Electronic Supporting Information

Sol-gel synthesis of alumina gel@zeolite X nanocomposite for high performance water defluoridation: Batch and column adsorption study

Adwitiya Chakraborty and Milan KantiNaskar*

Central Glass and Ceramic Research Institute (CSIR)

Kolkata 700 032

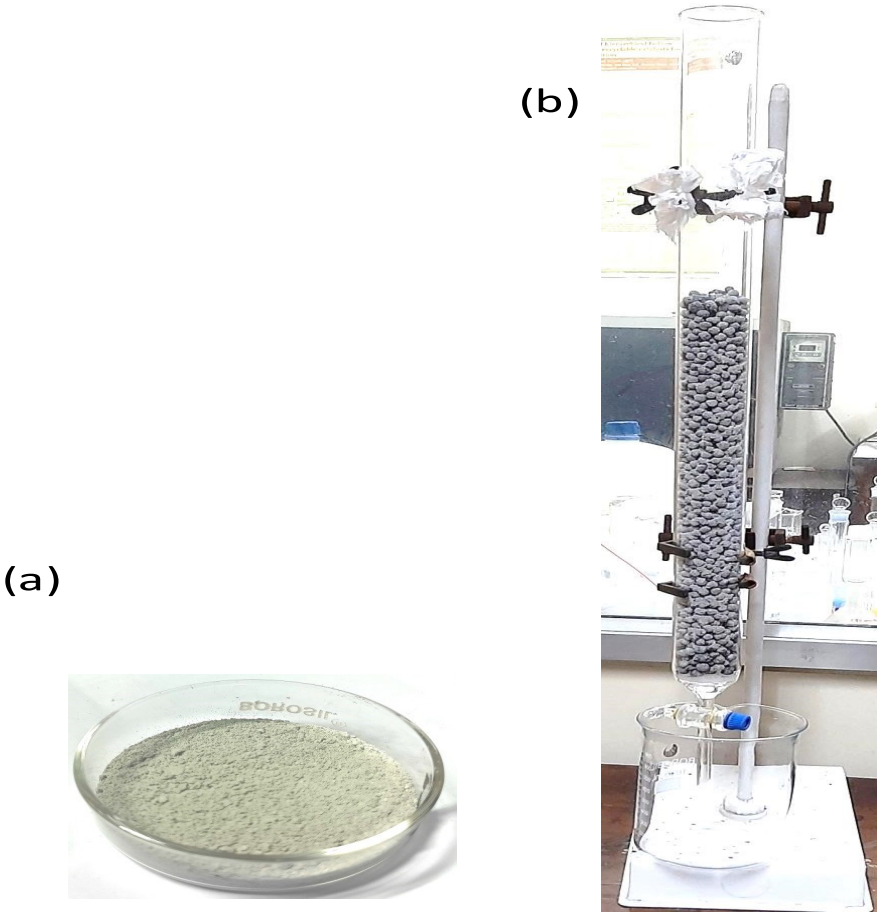

Fig. S1: (a) Synthesized alumina gel@zeolite X nanocomposite and (b) fixed bed column.

