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Synthesis of Fe-THC MOFs and Functionalizing of MOFs by MXene for Selective Removal of Lead (II) Ions from Wastewater

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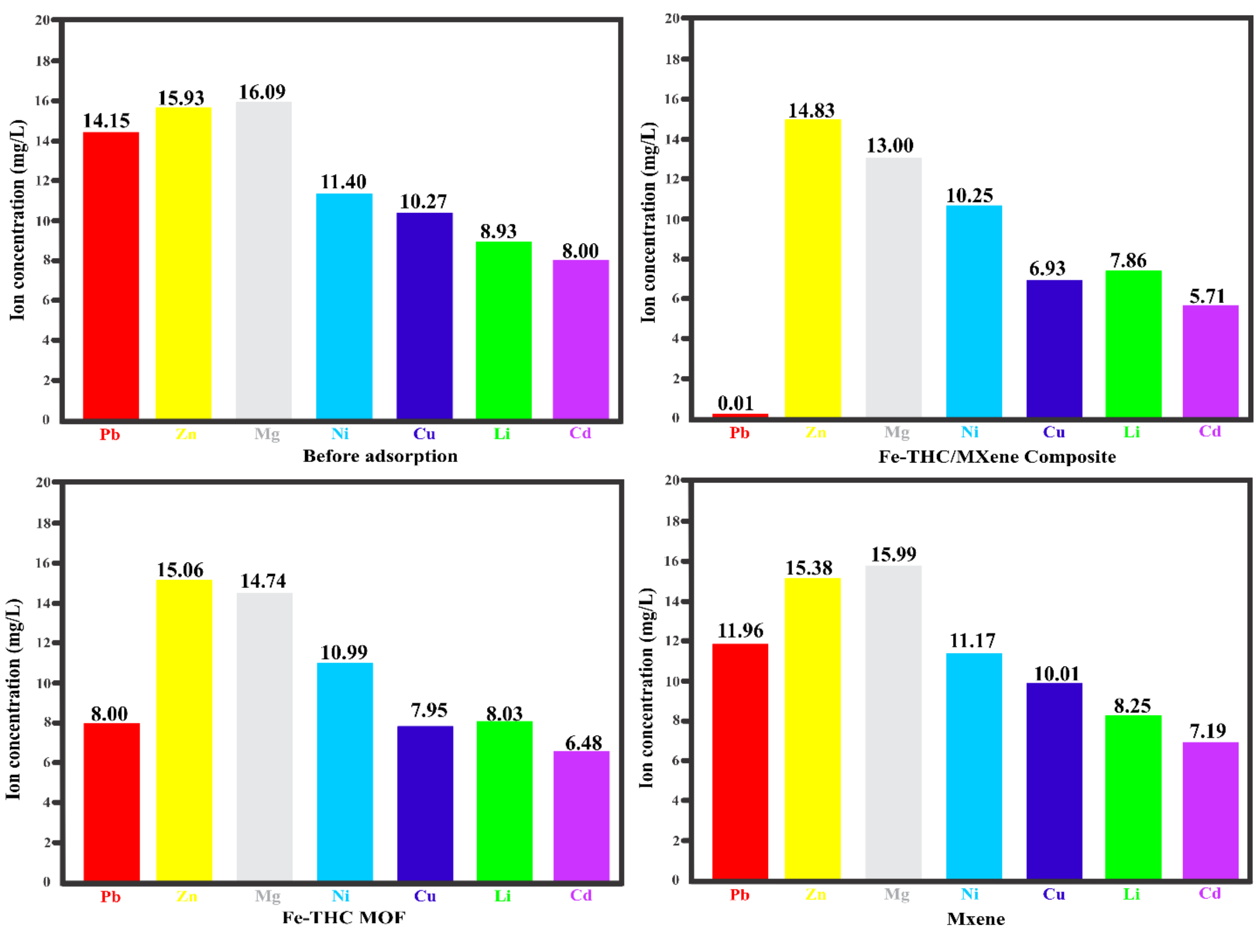
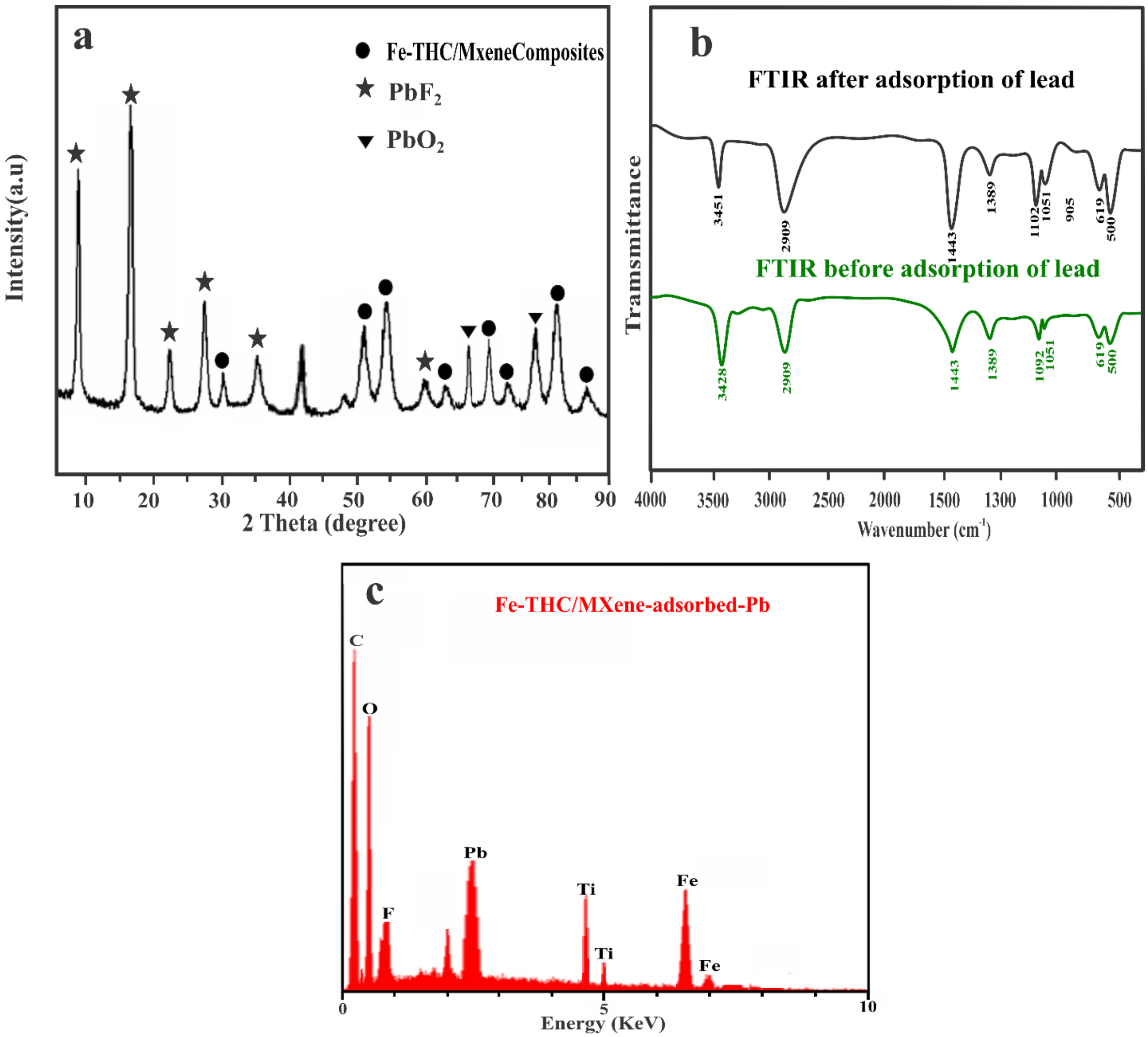


