Supplementary Information (SI) for New Journal of Chemistry.

Extending the Potential of MOF-derived $LaFeO_3$@C: A Sustainable Solution for Hexavalent Chromium Contamination

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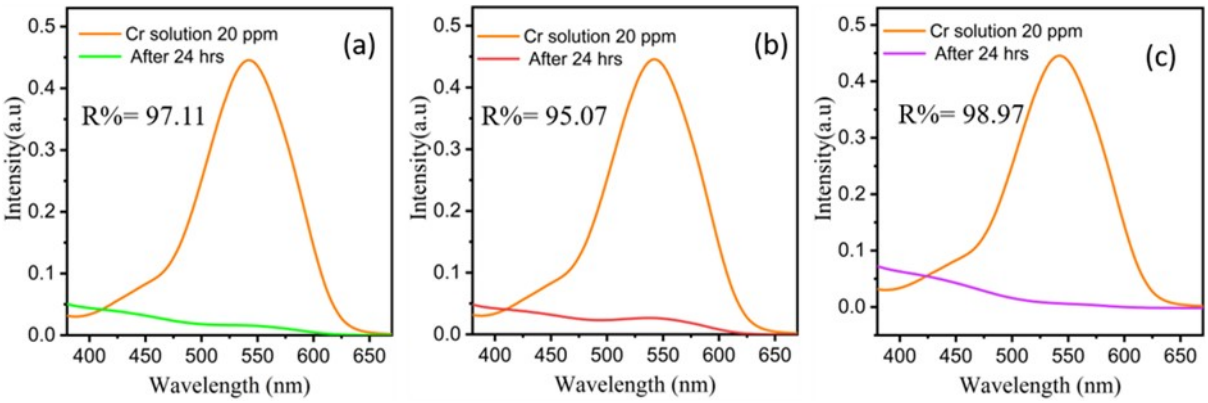


Figure S1. UV-Vis. absorption spectra representing the Cr (VI) removal by LaFeO3@C-700 when repeated the experiment under same conditions showing reproducibility.

Table S1. Thermodynamic parameters obtained from Vant Hoff's Plot

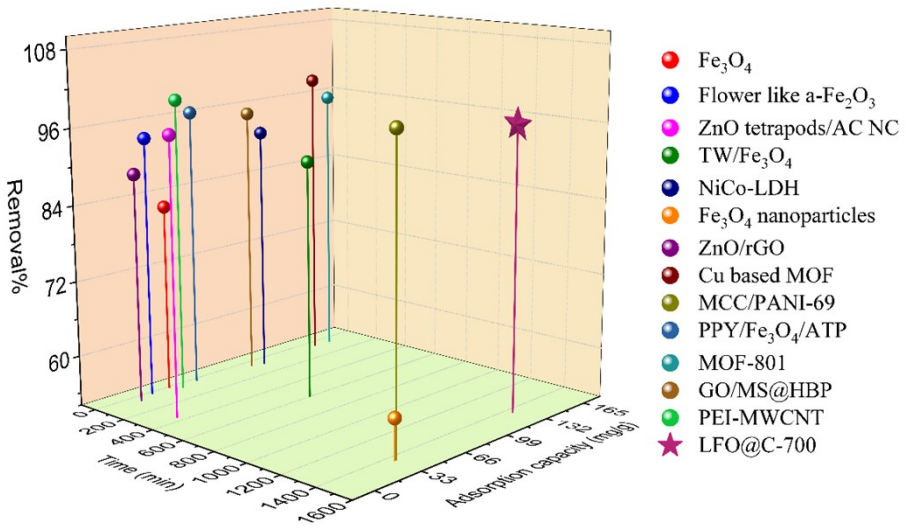
T(K)	**ΔG** (kJ/mol)	**ΔH** (kJ/mol)	**ΔS** (J/mol.K)	**R^2**
293	-6.886	50.97	197.27	0.9930
306	-9.193			
323	-12.795			

Table S2. Pseudo-first-order, pseudo-second-order, and intraparticle diffusion model parameters for Cr (VI) adsorption on LFO@C-700.

Adsorbate	**$Q_{e,exp}$ (mg/g)**	**Pseudo-first-order**			**Pseudo-second-order**		
		Q_e (mg/g)	K_1 (h^{-1})	R^2	Q_e (mg/g)	K_2 (h^{-1})	R^2
Cr (VI)	32.28	10.21	0.1839	0.7796	31.68	0.1181	0.9993
Intra-Particle diffusion model parameter							
Cr (VI)	Kd1	Kd2	Kd3	C1	C2	C3	R_1^2	R_2^2	R_3^2
	32.181	1.0695	2.7416	4.5927	26.481	22.883	0.6441	0.9591	0.9167

Table S3. The linear fitting parameters obtained from the Langmuir and the Freundlich adsorption models.