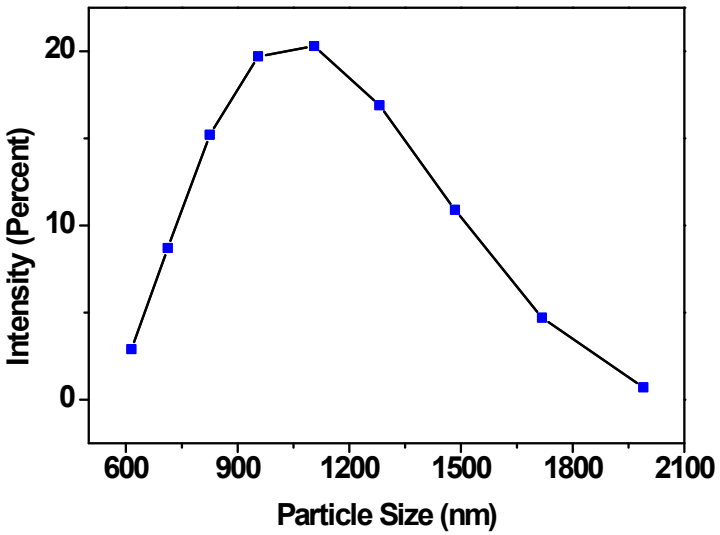

Fig. S2 : Particle size disribution of alumina gel@zeolite X nanocomposite

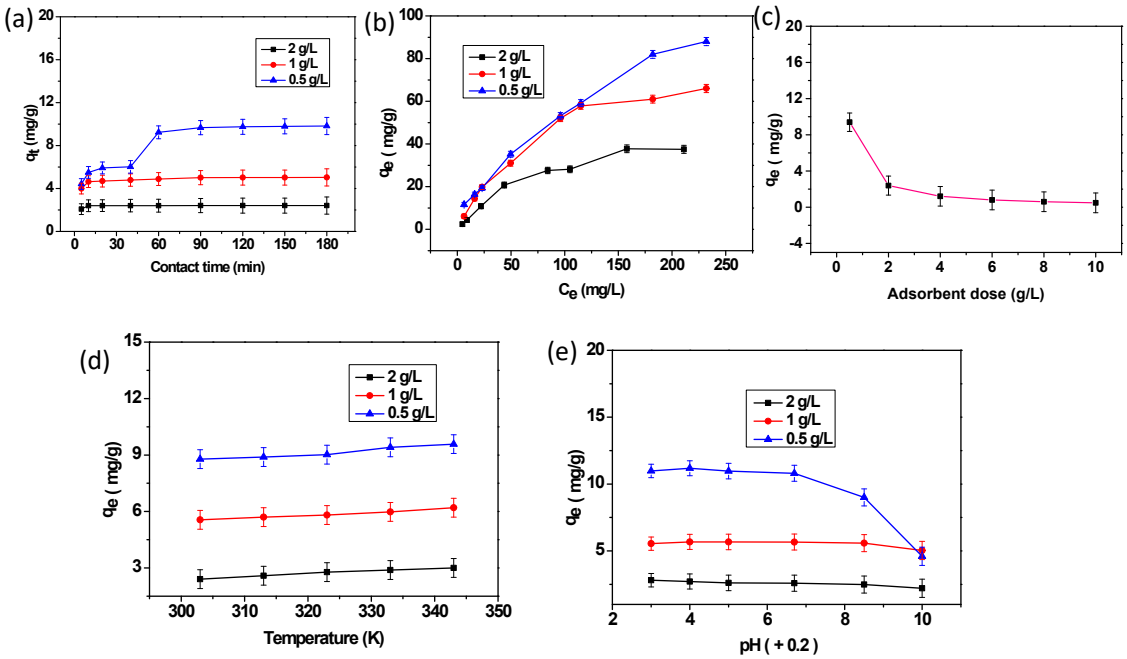

Fig. S3: Adsorption capacity with (a) contact time, (b) initial fluoride ion concentration, (c) adsorbent dose, (d) temperature and (e) pH on the adsorption of F^- ions by alumina gel@zeolite X nanocomposite

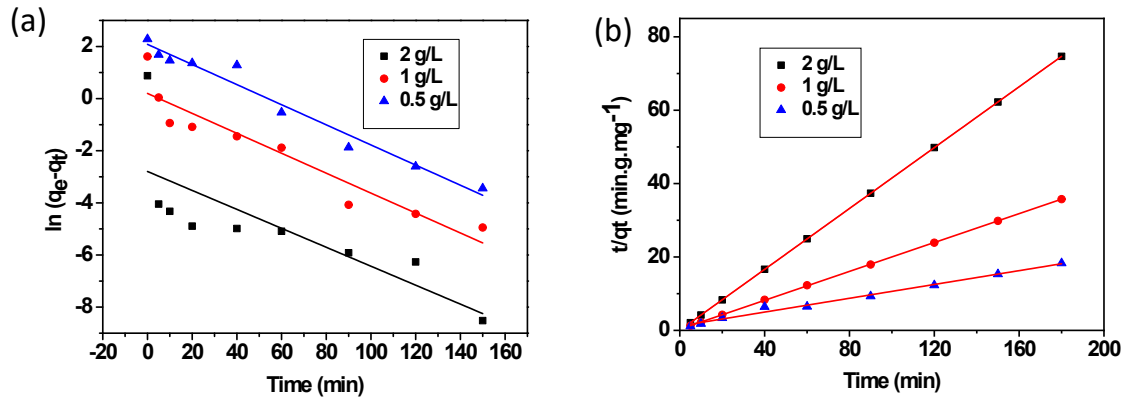

Fig. S4: Kinetics data with linear fitting of (a) pseudo-first-order and (b) pseudo-second-order

