

Hydrothermal synthesis of mineral-substituted hydroxyapatite nanocomposite material for fluoride removal from drinking water

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Supplementary Information (SI)

Figure 1(A) SEM image of HAp (B) EDAX graph of HAp.

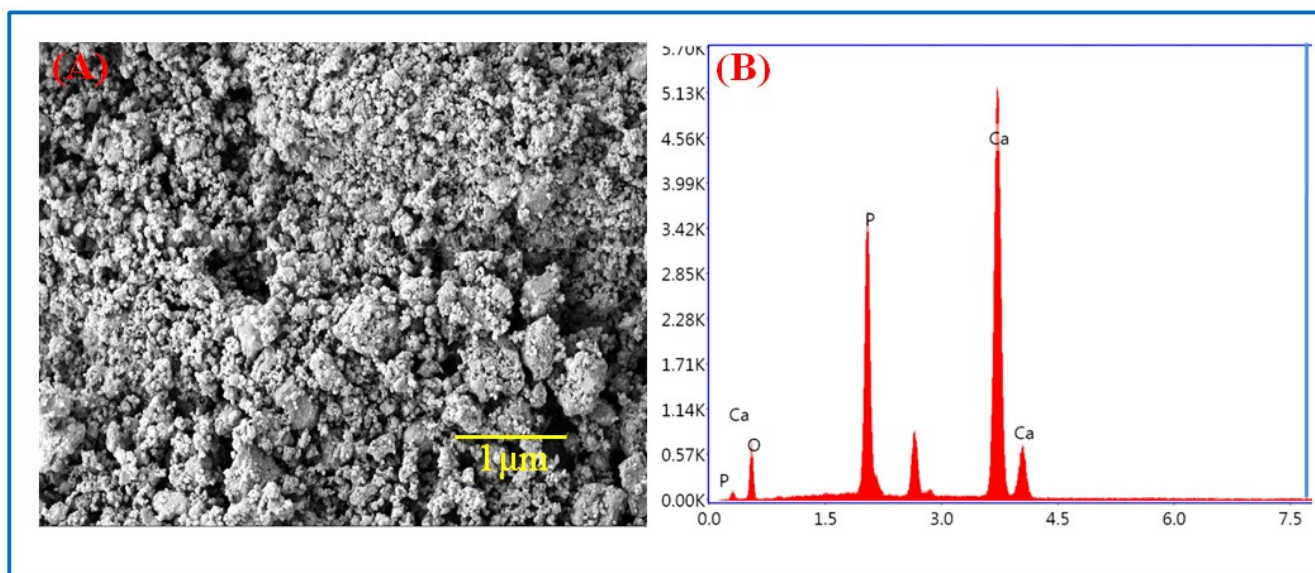


Figure 2. Dynamic Light Scattering (DLS, Particle size) image of HAp

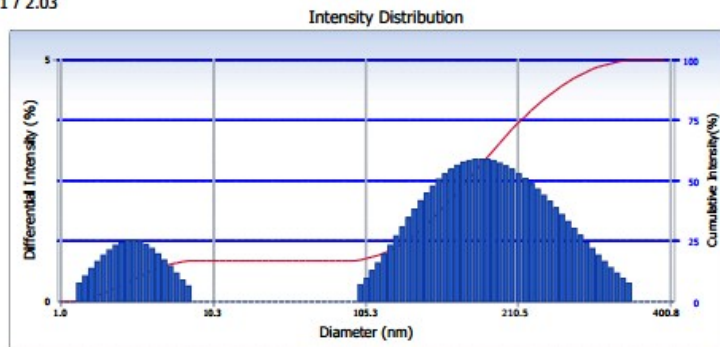
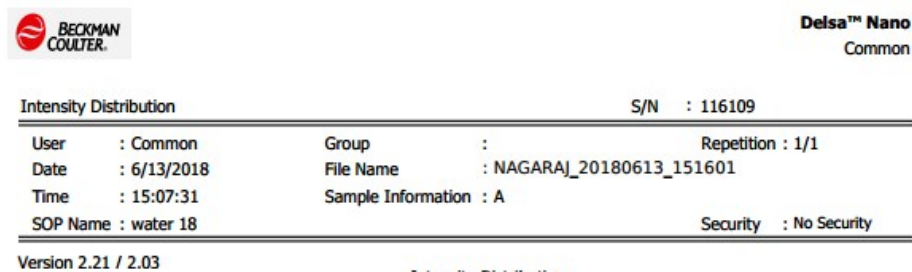


