Electronic Supplementary Material (ESI) for Environmental Science: Nano.

Supporting Information

Platform Selection of Engineered Nanomaterials for Water Decontamination Applications

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Search terms for Figure 1:

NM:

(TITLE-ABS-KEY (nanomaterial OR nano AND material OR nanoparticle OR nano AND particle) AND TITLE-ABS-KEY (water AND remediation OR decontamination OR water AND treatment OR water OR decontamination))

NM@S:

(TITLE-ABS-KEY(nanomaterial OR nano material OR nanoparticle OR nano particle) AND TITLE-ABS-KEY(Water Remediation OR decontamination OR water treatment OR water OR decontamination)AND TITLE-ABS-KEY(embedded OR infused OR incorporated OR affixed OR impregnated OR immobilized OR modified OR functionalized))

Table S1. Literature used for evaluation of the efficiency criterion for selected supports for metal oxide nanoadsorbents. The table summarizes the calculations and assumptions taken into account when adsorption performance of the supported nanomaterial (NM@S) was normalized to the performance of the nanomaterial in suspended form (NM).

Article	Platform group	Nanoadsorbent (NM)	Adsorbate	Nanoadsorbent performance (NM)	Nanoadsorbent performance on substrate (NM@S)	NM@S/NM	Assumptions
O. Thirunavukkarasu, Arsenic removal from drinking water using iron oxide-coated sand, 2003, Water, Air, and Soil Pollution[1]	Natural media Bead - Sand	α-FeOOH	As (III)	23 mg/g FeOOH [2]	41.1ug/gNM@S/45mgFe/gNM@S*65Fe/100FeO(OH)=0.59mgAs/g FeOOH	0.026	Iron oxide content 45 mg/g (4.5%) pH 7.6 phase: combination of goethite and hematite
			As(V)	1.14 mg/g FeOOH [3]	42.6ug/gNM@S/45mgFe/gNM@S*65Fe/100FeO(OH)=0.615mgAs/gFeOOH	0.539	
S.Lee, Iron oxide nano-particles-immobilized-sand material in the treatment of Cu(II), Cd(II) and Pb(II) contaminated waste waters, 2012, Chemical Engineering Journal[4]	Natural media Bead - Sand	Iron oxide	Cd(II)	7.4 mg/g Iron oxide [5]	0.5282/5.7*0.65*1000=60.23 mg/g Iron oxide	8.139	pH 4 and not 5 as in the NM@S paper
			Pb(II)	22.83 mg/g Iron oxide [5]	2.0877/5.7*0.65*1000=238.07 mg/g Iron oxide	10.43	
S. Kundu, Adsorptive removal of As(III) from aqueous solution using iron oxide coated cement (IOCC): Evaluation of kinetic, equilibrium and thermodynamic models Sanghamitra, 2006, Separation and Purification Technology[6]	Natural media - Cement	Fe_3O_4	As(III)	2.63 mg/g Fe_3O_4 [3]	0.69*0.2353=0.16 mg/g Fe_3O_4	0.061	
		Fe_3O_4	As(V)	2.63 mg/g Fe_3O_4 [3]	3.86*0.025*231/55.8=0.4 mg/g Fe_3O_4	0.152	
A. Yurum, Fast deposition of porous iron oxide on activated carbon by microwave heating and arsenic (V) removal from water, 2014, Chemical Engineering Journal[7]	Granular activated carbon	α-Fe_2O_3	As(V)	0.827 mg/g Fe_2O_3 [8]	136.37 mg/g Fe_2O_3	164.897	Took the oxidized activated carbon. WT%(Fe)=20.37% <u>Assumption</u>: Same pH range (pH=6.27 for N_{ads}-S, pH=7 for N_{ads})
A.M. Cooper, The effect of carbon type on arsenic and trichloroethylene removal capabilities of iron (hydr)oxide nanoparticle-impregnated granulated activated carbons, 2010, Journal of Hazardous Materials[9]	Granular activated carbon	δ -FeOOH	As(V)	7 mg/g δ-FeOOH [10]	45.1 mg/g FeOOH	6.443	Assumption: The same N_{ads} phase in both articles The same condition used to measure the adsorption capacity.

