

## Supporting Information

### **In-Situ Fixation of All-Inorganic Mo-Fe-S Clusters for Highly Selective Removal of Lead(II)**

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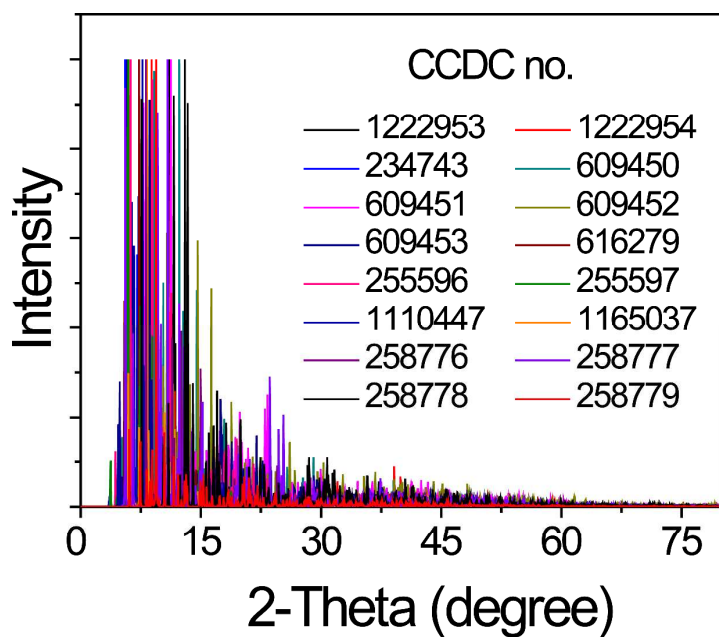
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Supporting Figures:



**Figure S1.** Simulated XRD patterns of 16 kinds Mo-Fe-S clusters according to their CCDC numbers (simulated by Materials Studio v7.0 software).

**Table S1** Hyperfine parameters of Mössbauer spectra of Fe<sub>3</sub>O<sub>4</sub> and FeMoS NPs.<sup>a</sup>

Sample	IS (mm s <sup>-1</sup> )	QS (mm s <sup>-1</sup> )	H (T)	A (%)	Site	Phase
Fe <sub>3</sub> O <sub>4</sub>	0.32	-0.01	48.57	51.22	A	Fe <sub>3</sub> O <sub>4</sub>
	0.46	0.00	44.95	48.78	B	
FeMoS	0.31	-0.01	48.36	43.37	A	Fe <sub>3</sub> O <sub>4</sub>
	0.52	0.00	44.62	56.63	B	

<sup>a</sup>IS: isomer shift relative to  $\alpha$ -Fe. QS: quadrupole splitting. H: magnetic field. A: relative subspectral area of each site.

**Table S2.** Selective capacity of Fe<sub>3</sub>O<sub>4</sub> NPs toward six mixed ions.

Mixed ions	Initial solution	Final solution	M <sup>n+</sup> removal	K <sub>d</sub> (mL/g)
	C <sub>0</sub>	C <sub>f</sub>	(%)	
Cu <sup>2+</sup>	10.756	10.594	1.506	15.29
Pb <sup>2+</sup>	10.651	10.620	0.2911	2.92
Cd <sup>2+</sup>	8.059	7.925	1.663	16.91
Ni <sup>2+</sup>	11.934	11.524	3.436	35.58
Mn <sup>2+</sup>	11.568	11.487	0.7002	7.05
Zn <sup>2+</sup>	10.425	10.279	1.400	14.20

**Table S3** Adsorption kinetics parameters of FeMoS NPs for Pb<sup>2+</sup> adsorption.

Pseudo-first-order			Pseudo-second-order		
$Q_{e,c}$ (mg g <sup>-1</sup> )	$k_1$ (min <sup>-1</sup> )	$R^2$	$Q_{e,c}$ (mg g <sup>-1</sup> )	$k_2 \times 10^{-2}$ (g mg min <sup>-1</sup> )	$R^2$
40.73.90±0.566	0.148±0.0104	0.991	42.55±0.578	0.598±0.0623	0.993

	Initial Phase			Secondary Phase		
	$K_{p1}$ (mg g <sup>-1</sup> min <sup>-0.5</sup> )	$C_l$	$R^2$	$K_{p2}$ (mg g <sup>-1</sup> min <sup>-0.5</sup> )	$C_l$	$R^2$
Intraparticle diffusion model	6.57±0.0754	8.68±0.258	0.999	0.159±0.0862	38.97±1.09	0.872

**Table S4.** Langmuir and Freundlich parameters of FeMoS NPs for Pb<sup>2+</sup> adsorption.

Langmuir isotherm			Freundlich isotherm		
$Q_m$ (mg g <sup>-1</sup> )	$K_L$ (L mg <sup>-1</sup> )	$R^2$	$K_F$ (mg g <sup>-1</sup> )	$1/n$	$R^2$
319.35±5.31	0.038±0.0033	0.995	87.54±13.16	0.217±0.029	0.974

**Table S5.** Comparison of adsorption capacities of various adsorbents for Pb<sup>2+</sup>.

Adsorbent	Q <sub>m</sub> (mg g <sup>-1</sup> )	Ref.
<b>FeMoS</b>	<b>319.35</b>	<b>This work</b>
MoS <sub>4</sub> -LDH	290	1
FA/PAA microgels	27	2
ATP/FA/PAA hydrogels	38	3
MPTS-CNTs/Fe <sub>3</sub> O <sub>4</sub>	65.4	4
MNP-CTS	140.1	5
Fe <sub>3</sub> O <sub>4</sub> /cyclodextrin	64.5	6
Fe <sub>3</sub> O <sub>4</sub> -GS	27.95	7
EDTA-modified chitosan/SiO <sub>2</sub> /Fe <sub>3</sub> O <sub>4</sub>	123.5	8
Fe <sub>3</sub> O <sub>4</sub> @SiO <sub>2</sub> -NH <sub>2</sub>	243.9	9
Magnetite-GO-LDH	173	10
NH-MNPs	167.8	11
Fe <sub>3</sub> O <sub>4</sub> /HA	92.4	12

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