Supplementary information

Harnessing Waste PET Bottles for Sustainable Ca-MOF Synthesis: A High-Efficiency Adsorbent for Uranium and Thorium

Manish Sharma[a], Anshika[b], Priya Sharma[b], Vikash Chandra Janu[c], Ragini Gupta[,a, b]*

[a]Materials Research Centre, Malaviya National Institute of Technology Jaipur, Jaipur 302017, India

[b]Department of Chemistry, Malaviya National Institute of Technology Jaipur, Jaipur 302017, India

[c]Defence Research and Development Organization Jodhpur, Jodhpur 342011, India

**rgupta.chy@mnit.ac.in*

Contents

Fig. S1. FTIR spectra of (a) BDC synthesised from plastic and (b) calcium waste.

Fig. S2. Pore size distribution of waste derived Ca-MOF.

Fig. S3. FESEM images of (a) chemically derived Ca-MOF and (b) waste-derived Ca-MOF.

Fig. S4. TGA of waste derived Ca-MOF.

Fig. S5. Effect of pH on the adsorption of U(VI) and Th(IV) ions using waste derived Ca-MOF.

Fig. S6. Comparison of removal efficiencies of U(VI) and Th(IV) ions using waste derived Ca-MOF and chemically derived Ca-MOF.

Fig. S7. Predicted *vs* actual diagram obtained from the ANOVA analysis for U(VI).

Fig. S8. Predicted *vs* actual diagram obtained from the ANOVA analysis for Th(IV).

Table S1 Experimental ranges and levels of independent variables

Table S2 Analysis of variance (ANOVA) for the removal of U(VI) ions optimization using waste Ca-MOF

Table S3 Analysis of variance (ANOVA) for the removal of Th(IV) ions optimization using waste Ca-MOF

Supplementary information

Text S1: Here, "calcium waste" refers to calcium derived from the marble industry (Kishangarh marble dumping yard), which primarily consists of calcium carbonate ($CaCO_3$). Calcium carbonate is an ionic species that does not have any specific type of chemical structure. Basically, the thermodynamically stable form of $CaCO_3$ under normal conditions is hexagonal β- $CaCO_3$ (the mineral calcite). But other forms are also found, like orthorhombic λ- $CaCO_3$ (the mineral aragonite) and hexagonal μ- $CaCO_3$, occurring as the mineral vaterite.

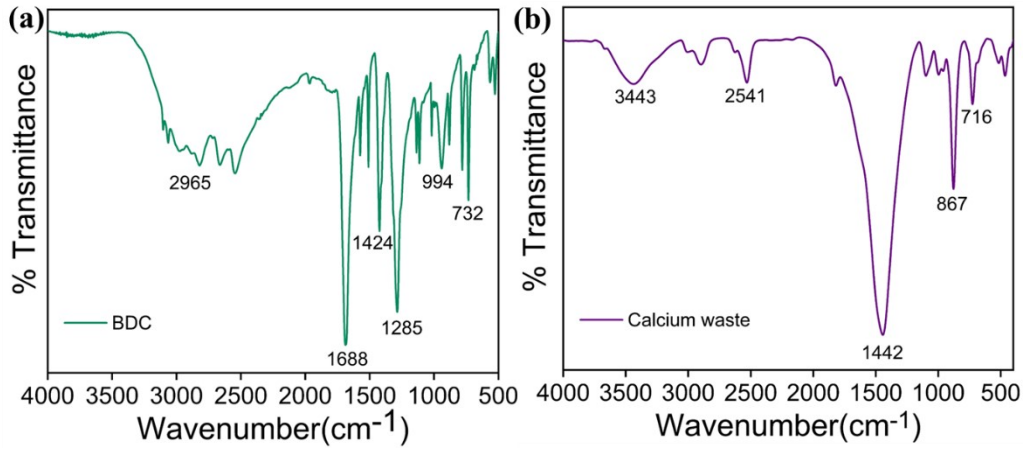

Fig. S1. FTIR spectra of (a) BDC synthesised from plastic and (b) calcium waste.