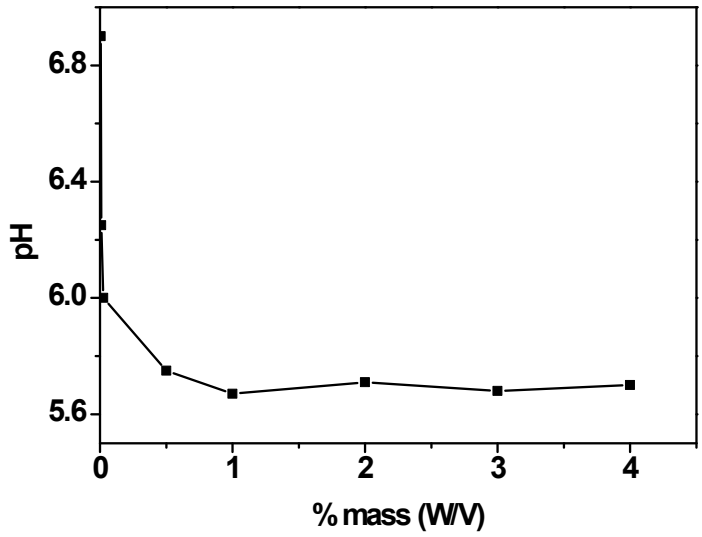

Fig. S5: pH vs percentage mass of the adsorbent

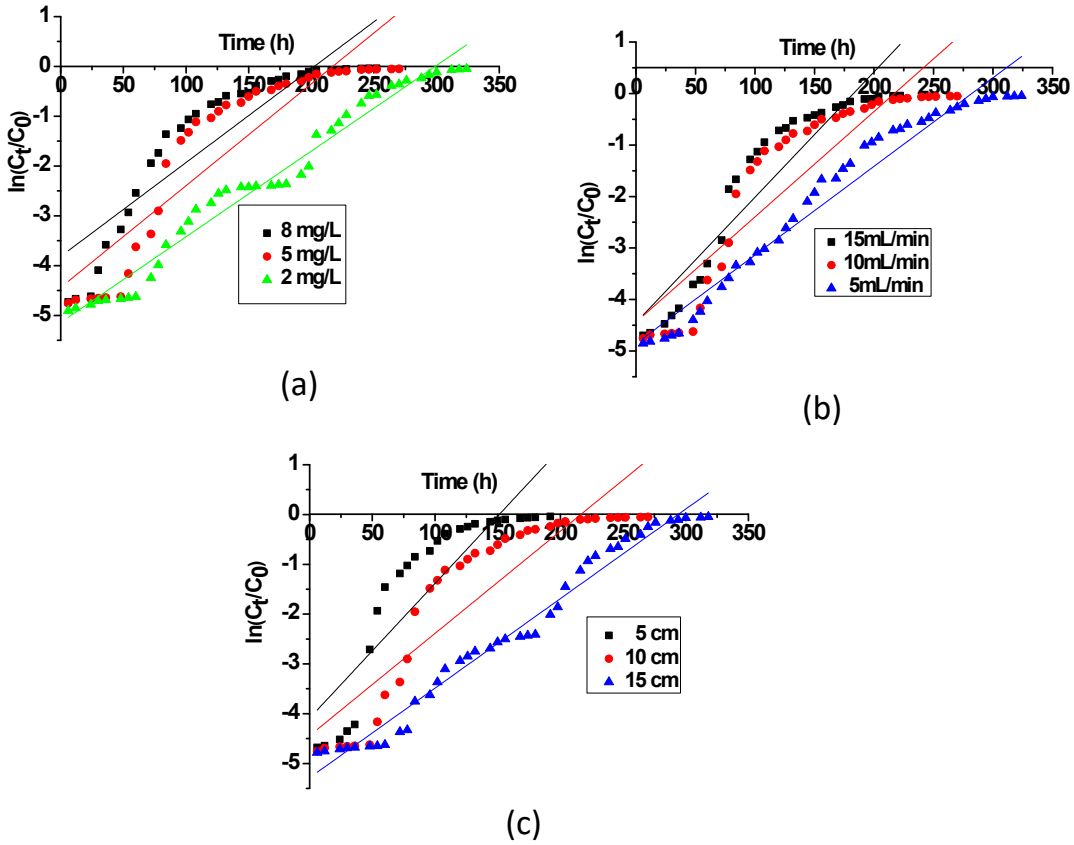

Fig. S6: Linear regression analysis of breakthrough curves using Adams-Bohart model at different (a) concentrations, (b) flow rates and (c) bed heights

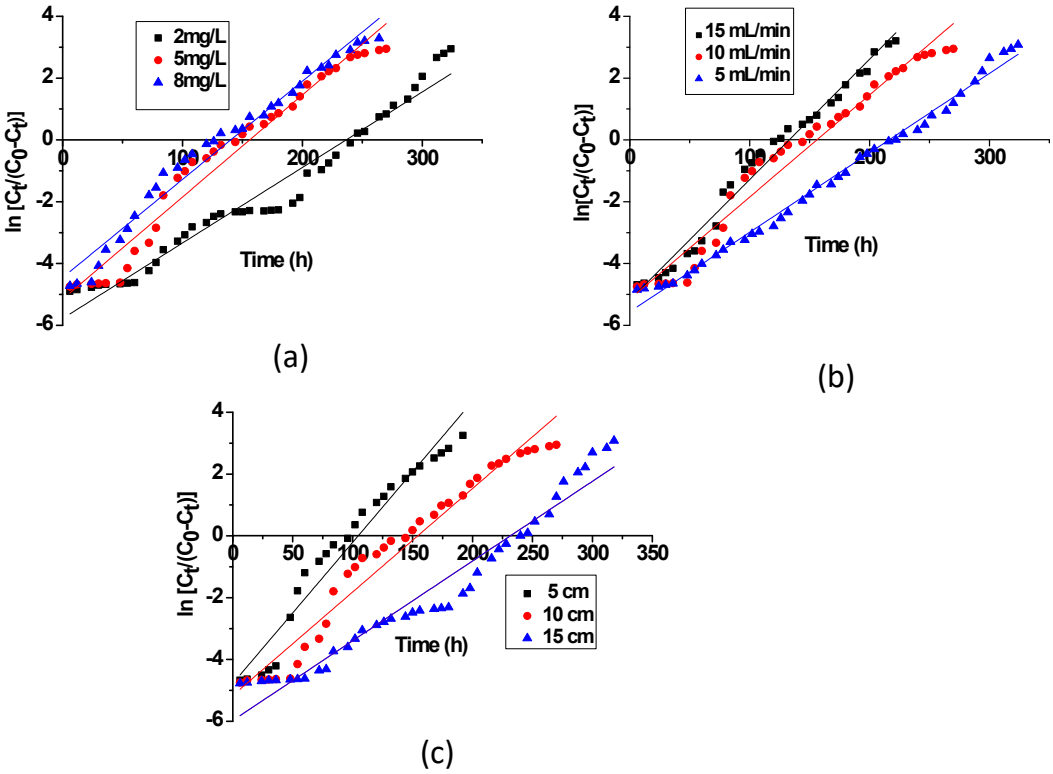

Fig. S7: Linear regression analysis of breakthrough curves using Yoon-Nelson modelat different (a) concentrations, (b) flow rates and (c) bed heights.