K. Hristovski, Effect of synthesis conditions on nano-iron (hydr)oxide impregnated granulated activated carbon, 2009, Chemical Engineering Journal[11]	Granular activated carbon	Amorphous FeOOH	As(V)	7 mg/g Amorphous FeOOH [12]	21.7 mg/g Amorphous FeOOH	3.100	Assumption: Adsorption capacity: the average amount of adsorption capacity (15.2-28.2 mg/g amorphous FeOOH)
M. Jain, Development of iron oxide/activated carbon nanoparticle composite for the removal of Cr(VI), Cu(II) and Cd(II) ions from aqueous solution,2018, Water Resources and Industry[13]	Activated carbon	Fe_3O_4 magnetite	Cr(IV)	5.5 mg/g Fe_3O_4	8.06/0.184*0.72 =31.54 mg/g Fe_3O_4	5.727	Phase: magnetite
			Cu(II)	2.7 mg/g Fe_3O_4	3.2/0.184*0.72=12.52 mg/g Fe_3O_4	4.637	
			Cd(II)	0.09 mg/g Fe_3O_4	2.15/0.184*0.72=8.41 mg/g Fe_3O_4	93.444	
D.Mohan, Cadmium and lead remediation using magnetic oak wood and oak bark fast pyrolysis bio-chars,2014, Chemical Engineering Journal [14]	Carbon biochar	Fe_3O_4 magnetite	Cd(II)	0.09 mg/g Fe_3O_4 [13]	7.4/0.513*0.72=10.39 mg/g Fe_3O_4	115.444	pH=5
			Cd(II)	0.09 mg/g Fe_3O_4 [13]	2.87/0.806*0.72=2.56 mg/g Fe_3O_4	28.444	
			Pb(II)	22.89 mg/g Fe_3O_4 [15]	30.2/0.513*0.72=42.39 mg/g Fe_3O_4	1.852	
			Pb(II)	0.1105mmol/g*207.2= 22.89 mg/g Fe_3O_4 [15]	10.13/0.806*0.72=9.05 mg/g Fe_3O_4	0.395	
S.M, Miller, Novel, bio-based, photoactive arsenic sorbent: TiO_2-impregnated chitosan bead, 2010, Water Research P.A. Nishad, Enhancing the antimony sorption properties of nano titania -chitosan beads using epichlorohydrin as the crosslinker, 2017, Journal of Hazardous Materials[16]	Chitosan beads	TiO_2	As(III)	3 mg/g TIO_2	2.099/0.298 =7.04 mg/g TiO_2	2.347	Data for NM is taken from fig. 4 in article, so we assume the experiment conditions are the same as for the NM@S. In article mentioned that TiO_2 mass is 29.8%. Assumption: pH is similar (pH-3.3 for N_{ads} and pH=4.3 for NM@S). Same NM used.[17] The ration between N_{ads} to S is given (1:5)
			As (V)	5.5 mg/g TIO_2	2.050/0.298 = 6.88 mg/g TiO_2	1.251	
P.A. Nishad, Nano-titania-crosslinked chitosan composite as a superior sorbent for antimony (III) and (V), 2014, Carbohydrate	Chitosan beads	TiO_2	Sb(III)	173.2 μmol/g TiO_2	170.3 6 = 1021.8 μmol/g TiO_2	5.9	pH=6.9 NM to S ration is 1:5
			Sv(III)	187.7 μmol/g TiO_2	1089 μmol/g TiO_2	5.802	pH=3.06

Polymers[17]			Sb(V)	799.1 µmol/g TiO_2	1215 µmol/g TiO_2	1.519	pH=3.33
J. Yamani, Enhanced arsenic removal using mixed metal oxide impregnated chitosan beads, 2012, Water Research[18]	Chitosan beads	Al_2O_3	As(V)	12 mg/g Al_2O_3	8.4 mg/g Al_2O_3	0.7	
A. I. Zouboulis, Arsenic Removal Using Iron Oxide Loaded Alginate Beads, 2002, Industrial and Engineering Chemistry Research[19]	Alginate beads	Hydrous FeO(OH)	As(V)	9 mg As / g-Fe [20]	5.79 mg As / g-Fe	0.643	Assumption: Same N_{ads} phase and experiment conditions.
J. Min, Removal of Selenite and Chromate Using Iron(III)-Doped Alginate Gels, 1999, Water Environment Research[21]	Alginate gel beads	Iron oxyhydroxide $Fe(OH)_3$	Se(IV)	2.4 mg / g-Fe [22]	0.15 g Se(IV) / g-Fe	0.062	
W. Biftu, Synthesis of nanoZrO_2 via simple new green routes and its effective application as adsorbent in phosphate remediation of water with or without immobilization in Al-alginate beads,2020, Water Science & Technology [23]	Al-alginate beads	$nZrO_2$	PO_4^{3-}	126.2 mg/g - $nZrO_2$	173.0 mg/g $nZrO_2$-Al-alginate = 24.22 mg/g $nZrO_2$	0.192	1.5 g of nano ZrO2 was added => 1.5/173= 86 => 86% Al-alginate beads and 14% NM
R. Pineda, Removal of Arsenic from Aqueous Solutions with Alginate Based-Magnetic Nanocomposites, 2009, Clean Technology [24]	Alginate	Magnetite (Fe_3O_4)	As(V)	11-17 mg/g Fe_3O_4 [25,26]	1.1 mg/g	0.418	Assumption: Same N_{ads} phase and experiment conditions. For NM@S/NM calculation we took the NM average
			As(III)	20-22 mg/g Fe_3O_4 [25,26]	1.04 mg/g	0.495	Assumption: Same N_{ads} phase and experiment conditions. For NM@S/NM calculation we took the NM average
J. Elton, Titanium Dioxide-Based Hybrid Ion-Exchange Media for Simultaneous Removal of Arsenic and Nitrate, 2013, Novel Solutions to Water Pollution[27]	Ion-Exchange beads	TiO_2	As	7 mg/g TiO_2 [28]	— 9.95 mg/g TiO_2	1.421	MW(Ti)=47.8 g/mol MW(TiO_2)=79.8 g/mol Assumption: Same N_{ads} phase and experiment conditions.

