Amberlite IRA 400 Cl^- ion exchange resin modified with Prosopis Juliflora seeds as an efficient Pb^{2+} adsorbent: Adsorption, kinetics, thermodynamics, and computational modeling studies by density functional theory

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Supplementary data

Table S1: The FT-IR spectral characteristics of surface modified ion exchange resin before and after adsorption.

FT-IR Peaks	Adsorption bands (cm^{-1})			Assignment
	Before adsorption	After adsorption	Differences	
1	3947.36	3793.51	153.85	
2	3420.57	3725.12	-304.55	Bonded –OH groups
3	2928.57	-	-	C–H stretching
4	2368.57	2346.58	21.99	
5	1599.67	1600.97	-1.3	C = O group
6	1354.98	1358.39	-3.41	S=O group
7	1190.34	1213.80	-85.03	S=O group
8	1128.77	-	-	S=O group
9	1040.50	1043.36	-2.86	C-X group
10	835.28	-	-	C-X group
11	776.85	779.32	-2.47	C-X group
12	679.39	-	-	C-X group
13	621.20	-	-	-
14	583.93	-	-	–C–C– group

Table S2: Parameters of the various isotherm models in adsorption of Pb^{2+} onto SMA resin.

Isotherms	Parameters	Temperatures (K)				
		298	308	318	328	338
Langmuir	K_L (L g^{-1})	0.12	0.18	0.141	0.115	0.041
	q_{max} (mg g^{-1})	106.5	66.36	64.79	63.75	105.7
	R^2	0.989	0.996	0.995	0.998	0.955
Freundlich	K_F (mg g^{-1})	0.00184	0.00049	0.000584	0.0018	0.014
	N	0.447	0.359	0.354	0.389	0.51
	R^2	0.924	0.904	0.963	0.949	0.992
Koble-Corrigan	A	22.82	16.39	15.29	13.23	874.8
	B	0.32	0.0334	0.113	0.143	35.96
	N	-0.98	-0.365	-0.458	-0.543	-0.891
	R^2	0.956	0.974	0.997	0.999	0.021
Dubinin-Radushkevich	E (k J mol^{-1})	0.826	1.11	0.978	0.876	7.82
	q_s(mg g^{-1})	65.96	42.95	43.64	42.48	49.65
	R^2	0.873	0.751	0.816	0.799	0.777
Temkin	A (L g^{-1})	0.756	0.734	0.722	0.675	1.21
	B (k J mol^{-1})	12.32	11.23	10.43	8.45	29.32
	R^2	0.877	0.931	0.919	0.925	0.879

Table S3: The kinetic models of adsorption on Pb^{2+} - loaded SMA resin at various temperatures

Kinetic model	Parameters	Temperature (K)				
		298	308	318	328	338
Pseudo first order	K_1 (min^{-1})	0.018	0.048	0.046	0.049	0.022
	q_e (mg g^{-1})	26.28	29.96	24.68	25.13	38.55
	R^2	0.976	0.967	0.945	0.950	0.948
	Δq_e (%)	47.17	30.91	34.75	32.69	23.69
Pseudo second order	K_2 (mg g^{-1})	0.228	0.070	0.235	0.293	0.144
	q_e (g mg^{-1} mim^{-1})	62.5	76.92	62.5	58.82	66.67
	R^2	0.999	0.997	0.999	0.999	0.996
	Δq_e (%)	10.95	-16.05	-3.07	1	-4.43
First order reaction	K_1 (min^{-1})	0.121	0.066	0.063	0.052	0.082
	q_e (mg g^{-1})	49.99	50.68	49.76	49.75	49.57
	R^2	0.794	0.362	0.326	0.317	0.537
	Δq_e (%)	23.46	10.19	9.67	8.07	12.67
Weber and Morris model	K_{id} (mg g^{-1} $min^{1/2}$)	2.487	1.575	1.526	1.262	1.819
	I	39.28	43.13	42.39	43.66	41.26
	R^2	0.932	0.568	0.523	0.509	0.734

Table S4: The thermodynamic parameters for the adsorption of Pb^{2+} onto SMA resin

Temperature (K)	Equilibrium constant (K)	Thermodynamic parameters		
		ΔG^o (K J mol^{-1})	ΔH^o (K J mol^{-1})	ΔS^o (J mol^{-1} K^{-1})
298	2.77	-2.52	-10.13	-24.45
308	1.56	-1.13		
318	1.46	-1.01		
328	1.37	-0.86		
338	1.65	-1.4		

Table S5: The computational study for the adsorption of Pb^{2+} on the SMA ion exchange resin

Binding state	BE in K cal / mol Pb^{2+} ion in singlet state	BE in K cal / mol Pb^{2+} ion in triplet state	Bond distance between hetero atom and Pb^{2+} ion in singlet state (Å)	Bond distance between hetero atom and Pb^{2+} ion in triplet state (Å)
Pyrene-CHO	115.13179823	328.74986146	3.300000	3.300000
Pyrene-OH	112.036268229	327.69215009	3.30000	3.300000
Pyrene-COOH (chelate type)	98.4458220152	305.871852617	3.261254 (-C=O)	3.261254
			3.256463 (-O-H)	3.256463
Pyrene-CO	153.573444695	298.919717595	3.3000	3.300000
Pyrene-aromatic	129.90420271	291.94962952	5.452	5.452
Pyrene SH	92.234411885	289.77034513	3.825000	3.825000

Table S6: Maximum adsorption capacity calculated according to Langmuir isotherm for various adsorbent for the adsorption of Pb^{2+}.

Adsorbents	q_{max} (according to Langmuir) (mg/g)	Reference
Amberlite 400 Cl	32.491	[21]
Hazelnut husk AC	13.05	[33]
Tamarind wood AC	43.859	[34]
cellulose modified bone char	89.9	[35]
Palm Oil mill effluent AC	94.34	[36]
polyaniline coated PJ seed	90.91	[37]
ARASA	270.2	[38]
modified Aloji clay	142.57	[39]
sludge based bio-char	16.70 and 49.47	[40]
SMA resin	106.5	This Study