Figure.S1: Selectivity of Pb^{2+}adsorption before adsorption (a), on Fe-THC/MXene (b), Fe-THC MOFs (c), MXene (d)



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14 **Figure.S2: XRD (a), FTIR (b), and EDX spectrums (c) of Fe-THC MOFs composites after adsorption of lead**

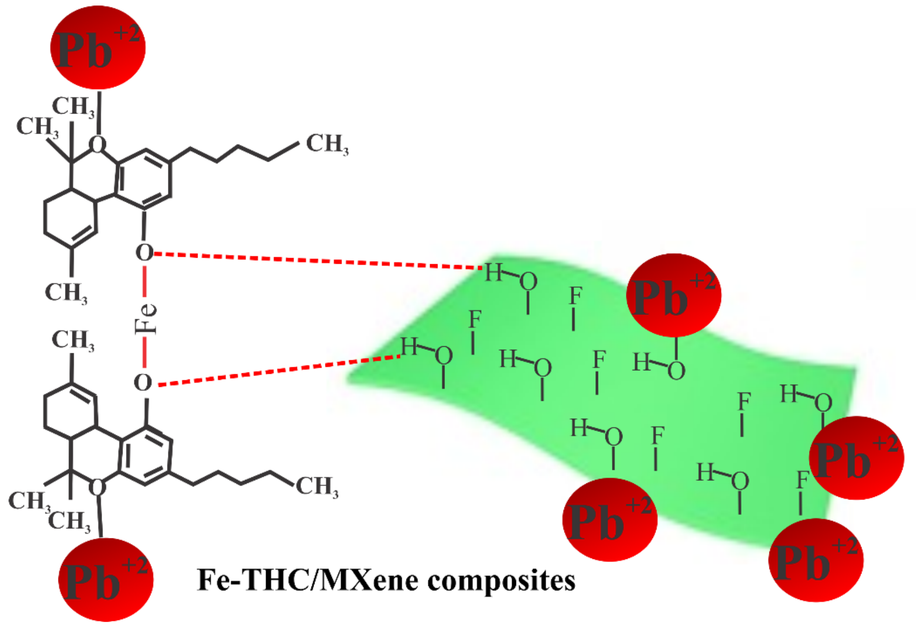

Figure.S3: Possible mechanism of adsorption of lead on the Fe-THC/Composite

Kinetic Models	**10 mg L^{-1}**	**20 mg L^{-1}**	**30 mg L^{-1}**
PFO			
q_e (mg g^{-1})	120.36	36.09	11.85
K_1(min^{-1})	10.79	0.0805	8.56
R^2	0.9836	0.9773	0.9541
PSO			
q_e (mg g^{-1})	466.99	335.53	213.27
K_2 [(g mg^{-1})min^{-1})]	3.36	2.88	3.94
R^2	0.9999	0.9995	0.9766

Table.S1: Adsorption kinetic parameters of Pb^{2+}adsorption on Fe-THC/MXene

Adsorbent cons (mg L^{-1})	**R^2**				**C (mg/g)**				**K (mg/g-$min^{0.5}$)**			
	Total	$1R^2$	$2R^2$	$3R^2$	Total	C_1	C_2	C_3	Total	K_1	K_2	K_3
10 mg L^{-1}	0.56	0.97	0.82	0.78	89.9	8.32	8.67	9.36	0.03	0.29	0.08	0.02

20 mg L^{-1}	0.60	0.99	0.93	0.62	12.64	13.53	7.39	15.6	0.30	0.36	0.19	0.04
30 mg L^{-1}	0.78	1.0	0.97	0.57	15.66	12.30	19.46	18.62	0.29	1.36	0.49	0.08

Table.S2: Intra-particle diffusion kinetic parameters of Pb^{2+}adsorption on Fe-THC/MXene

Isothermal model	**Para meters**	**305 K**	**310 K**	**315 K**
Langmuir	$q_{m\ exp}$ (mg g^{-1})	680	298	84
	$q_{m\ cal}$ (mg g^{-1})	674	293	77
	K_L	0.1680	0.3543	0. 1268
	R^2	0.9999	0.9986	0.9939
Freundlich				
	$K_{F\ exp}$ (mg g^{-1})	160	50	20
	$K_{F\ cal}$ (mg g^{-1})	148	39	17
	n	3.51	0.622	2.59
	R^2	0.9820	0.9563	0.81
Temkin				
	K_T	0.12	17.26	1.91
	B	123	45.99	6.469
	R^2	0.9885	0.9636	0.9203

Table.S3: Adsorption isotherm parameters of Pb^{2+}adsorption time on Fe-THC/MXene

Temperature (K)	**ΔG(KJ mol^{-1})**	**ΔH(KJ $mol^{-1}K^{-1}$)**	**ΔS(K mol^{-1})**
305 K	-8.539	-40.365	-0.359
310 K	-4.688		
315 K	-2.967		

Table.S4: Thermodynamic parameters of Pb^{2+}adsorption on Fe-THC/MXene

	Fe-THC/MXene composite		**Fe-THC MOFs**		**MXene**	
Heavy metals ion	**K_Q(mL g^{-1})**	**K**	**K_Q(mL g^{-1})**	**K**	**K_Q(mL g^{-1})**	**K**

Pb (II)	19, 206.6	21,935.9	12,403.2	13,967.9	750.0	1347.2
Zn (II)	93.9	112.3	89.8	96.1	68.8	73.7
Mg (II)	87.4	107.3	74.2	91.9	57.4	68.7
Ni(I)	56.5	196.0	49.9	148.5	33.6	98.4
Cu (II)	33.9	218.2	29.5	79.3	17.69	59.5
Cd (II)	25.8	92.7	17.0	63.7	10.0	49.6
Li (I)	12.5	59.9	4.88	42.6	3.7	18.2

Table.S5: Selectivity parameters of Pb^{2+}adsorption on Fe-THC/MXene

Adsorbents	Temperature	Equilibrium time	pH	q_e (mg/g)	References
nFe@ZIF-8 composite	313K	60 min	5	175.43	[54]
Melamine-modified Zr-MOFs	313K	120	5	122.0	[55]
CAU-7-TATB	-	45	5	63	[56]
FSAC	398		4	80.6	[57]
MIL-101(Fe)/GO	-	15	6	128.6	[58]
Fe-THC/MXene	305K	12	4.5	674	This Work

Table.S6: Comparative study with previous literature