					— 14.92 mg/g TiO_2	2.131	MW(Ti)=47.8 g/mol MW(TiO_2)=79.8 g/mol Assumption: Same N_{ads} phase and experiment conditions.
					— 16.36 mg/g TiO_2	2.336	MW(Ti)=47.8 g/mol MW(TiO_2)=79.8 g/mol Assumption: Same N_{ads} phase and experiment conditions.
M. Gifford, Ranking traditional and nano-enabled sorbents for simultaneous removal of arsenic and chromium from simulated groundwater, 2017, Science of the Total Environment[29]	Ion-Exchange beads	TiO_2	As	107.5 μmol/g TiO_2	12.4/0.16 □mol/g = 77.5 □mol/g TiO_2	0.721	From J. Elton et al. assuming mass of synthesized TiO_2@S is 11-21% (16% avg)[27]. From K. Hristovski el al. assuming that mass of amorphous iron (hydro)oxide synthesized is 16% of Fe[30]. Mw(Fe) = 55.8 g/mol Mw($Fe(OH)_2$) = 89.8 g/mol
			Cr	5.7 μmol/g $Fe(OH)_2$	— — $Fe(OH)_2$	8.246	
		amorphous $Fe(OH)_2$	As	172.1 μmol/g $Fe(OH)_2$	— — $Fe(OH)_2$	0.341	From J. Elton et al. assuming mass of synthesized TiO_2@S is 11-21% (16% avg)[27]. From K. Hristovski el al. assuming that mass of amorphous iron (hydro)oxide synthesized is 16% of Fe[30]. Mw(Fe) = 55.8 g/mol Mw($Fe(OH)_2$) = 89.8 g/mol From K. Hristovski el al. assuming that mass

							of amorphous iron (hydro)oxide synthesized is 16% of Fe[30]. Mw(Fe) = 55.8 g/mol Mw($Fe(OH)_2$) = 89.8 g/mol
J. Wang, Hydrous ferric oxide–resin nanocomposites of tunable structure for arsenite removal: Effect of the host pore structure, 2011, Journal of Hazardous Materials[31]	Ion-Exchange beads	Amorphous $Fe(OH)_2$	As(III)	28.0 mg/g $Fe(OH)_2$ [16]	225*0.65=146.25 mg/g $Fe(OH)_2$	4.223	
					200*0.65=130 mg/g $Fe(OH)_2$	4.643	
					190*0.65=123.5 mg/g $Fe(OH)_2$	4.411	
					200*0.65=130 mg/g $Fe(OH)_2$	4.643	
					175*0.65=113.75 mg/g $Fe(OH)_2$	4.063	
Q. Su, Fabrication of polymer-supported nanosized hydrous manganese dioxide (HMO) for enhanced lead removal from waters, 2009, Science of the Total Environment[32]	Ion-Exchange beads	$Mn(OH)_2$	Pb(II)	352.55 mg/g $Mn(OH)_2$	395 mg/g /(7.33%Mn*55/89Mn in MN(OH)2)= 3381.85 mg/g $Mn(OH)_2$	9.592	
L. Zhang, Removal of phosphate from water by activated carbon fiber loaded with lanthanum oxide, 2011, Journal of Hazardous Materials[33]	Carbon fibers	LaO	PO_4^{3-}	46.95 mg/g LaO [34]	5.85/0.1178 = 49.66 mg/g LaO	1.058	WT%(LaO)=11.78% Assumption: Same LaO phase and experiment condition
J. Zhang, Synthesis of magnetic iron oxide nanoparticles onto fluorinated carbon fabrics for contaminant removal and oil-water separation, 2017, Separation and Purification Technology[35]	Carbon fibers	Fe_3O_4	Cu(II)	8.9 mg/g Fe_3O_4 [36]	62.5 mg/g Fe_3O_4	7.022	pH=5
Q. Zhou, Phosphorus removal from wastewater using nano-particulates of hydrated ferric oxide doped activated carbon fiber prepared by Sol–Gel method, 2012, Chemical Engineering Journal journal[37]	Carbon fibers	FeOOH	P	139.5 mg/g FeOOH [38]	12.86/0.44=29.227 mg/g FeOOH	0.21	From fig2 WT% (FeOOH)=44 12.86 mg/g-NM@S 12.86/0.44 = 29.227 mg/g FeOOH pH range of 2.0–6.0 assume: amorphous phase, FeOOH adsorption capacity:

							134-145 mg/g [38], we took the average
Y. Zheng, Adsorptive removal of arsenic from aqueous solution by a PVDF/zirconia blend flat sheet membrane, 2011, Journal of Membrane Science[39]	Carbon fibers	$Zr(OH)_4$	As	38.9 mg/g $Zr(OH)_4$	43 mg/g mg/g $Zr(OH)_4$	1.105	
K.E. Greenstein, Performance comparison of hematite (□-Fe_2O_3)-polymer composite and core-shell nanofibers as point-of-use filtration platforms for metal sequestration, 2019, Water Research[40]	Polymeric fibers	α-Fe_2O_3	As(V)	17 mg/g α-Fe_2O_3	9.3 mg/g α-Fe_2O_3	0.547	
			Cu(II)	70 mg/g α-Fe_2O_3	35 mg/g α-Fe_2O_3	0.5	
			Cr(VI)	9.5 mg/g α-Fe_2O_3	7.3 mg/g α-Fe_2O_3	0.768	
			Pb(II)	94 mg/g α-Fe_2O_3	57 mg/g α-Fe_2O_3	0.606	
K.T. Peter, Functionalized polymer-iron oxide hybrid nanofibers: Electrospun filtration devices for metal oxyanion removal, 2017, Water Research [41]	Polymeric fibers (polyacrylonitrile, PAN)	Ferrihydrite iron oxide	Cr	19 mg-Cr/g-Fh	17 mg-Cr/g-Fh	0.89	
			As	31 mg-As/g-Fh	26 mg-As/g-Fh	0.84	
K.T. Peter , Surfactant-assisted fabrication of porous polymeric nanofibers with surface-enriched iron oxide nanoparticles: composite filtration materials for removal of metal cations, 2018, Environmental Science[42]	Polymeric fibers (PAN)	Amorphous Fe_2O_3	Pb	13 mg-Pb/g-Fe_2O_3	27 mg-Pb/g-Fe_2O_3	2.08	
			Cu	75 mg-Cu/g-Fe_2O_3	25 mg-Cu/g-Fe_2O_3	0.33	
			Cd	105 mg-Cd/g-Fe_2O_3	100 mg-Cd/g-Fe_2O_3	0.95	
	Polymeric fibers (PAN-based)	Amorphous Fe_2O_3	Pb	13 mg-Pb/g-Fe_2O_3	101 mg-Pb/g-Fe_2O_3	7.77	
			Cu	75 mg-Cu/g-Fe_2O_3	170 mg-Cu/g-Fe_2O_3	2.27	
			Cd	105 mg-Cd/g-Fe_2O_3	57 mg-Cd/g-Fe_2O_3	0.54	
X.Zhang, Preparation, performance and adsorption activity of TiO_2 nanoparticles entrapped PVDF hybrid membranes, 2012, Applied Surface Science [43]	PVDF membrane	TiO_2	Cu(II)	6.86 mg/g TiO_2 [44]	86 ug/cm^2 / (1.087*1.78)g/cm^3 density of pVDF and added weiget by TiO2 / 0.1 cm thick mem / 8.76% TIO2 = 0.5 mg/g TiO2	0.073	8.74% loaded TiO_2 20mm×20mm membrane area (4cm^2) pH>7 (for pH>7 adsorption is the same) Lagergren model
B. Gohari, Polyethersulfone Membranes Prepared with 3-Aminopropyltriethoxysilane Modified Alumina Nanoparticles for Cu(II) Removal from Water, 2018, ACS OMEGA[45]	PES membrane	γ-alumina	Cu(II)	51.3 mg/g	$\frac{44.84\frac{mg}{g}}{0.05}$ = 896.8 mg/g	17.48	5% alumina
X. Zhang, Preparation, performances of PVDF/ZnO hybrid	PVDF membrane	hexagonal ZnO	Cu(II)	54.3 mg/g [47]	87.5 ug/cm^2 / (1.05*1.78)g/cm^3 density of pVDF and added	0.172	

membranes and their applications in the removal of copper ions, 2014, Applied Surface Science[46]					weiget by ZnO / 0.1 cm thick mem / 5% ZnO = 9.35 mg/g ZnO		
L. Chen, In situ formation of La(OH)3-poly(vinylidene fluoride) composite filtration membrane with superior phosphate removal properties, 2018, Chemical Engineering Journal [48]	PVDF membrane	$La(OH)_3$	PO_4	61.7 mg /g-La	256.6 mg/g-La	4.159	

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