

5 *Electronic supplementary information for*

Cyclodextrin functionalized magnetic iron oxide nanocrystals: a host-carrier for magnetic separation of non-polar molecules and arsenic from aqueous media

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Supplementary information

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S1. Infrared spectral assignments of CMCD and CMCD-Fe₃O₄ nanocrystals.

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Table S1. Infrared spectral assignments of CMCD and CMCD-Fe₃O₄ nanocrystals.

Infrared (cm ⁻¹)		
CMCD	CMCD-Fe ₃ O ₄	Assignment
759	757	Internal rotation modes about CH ₂ OH (side)
948	947	C-C stretch
1158	1156	Hydroxyl C-O stretch
1206,1243,1330	1205,1245,1325	C-O-H bending (coupled modes)
1420	1411	Symmetric C-O stretching of COO ⁻ group
1457	1457	O-C-H
1605	1595	asymmetric C-O stretching of COO ⁻ group
2929	2927	C-H stretch

Table S2. Summary of the Rietveld refinement results for CMCD-Fe₃O₄ nanocrystals.

	Phase 1	Phase 2
	Fe ₃ O ₄ (magnetite)	FeO (wustite)
Space group	F d -3 m	F m -3 m
Lattice parameters	a = 8.3667 Å	a = 4.1965 Å
Preferred Orientation	Nil	3.9478 along (220) plane
Weight Percentage	97.9%	2.1%
Statistical indices, χ^2	1.51	

Table S3. Atomic positions of the CMCD-Fe₃O₄ nanocrystals as obtained from a Rietveld analysis of the X-ray diffraction pattern.

Magnetite	Atom	Oxidation state	x	y	z	site	occupancy
	Fe	+3	0.12500	0.12500	0.12500	8a	1.00000
	Fe	+2	0.50000	0.50000	0.50000	16d	1.00000
	O	-2	0.24726	0.24726	0.24726	32e	1.00000
Wustite	Atom	Oxidation state	x	y	z	site	occupancy
	Fe	+2	0.12500	0.12500	0.12500	4a	1.00000
	O	-2	0.50000	0.50000	0.50000	4a	1.00000

Figure S4. Arsenic (III) adsorption capacity of CMCD-Fe₃O₄ for differing equilibration times.

The effect of equilibration time on the adsorption of arsenic on CMCD-Fe₃O₄ was studied at the maximum adsorption capacity of CMCD-Fe₃O₄ nanocrystals, corresponding to the last data point in the adsorption isotherm shown in Figure 5b.

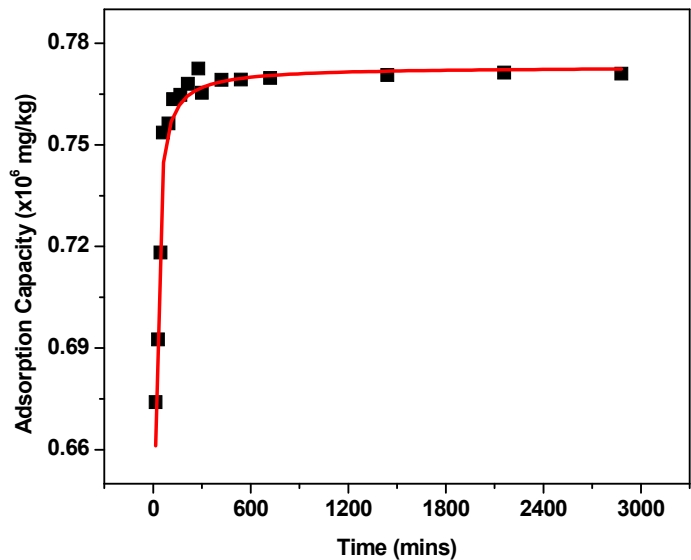


Figure S5. Arsenic (III) adsorption capacity of CMCD-Fe₃O₄ in the presence of different anions.

The effect of interfering anions on the adsorption of arsenic was studied at the maximum adsorption capacity of the CMCD-Fe₃O₄ nanocrystals, corresponding to the last data point in the adsorption isotherm shown in Figure 5b. The anions concentration in the solution was maintained at 0.01M.

