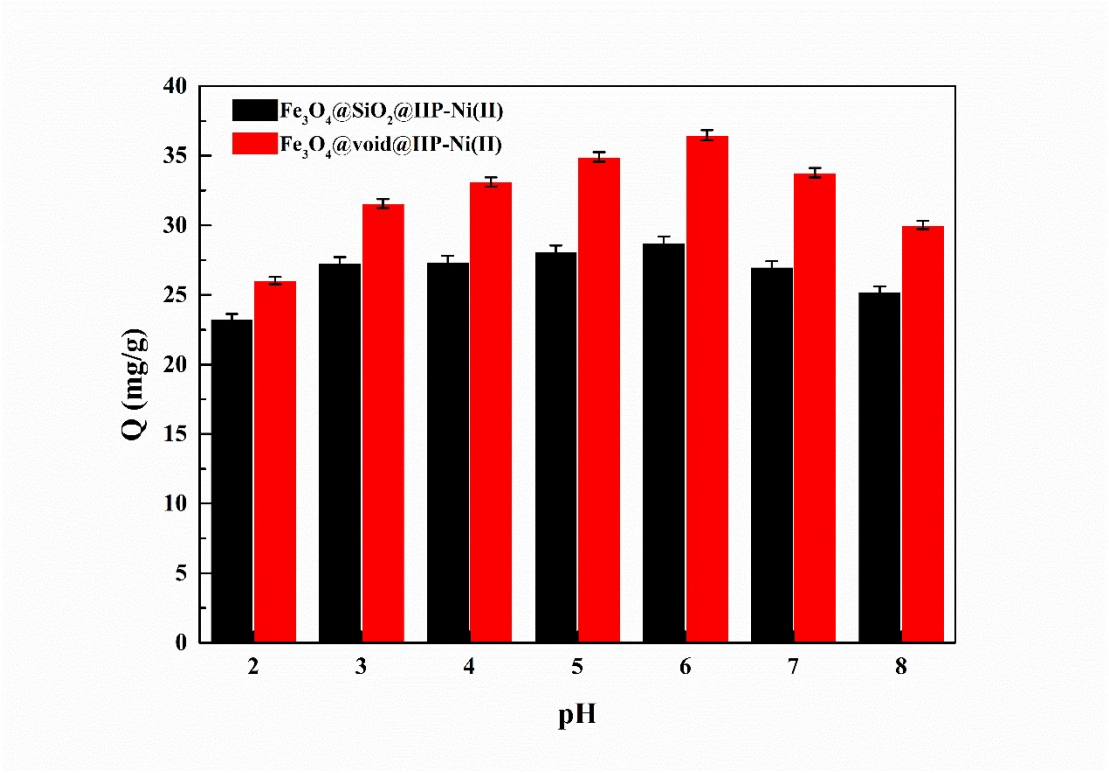

Fig. S3. Effect of pH on the adsorption.