Adsorption Isotherm parameters						
Adsorbate	Langmuir constant			Freundlich constant		
	Q_{max}(mg/g)	K_L(L/mg)	R^2	K_F(L/mg)	n	R^2
Cr (VI)	127.71	0.1706	0.9859	28.09	2.753	0.9397



Fe_3O_4 [1]; α-Fe_3O_4[2]; ZnO tetrapods/AC NC [3];TW/Fe_3O_4[4]; NiCo-LDH[5]; ZnO/rGO[6]; Cu-based MOF[7]; MCC/PANI-69wt%[8]; GO/MS@HBP[9]; PEI-MWCNT[10]

Figure S2. Comparison of Cr (VI) adsorption efficiency of LFO@C-700 with recently reported materials.

Table S4. Comparison of different detoxification methods for Cr(VI) removal reported in literatures.

Sl No.	Materials	Removal Mechanism	Time	Removal (%)	Qe (mg/g)	Ref
1	MXene@MIL-53-NH_2	Adsorption and Reduction	20 h	91.0	224.46	[11]
2	Cu@MIL-53(Fe)	Adsorption and Reduction	180 min	99.05	726.4	[12]
4	CdS@MOF@C_3N_4	Photocatalysis	100 min	86.7	-	[13]
	MIL-53(Fe)/WO_3	Photocatalysis	240 min	94.0	-	[14]
5	Ni@C/NiFeOx	Electrochemical Reduction	80 min	96.6	-	[15]
6	nZVI-MOF-74(Co)-PDA@PVDF	Membrane Process	-	-	83.12	[16]
7	Cs-2@ZIF-8	Ion Exchange	300 min	90.23	61.05	[17]
9	Fe_3O_4/CS/PPy	Adsorption	720 min	100.0	193.23	[18]
8	Silver-triazolate MOF	Anion Exchange	240 min	-	38.6	[19]
10	$LaFeO_3$@C-700	Adsorption and reduction	24 h	97.0	127.71	This work

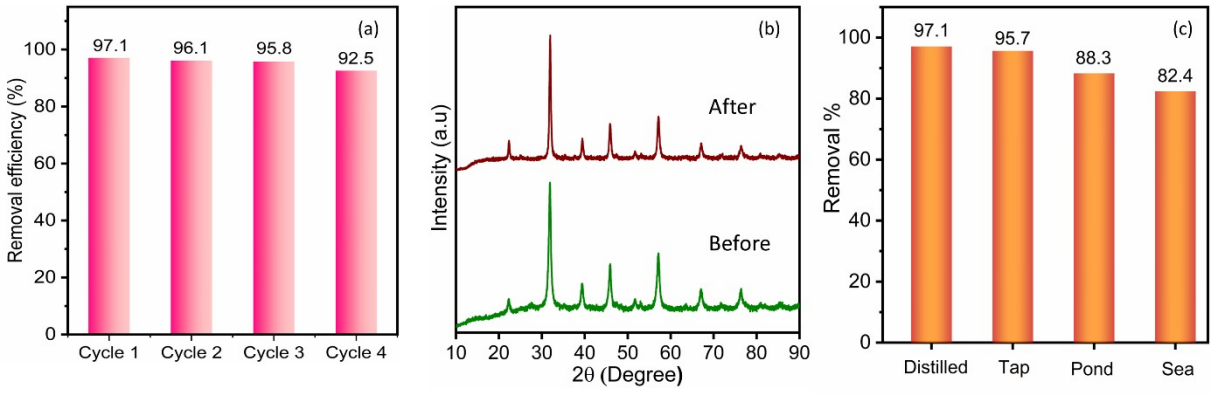


Figure S3. (a) Recyclability study of LFO@C-700 for Cr (VI) adsorption, (b) chemical stability, and (c) environmental application of LFO@C-700.

Table S5. The binding energy positions and atomic percentage of elemental states LFO@C-700 before and after adsorption.

Elements		LFO@C-700 (Before adsorption)		Ref.	LFO@C-700 (After adsorption)		Ref.
		BE (eV)	Atomic %		BE (eV)	Atomic %	
La	La $3d_{3/2}$	835.0	32.60		-	-	
	satellite	838.8	23.26		-	-	
	plasmon	847.2	5.09		-	-	
	La $3d_{3/2}$	851.7	24.93		-	-	
	satellite	855.5	14.12		-	-	
Fe	Fe $2p_{3/2}$	710.5	31.40		710.5	41.72	
	Fe $2p_{3/2}$	712.3	27.04		712.3	14.35	
	satellite	718.7	12.47		718.4	12.05	
	Fe $2p_{1/2}$	724.2	23.00	[20]	724.2	24.97	This work
	Fe $2p_{1/2}$	726.3	6.10		726.4	6.91	
O	O_L	528.9	24.22		528.8	20.85	
	O_V	530.3	31.56		530.2	38.43	
	$O_{OH/ads}$	531.8	31.85		531.8	28.51	
	O_{H2O}	533.1	12.36		533.1	12.21	
C	C-C/C=C	284.8	31.87		284.8	37.61	
	C-O-C	286.2	46.41		286.4	42.58	
	O-C=O	289.7	21.72		288.4	19.81	
Cr	Cr $2p_{3/2}$	-	-		576.8	63.39	
	Cr $2p_{1/2}$	-	-		586.4	36.61	

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