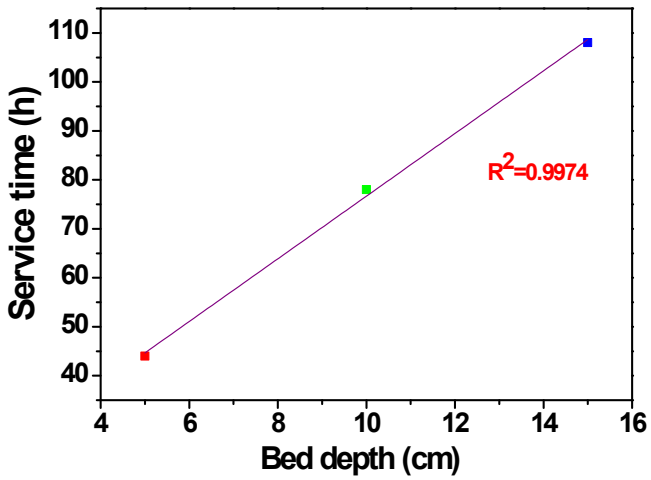

Fig. S8: Linear Plot of BDST for fluoride adsorption

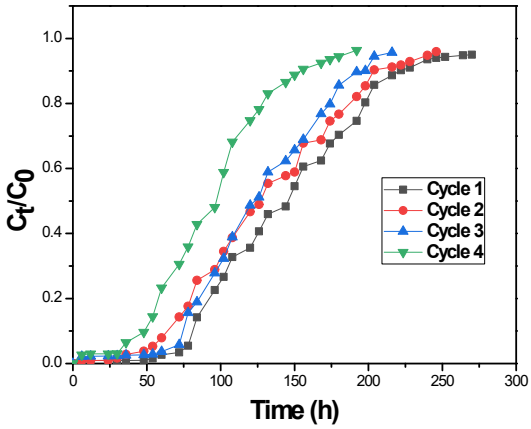

Fig. S9: Desorption-regeneration cycle for fluoride removal

Table S1: Adsorption capacity (mg/g) of zeolite X and alumina gel@zeolite X nanocomposites

Time (min)	Initial adsorbate conc. (ppm)	Adsorbent dose(gm/L)	Adsorption capacity (mg/g) of zeolite X	Adsorption capacity (mg/g) of alumina gel@zeolite X
120	5	0.50	2.6	9.75
		1.00	0.70	5.02
		2.00	0.55	2.40

Table S2**:** Kinetic parameters for the adsorption of fluoride ions

Model	Mathematical expression		**Adsorbent dose (g/L)**		
			0.5	1.0	2.0
Pseudo-first order kinetics	$\ln (q_e-q_t) = -k_1 t + \ln q_e$	k_1 (min^{-1})	0.03861	0.03824	0.03636
		q_e(mg/g)	8.026	1.2200	0.06110
		R^2	0.9657	0.8823	0.5616
		S.E (Intercept)	0.346	0.375	0.729
		S.E(Slope)	0.003	0.004	0.008

Pseudo-second order kinetics	$t/q_t = 1/k_2q_e^2 + (1/q_e)t$	k_2 (g/mg·min)	0.0729	0.1239	4.52
		q_e(mg/g)	10.62	5.07	2.411
		R^2	0.9999	0.9999	0.9999
		S.E (Intercept)	0.198	0.056	0.011
		S.E(Slope)	0.002	0.0005	0.0001

Note: $q_e$andq_t (mg/ g) are the amounts of fluoride adsorbed at equilibrium and time t (min), and k_1 (min^{-1}) and k_2 ($g.mg^{-1}min^{-1}$) are thefirst and second-order rate constants, respectively, SE = Standard Error.

Table S3: Theparameters obtained from Langmuir and Freundlich models

Adsorbent dose (g/L)			0.5	1.0	2.0
Langmuir isotherm	$C_e/q_e=C_e/q_m+1/K_L.q_m$	K_L (L/mg)	0.0217	0.0972	0.26431
		q_m (mg/g)	103.62	68.119	37.608
		R^2	0.8973	0.9877	0.9822
		S.E (Intercept)	0.113	0.0476	0.080
		S.E (Slope)	0.001	0.0006	0.001
Freundlich isotherm	$\log q_e = \log K_F + 1/n_F \log C_e$	K_L (L/mg)	10.452	11.668	10.739
		q_m (mg/g)	2.653	2.764	3.495
		R^2	0.8781	0.9826	0.9245
		S.E (Intercept)	0.197	0.061	0.106
		S.E(Slope)	0.052	0.018	0.030

Note: q_e is the amounts of fluoride adsorbed at equilibrium and $q_m$isq_e for a complete monolayer, i.e., maximum adsorption capacity (mg/g), K_L is adsorption equilibrium constant (L/mg); K_F and n_F are empirical constants, indicating the adsorption capacity and adsorption intensity,respectively, SE = Standard Error.