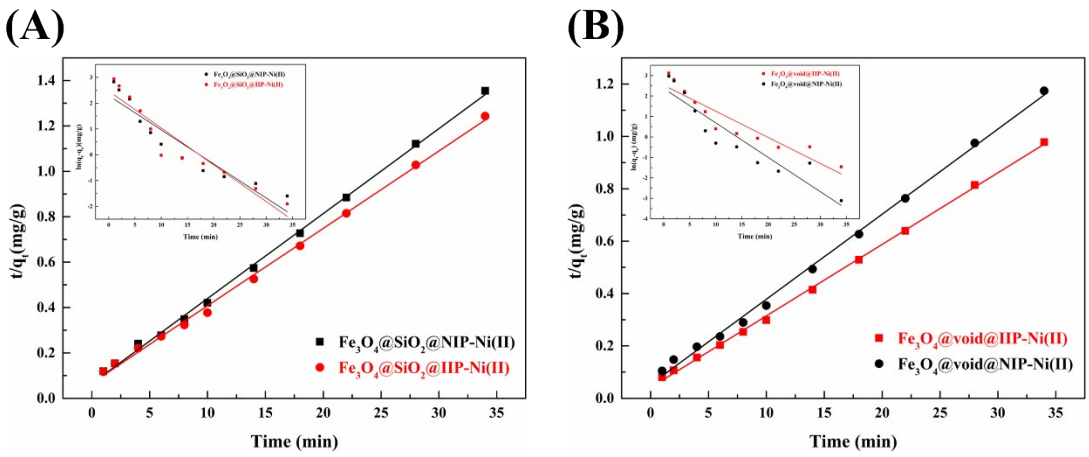

Fig. S4. Pseudo-second-order kinetic model of Fe_3O_4@SiO_2@IIP (or NIP) and Fe_3O_4@void@IIP (or NIP). (the inset was the Pseudo-first-order kinetic model).

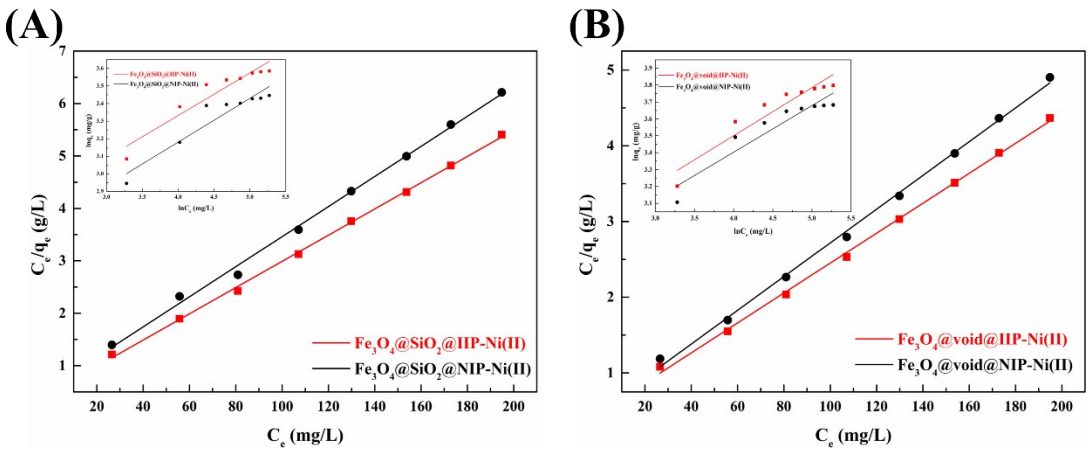

Fig. S5. Langmuir isotherm models of Fe_3O_4@SiO_2@IIP (or NIP) and Fe_3O_4@void@IIP (or NIP). (the inset was the Freundlich isotherm models).

