

Supplementary information

3D rhombohedral nanocrystals decorated with Graphene oxide for the effective removal of Hexavalent Chromium: Adsorption and DFT Investigations

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Supplementary Table 1. The physical measurements were determined from simulation and examined in comparison with PXRD data of the UiO-66-NDC system

Method	a(Å)
DFT Simulation (PBE)	20.7386
Experiment	20.7462

Supplementary Table 2. GO/UiO-66-NDC nanocomposite adsorption isotherms for Cr(VI)

Nanocomposite GO/UiO-66-NDC adsorption model for Cr(VI)					
Langmuir Isotherm					
Intercept	Slope	q _{max} (mg/g)	K _L	R _L	R ²
0.00636	0.14757	157.23	0.04	0.32	0.999
Freundlich Isotherm					
Intercept	Slope	1/n	K _f	R ²	
0.88526	0.7805	0.7805	7.67821	0.995	
Temkin Isotherm					
Intercept	Slope	B _T	K _T	R ²	
-12.085	26.7321	26.7321	0.636306	0.97456	

Supplementary Table 3. Thermodynamic behavior of Cr(VI) adsorption GO/UiO-66-NDC nanocomposite

Temperature (K)	K_L	ΔG (KJ/mol)	ΔH (KJ/mol)	ΔS	R^2
298.15	6.18328	-4.51603	2.07979	22.18233	0.9837
303.15	6.333	-4.65207			
313.15	6.4033	-4.75708			
318.15	6.474576	-4.86309			