Figure 3. Dynamic Light Scattering (DLS, Particle size) image of HAp

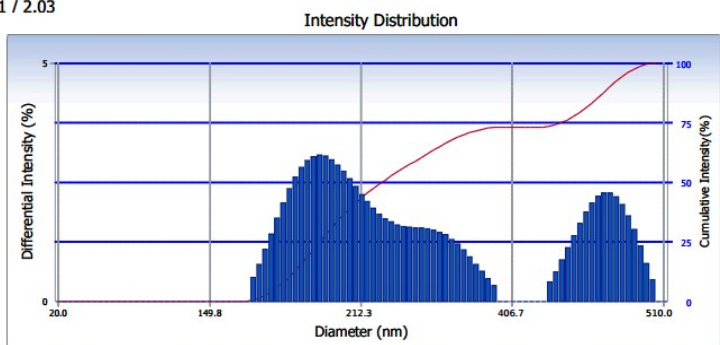
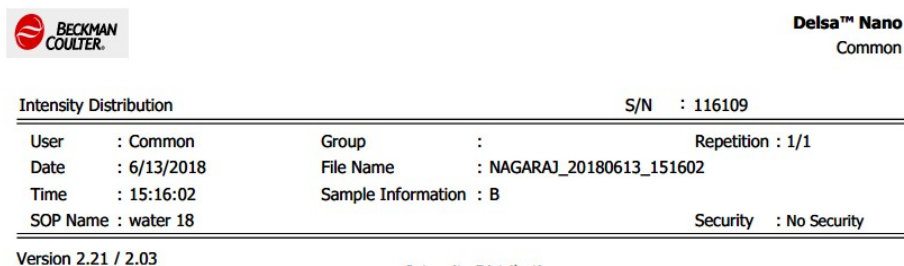