Table S4: A comparative data on maximum adsorption capacity, kinetics and rate constant for fluoride ion adsorption by alumina gel@zeolite X nanocomposite and reported adsorbents

Adsorbents	Maximum adsorption capacity (mg/g) at 25 ^{0}C	Kinetics	Value of rate constant *k*	Ref
Bentonite/chitosan beads	1.164	Pseudo second order	149.67 (g/mg.min)	1
Crystalline gamma alumina	32	Pseudo second order	0.02678 (g/mg.min)	2
PVA-alginate/CTAB	12.93	Pseudo second order	1.149 (g/mg.min)	3
Perchloric acid cross-linked calcium alginate	44	Pseudo second order	0.026 (g/mg.min)	4
Aluminium impregnated chitosan	1.73	First order	0.101 min^{-1}	5
Aluminium coated modified zeolite	11.52	Pseudo second order	0.6804 (g/mg.min)	6
Alumina gel@zeolite X	103.62	Pseudo second order	0.0729 (g/mg.min)	Present work

Table S5

(a) Adams-Bohart Model Parameters

C_0 (mg/L)	Q(ml/min)	Z(cm)	$K_{AB}\times10^{-3}$ (L/mg h)	N_0(mg/L)	R^2
2	10	10	8.60	5072.13	0.9729
5	10	10	4.09	9214.74	0.8258
8	10	10	2.35	13782.75	0.8120
5	5	10	3.18	6481.32	0.9584
5	10	10	3.78	9970.38	0.8258
5	15	10	4.50	12564.18	0.8727
5	10	5	5.00	13886	0.7802
5	10	10	3.80	9917.06	0.8250
5	10	15	3.29	8983.81	0.9776

(b) Thomas Model Parameters

C_0 (mg/L)	Q(ml/min)	Z(cm)	$K_{Th}\times10^{-3}$ (L/mg h)	q_0(mg/g)	R^2
2	10	10	12.22	4.729	0.9621
5	10	10	6.602	7.799	0.9638
8	10	10	3.96	11.232	0.9728
5	5	10	4.73	5.86	0.9918
5	10	10	6.11	8.425	0.9638
5	15	10	7.21	10.77	0.9827
5	10	5	8.45	11.302	0.9516
5	10	10	6.20	8.326	0.9631
5	10	15	4.77	8.335	0.95233

(c) Yoon-Nelson Model Parameters

C_0 (mg/L)	Q(ml/min)	Z(cm)	$K_{YN} \times 10^{-3}$ (hr^{-1})	τ(hr)	R^2
2	10	10	24.43	236.54	0.9622
5	10	10	33.01	156	0.9638
8	10	10	31.77	140	0.9732
5	5	10	25.71	216.24	0.9961
5	10	10	33.01	155.99	0.9638
5	15	10	38.95	132.95	0.9827
5	10	5	45.66	104	0.9513
5	10	10	33.48	154.21	0.9631
5	10	15	25.79	231.51	0.9523

(d) BDST Model Parameters

C_0 (mg/L)	Q(ml/min)	Z(cm)	N_0(mg/L)	K_a (L/mg hr)	R^2
5	10	5	2933.55	0.0430	0.9974
5	10	10			
5	10	15			

References

1 Y. Zhang, D. Wang, B. Liu, X. Gao, W. Xu, P. Liang, and Y. Xu, ***Am. J. Anal. Chem., 2013, 4, 48-53.***

2 P. Chinnakoti, A.L.A Chunduri, R.K. Vankayala, S. Patnaik, and V. Kamisetti, ***Appl. Water Sci.,*** **2017, 7, 2413-2423.**

3 P. Kathane and A. Tiwari ***Adv. Phys. Lett.,*** **2016, 3, 2349-1108.**

4 V. Yarramuthi, J. M. Jagadeeson, K. D. Rachapudi and R. K. Challagundla , ***Indian J. Adv. Chem. Sci.*****, 2018; 6(2), 88-95.**

5 S. K. Swain, R. K. Dey, M. Islam, R. K. Patel,.U. Jha, T. Patnaik, and C. Airoldi, ***Sep. Sci. Techno*****l., 2009, 44, 2096–2116**.

6 Y.D. Wirtu, F. Melak, M. Yitbarek and H. Astatkie, ***Groundwater Sustain. Dev*****., 2021, 12, 100525.**