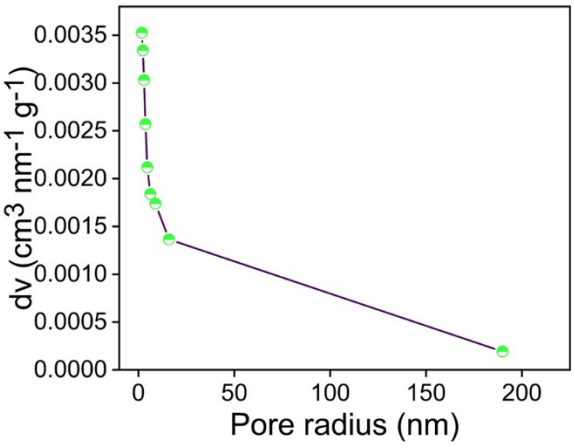

Fig. S2. Pore size distribution of waste derived Ca-MOF.

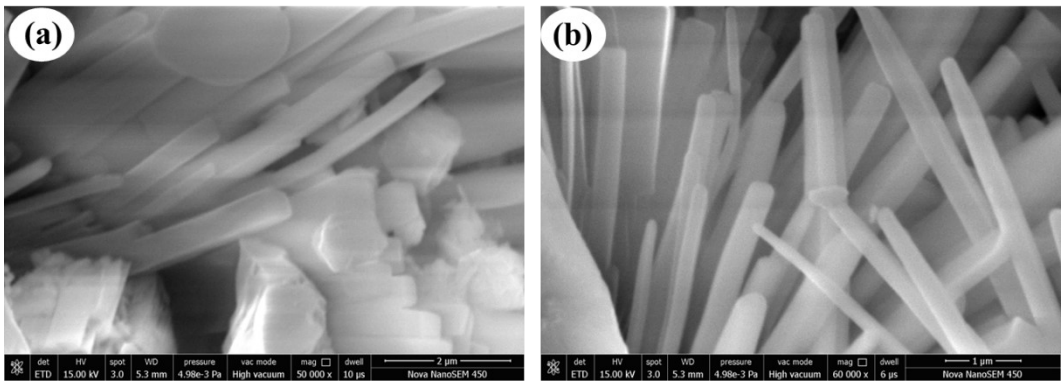

Fig. S3. FESEM images of (a) chemically derived Ca-MOF and (b) waste-derived Ca-MOF.

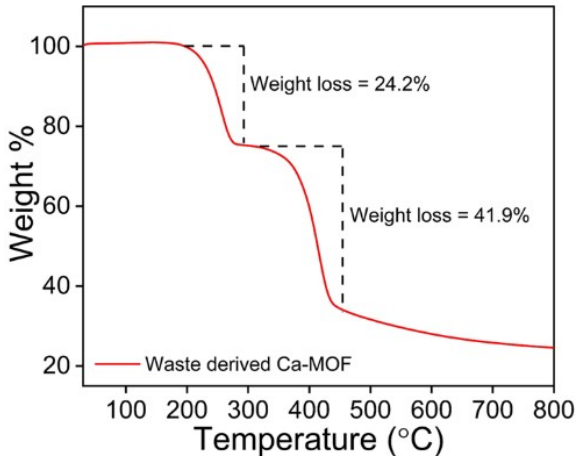

Fig. S4. TGA of waste derived Ca-MOF.

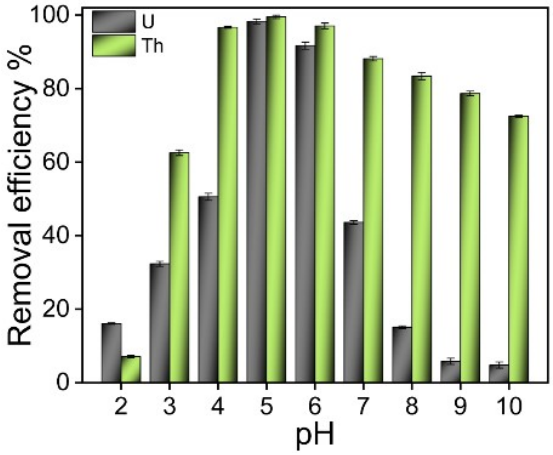

Fig. S5. Effect of pH on the adsorption of U(VI) and Th(IV) ions using waste derived Ca-MOF.