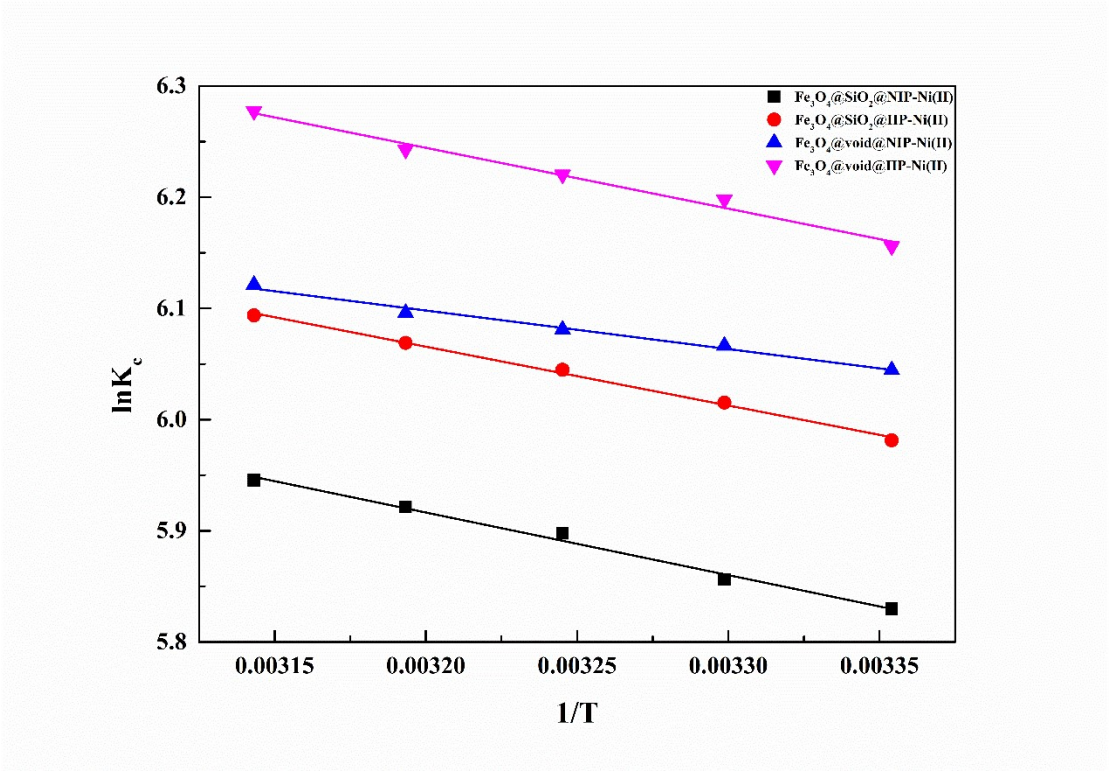

Fig. S6. Plot of lnKc versus 1/T.

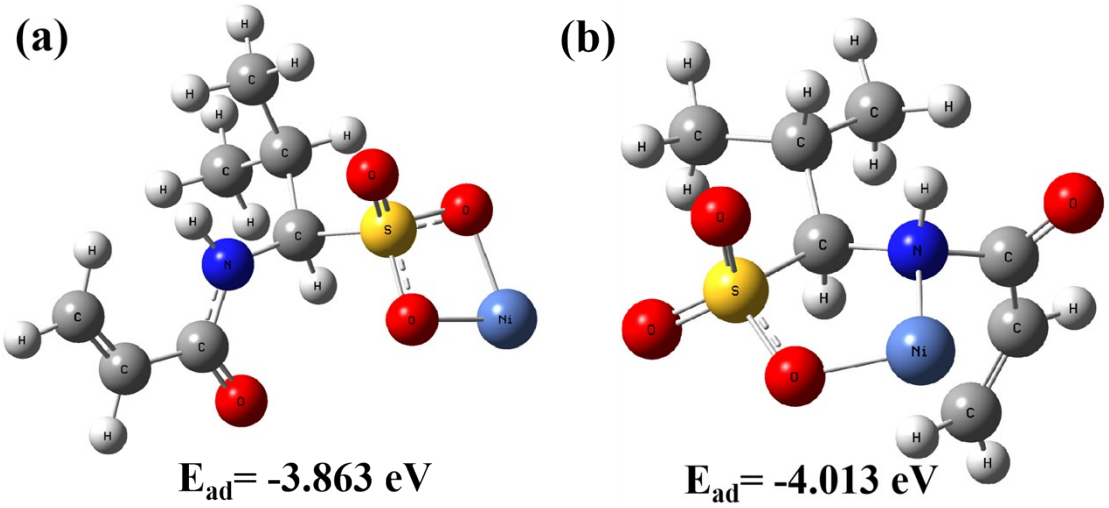

Fig. S7 The optimized structure of the complexes formed by functional group with Ni(II).

Table S1. Comparison of adsorption properties of adsorbents for Ni(II)

Adsorbents	Equilibrium time	Adsorption capacity	Removal rate	Reference
IICFMPSs	20 min	41.95 mg/g	NA	1
Ni-MIIP	60 min	18.50 mg/g	NA	2
FPCC	2 h	19.00 mg/g	99.7%	3
Ni (II)-IIP	15 min	40.29 mg/g	NA	4
SMIA	100 min	38.49 mg/g	NA	5
IIPClO4	NA	11.74 mg/g	NA	6
Fe_3O_4/SBP	40 min	9.39 mg/g	81.2%	7
CMF	NA	11.63mg/g	NA	8
CTS-REC	NA	13.32mg/g	NA	9
Fe_3O_4@void@IIP-Ni(II)	10 min	44.64 mg/g	99.97%	This work

Table S2. Thermodynamic parameters for Ni(II) adsorption.