Figure 4. pH zero point charge (pH_{zpc}) image of HAp

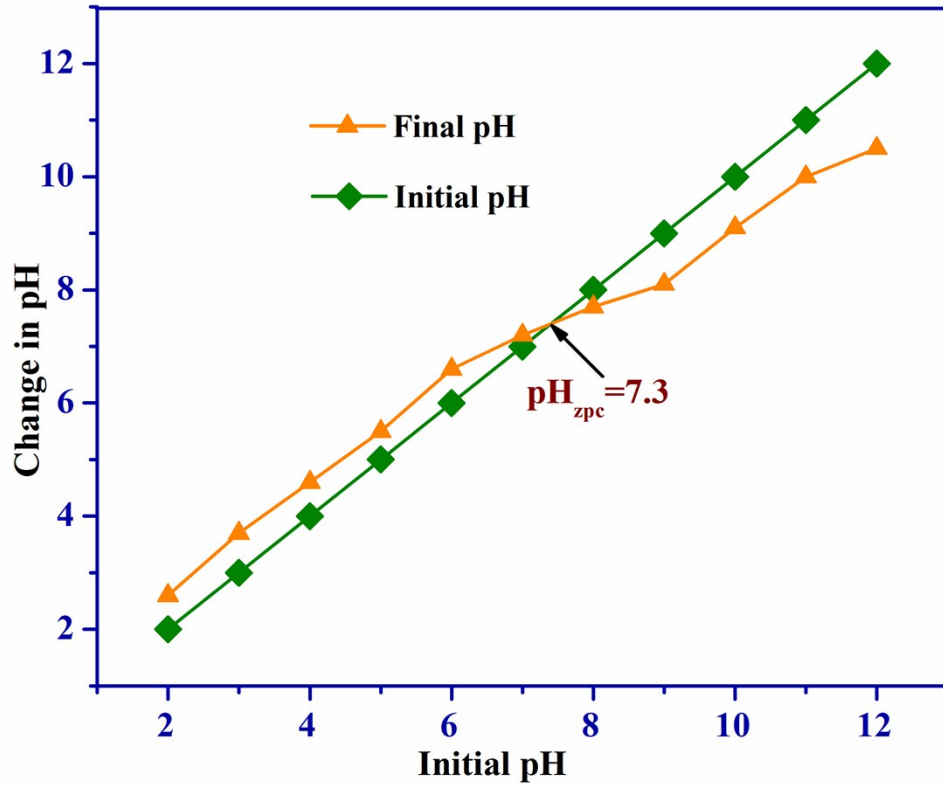


Table 1. Adsorption isotherm parameters of the mHAp nanocomposite adsorbent

Isotherms	Parameters	Temperature		
		303 K	313 K	323 K
Freundlich	1/n	0.1780	0.1872	0.2211
	N	5.6052	5.3521	4.5201
	$k_F(\text{mg}\cdot\text{g}^{-1}) (\text{L}\cdot\text{mg}^{-1})^{1/n}$	3.1872	3.3006	3.4041
	R	0.9918	0.9997	0.9999
	Sd	0.0074	0.0219	0.0246
	χ^2	0.2021	0.3410	0.4232
Langmuir	$Q^\circ (\text{mg}\cdot\text{g}^{-1})$	4.7081	4.9032	5.3789
	$b (\text{L}\cdot\text{g}^{-1})$	1.7277	1.8113	1.5326
	R_L	0.0344	0.0391	0.0212
	R	0.9995	0.9975	0.9949
	Sd	0.0137	0.0293	0.0341
	χ^2	0.3891	0.8762	0.9785
Dubnin – Radushkevich	$X_m (\text{mg}\cdot\text{g}^{-1})$	4.8271	4.7293	4.6751
	$E (\text{kJ}\cdot\text{mol}^{-1})$	8.7261	9.2507	9.9031
	R	0.9808	0.9317	0.9262
	Sd	0.0250	0.0551	0.0654
	χ^2	0.7659	1.4709	1.8203

Table 2. Kinetic models and their estimated parameters for the mHAp nanocomposite adsorbent

Kinetic models	Parameters	Temperature at 303 K				
		2 mg/g	4 mg/g	6 mg/g	8 mg/g	10 mg/g
Pseudo-first-order	k_{ad} (min ⁻¹)	0.1461	0.1560	0.1173	0.1671	0.1752
	R	0.9969	0.9980	0.9912	0.9785	0.9531
	Sd	1.0993	1.0172	0.0918	1.0685	1.0721
Pseudo-second-order	q_e (mg/g)	2.3376	1.4409	1.2081	1.0133	1.3011
	k (g/mg min)	0.2461	0.2524	0.3412	0.3423	0.3132
	h (mg/g min)	3.9290	3.8169	3.7428	3.3421	3.3422
	R	0.9999	0.9999	0.9992	0.9995	0.9999
	Sd	0.0220	0.0172	0.0918	0.0685	0.0721
Particle diffusion	k_p (min ⁻¹)	0.1530	0.1321	0.1412	0.1142	0.1317
	R	0.9891	0.9801	0.9968	0.9805	0.0981
	Sd	0.029	0.036	0.035	0.031	0.035
Intraparticle diffusion	k_i (mg/g min ^{0.5})	0.1357	0.1345	0.1420	0.0390	0.0398
	R	0.9778	0.9730	0.9689	0.9765	0.9614
	Sd	0.0168	0.0379	0.0625	0.0855	0.0603

Table 3 Thermodynamic parameters of the mHAp nanocomposite adsorbent

Temperature (K)	Thermodynamic parameters		
	ΔG° (KJ mol ⁻¹)	ΔH° (KJ mol ⁻¹)	ΔS° (KJ mol ⁻¹ K ⁻¹)
313	-0.73	0.6301	2.6301
323	-0.91		
333	-1.12		

Table 4. Field study results for the adsorbent of mHAp and HAp nanocomposites.

Water quality parameters	Adsorbent mHAp		Adsorbent HAp	
	Before	After	Before	After
Fluoride (mg L ⁻¹)	2.42	0.51	2.42	0.91
pH	7.3	6.9	7.3	6.7
Chloride (mg L ⁻¹)	443	272	443	290
Sulfate (mg L ⁻¹)	166	147	166	150
Nitrate (mg L ⁻¹)	47	31	47	35
Bicarbonate (mg L ⁻¹)	132	114	132	120
Total Hardness (mg L ⁻¹)	493	371	493	380
Total Dissolved Solids(TDS) (mg L ⁻¹)	256	223	256	233
Electrical Conductivity (m Sm ⁻¹)	7.2	3.1	7.2	3.7