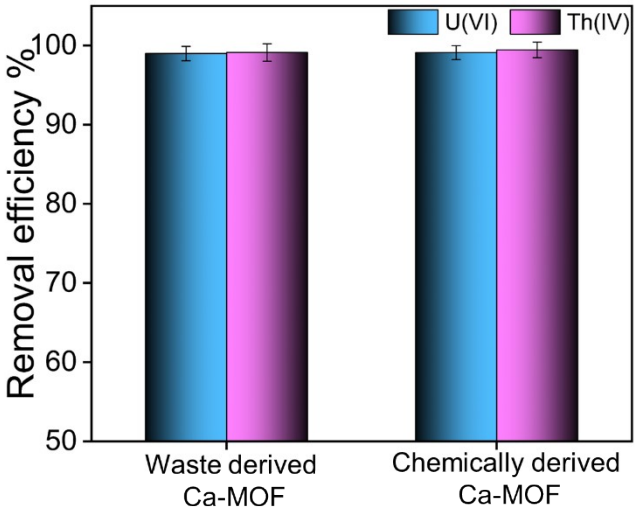

Fig. S6. Comparison of removal efficiencies of U(VI) and Th(IV) ions using waste derived Ca-MOF and chemically derived Ca-MOF.

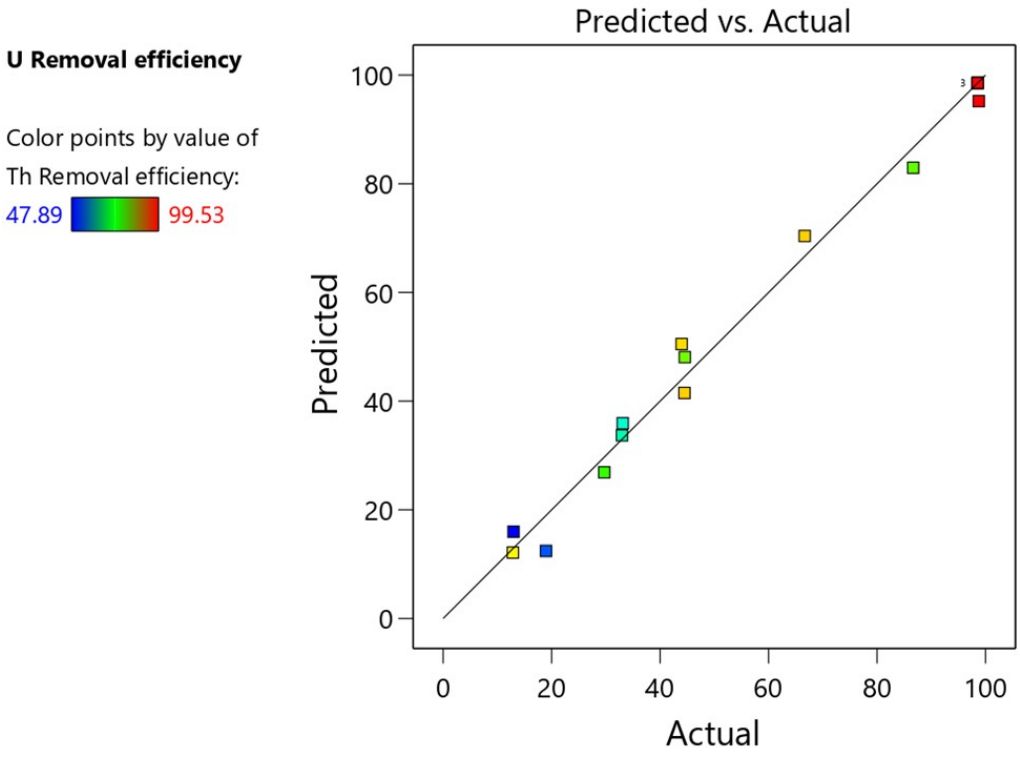

Fig. S7. Predicted *vs* actual diagram obtained from the ANOVA analysis for U(VI).