Adsorbent	Temperature (K)	ΔG (kJ/mol)	ΔH (kJ/mol)	ΔS (J/mol·K)
Fe_3O_4@void@IIP-Ni(II)	298	-15.259	45.480	66.470
	303	-15.621		
	308	-15.936		
	313	-16.253		
	318	-16.604		
Fe_3O_4@void@NIP-Ni(II)	298	-14.984	28.825	59.924
	303	-15.230		
	308	-15.579		
	313	-15.871		
	318	-16.192		
Fe_3O_4@SiO_2@IIP-Ni(II)	298	-14.827	44.018	64.516
	303	-15.161		
	308	-15.487		
	313	-15.801		
	318	-16.119		
Fe_3O_4@SiO_2@NIP-Ni(II)	298	-14.451	46.801	64.166
	303	-14.760		
	308	-15.109		
	313	-15.417		
	318	-15.726		

Table S3. Selectivity parameters of IIPs and NIPs .

Metal ion	Sorbent	Distribution ratio D (mL/g)	Selectivity coefficient (k)	Relative selective coefficient (k')
Ni(II)	Fe_3O_4@SiO_2@IIP-Ni(II)	87546.30		
	Fe_3O_4@SiO_2@NIP-Ni(II)	4259.83		
	Fe_3O_4@void@IIP-Ni(II)	3249293.29		
	Fe_3O_4@void@NIP-Ni(II)	157930.44		
Co(II)	Fe_3O_4@SiO_2@IIP-Ni(II)	19031.14	4.60	4.30
	Fe_3O_4@SiO_2@NIP-Ni(II)	3984.82	1.07	
	Fe_3O_4@void@IIP-Ni(II)	695750.49	4.67	3.65
	Fe_3O_4@void@NIP-Ni(II)	123362.69	1.28	
Cu(II)	Fe_3O_4@SiO_2@IIP-Ni(II)	17099.37	4.12	3.65
	Fe_3O_4@SiO_2@NIP-Ni(II)	3767.01	1.13	
	Fe_3O_4@void@IIP-Ni(II)	647093.86	4.62	3.58
	Fe_3O_4@void@NIP-Ni(II)	125560.36	1.29	
Pb(II)	Fe_3O_4@SiO_2@IIP-Ni(II)	9991.70	8.76	6.84
	Fe_3O_4@SiO_2@NIP-Ni(II)	3326.52	1.28	
	Fe_3O_4@void@IIP-Ni(II)	363544.54	8.94	6.80
	Fe_3O_4@void@NIP-Ni(II)	120095.65	1.32	
Zn(II)	Fe_3O_4@SiO_2@IIP-Ni(II)	9694.39	9.03	5.15
	Fe_3O_4@SiO_2@NIP-Ni(II)	2428.03	1.75	
	Fe_3O_4@void@IIP-Ni(II)	335423.83	9.69	4.75
	Fe_3O_4@void@NIP-Ni(II)	77422.02	2.04	

Table S4. Fukui function (f^-) of atoms on potential adsorption sites from $AMPS^-$ molecule.

Atom	f^- Fukui function
N (9)	0.2744
S (10)	-0.0213
O (11)	0.1135
O (12)	0.0873
O (13)	0.0691

Table S5. Partial bond lengths and Wiberg bond order of $AMPS^-$ and AMPS-Ni(II)

Items	Bond lengths Å			Wiberg bond order		
	S10-O13	C1-N9	C5-N9	S10-O13	C1-N9	C5-N9
$AMPS^-$	1.463	1.437	1.342	2.213	1.256	1.610
AMPS-Ni(II)	1.536	1.492	1.472	1.683	1.159	1.183

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