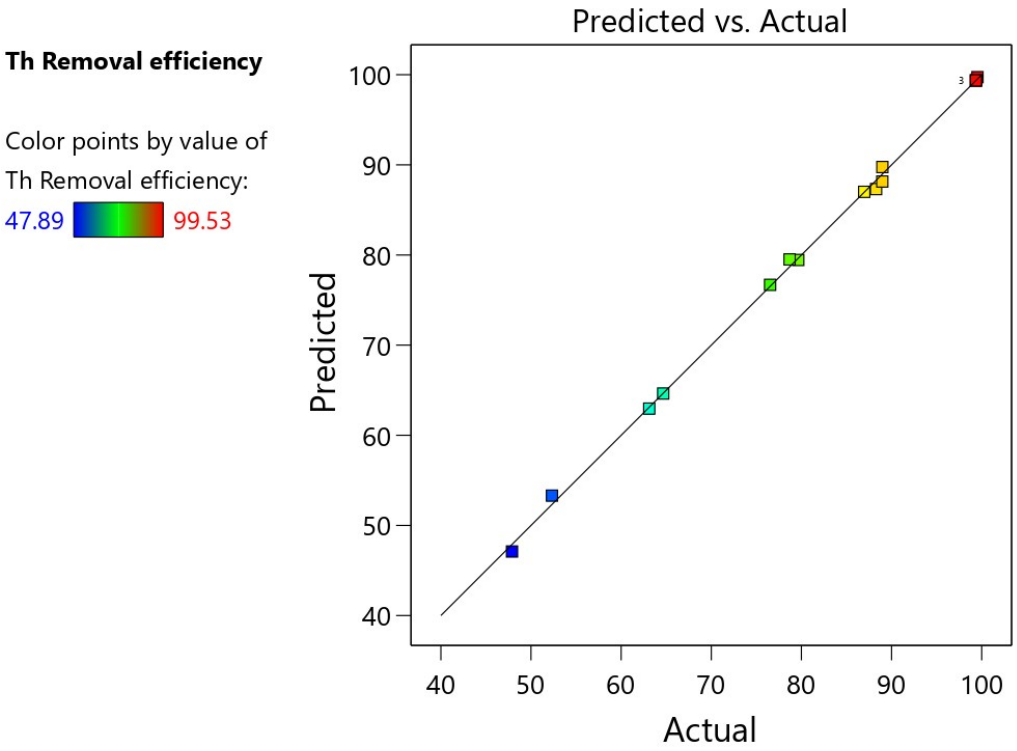

Fig. S8. Predicted *vs* actual diagram obtained from the ANOVA analysis for Th(IV).

Table S1 Experimental ranges and levels of independent variables

S. No.	Variables	Factors range and levels		
		-1	0	1
1.	Mas (mg)	2	6	10
2.	pH	3	5	7
3.	Time (min)	5	15	25

Table S2 Analysis of variance (ANOVA) for the removal of U(VI) ions optimization using waste Ca-MOF

Source	Sum of Squares	df	Mean Square	F-value	P-value	
Model	15355.80	9	1706.20	49.30	0.0002	significant
A-pH	136.13	1	136.13	3.93	0.1042	
B-Time	597.54	1	597.54	17.26	0.0089	
C-Mass	1779.66	1	1779.66	51.42	0.0008	
AB	7.13	1	7.13	0.2060	0.6690	
AC	73.10	1	73.10	2.11	0.2059	
BC	25.10	1	25.10	0.7252	0.4333	
A^2	12303.42	1	12303.42	355.48	< 0.0001	
B^2	427.49	1	427.49	12.35	0.0170	
C^2	686.45	1	686.45	19.83	0.0067	
Residual	173.05	5	34.61			
Lack of Fit	173.05	3	57.68			
Pure Error	1.78	2	0.86			
Cor Total	15528.86	14				
R^2	0.9889					
Adjusted R^2	0.9688					
Predicted R^2	0.8217					
Adeq Precision	17.9920					

Table S3 Analysis of variance (ANOVA) for the removal of Th(IV) ions optimization using waste Ca-MOF

Source	**Sum of Squares**	**df**	**Mean Square**	**F-value**	**P-value**	
Model	4098.76	9	455.42	495.40	< 0.0001	significant
A-pH	1589.35	1	1589.35	1728.89	< 0.0001	
B-Time	418.18	1	418.18	454.90	< 0.0001	
C-Mass	67.63	1	67.63	73.57	0.0004	
AB	1.93	1	1.93	2.10	0.2068	
AC	30.36	1	30.36	33.03	0.0022	
BC	33.18	1	33.18	36.09	0.0018	
A^2	1777.75	1	1777.75	1933.83	< 0.0001	
B^2	254.21	1	254.21	276.53	< 0.0001	
C^2	70.27	1	70.27	76.44	0.0003	
Residual	4.60	5	0.9193			
Lack of Fit	4.60	3	1.53			
Pure Error	1.56	2	0.56			
Cor Total	4103.35	14				
R^2	0.9989					
Adjusted R^2	0.9969					
Predicted R^2	0.9821					
Adeq Precision	67.2124					