Electronic Supplementary Material (ESI) for Nanoscale

Electronic Support Information (ESI)
Figures & Tables

Table S1: Abbreviations and main components of the test media and the numerically estimated ionic strengths. The data were numerically estimated using the USGS software PHREEQCi 2.18 using the database *minteq.v4* omitting the following components: amino acids, proteins, vitamins and glucose.

Medium abbreviation	Test system	Main components	Concentration [mM]	Ionic strength [mM]
Elendt	*Daphnia magna*	$CaCl_2$	2.0	8.3
		$NaHCO_3$	0.8	
		$MgSO_4$	0.5	
DMEM+FCS	OLN-93 cells	NaCl	109.5	167.8
		$NaHCO_3$	44.6	
		KCl	5.4	
		$CaCl_2$	1.8	
		NaH_2PO_4	0.9	
		$MgSO_4$	0.8	
		proteins, amino acids, glucose		
DSM	*Arthrobacter globiformis*	NaCl	28.6	28.6
		glucose, proteins		
AS	Activated sludge	Sodium acetate	52.1	207.9
		Na_2HPO_4	49.0	
		KH_2PO_4	27.6	
		$NaNO_3$	9.8	
		$CaCl_2$	0.25	
		$MgSO_4$	0.09	
AchE	Enzyme inhibition for acetylcholine esterase	Na_2HPO_4	20.0	52.3
		$NaHCO_3$	0.6	
GR	Enzyme inhibition for glutathione reductase	KH_2PO_4 / K_2HPO_4	100.0	205.9

Table S2a: Application scenario A: "Polyvinylpyrrolidone coated iron oxide (Fe_3O_4; magnetite) nanoparticles as contrast agent for magnetic resonance imaging (MRI)" (tested with the "precautionary matrix" [Höck et al. 2010]).

Scenarios	Precautionary need			
	Workers, general **[WG]**	Workers, worst case **[WWC]**	Consumers **[C]**	Environment **[E]**
MRI: production, liquid [**PL**] *Life cycle stage*: production of the IONP *Medium*: IONP in suspension	Precautionary need for workers in general *Workers*: all persons getting potentially into contact with the IONP during production Assumptions refer to normal production process	Precautionary need for workers in the worst case *Workers*: all persons getting potentially into contact with the IONP during production Assumptions refer to worst case	[Not applicable]	Precautionary need for the environment
MRI: production, dry [**PD**] *Life cycle stage*: production of the IONP *Medium*: IONP as dry powder				
MRI: use, liquid [**UL**] *Life cycle stage*: use of the IONP as contrast agent in clinical settings *Medium*: IONP in suspension	Precautionary need for workers in general *Workers*: all clinical personnel getting potentially into contact with the IONP at the clinic Assumptions refer to normal handling of pharmaceuticals and medical products	Precautionary need for workers in worst case *Workers*: all clinical personnel getting potentially into contact with the IONP at the clinic Assumptions refer to worst case handling of pharmaceuticals and medical products	Precautionary need for consumers *Consumers*: patients that are administered the IONP as contrast agent for MRI scanning purposes	Precautionary need for the environment
MRI: use, dry [**UD**] *Life cycle stage*: use of the PVP-IO-NP as contrast agent in clinical settings *Medium*: IONP in suspension				

Table S2b: Application scenario B: "Iron oxide (Fe_3O_4; magnetite) or zero valent iron (Fe^0; nZVI) nanoparticles as adsorbent or reductive agent for soil or groundwater remediation purposes" (tested with the "precautionary matrix" [Höck et al. 2010]).

Scenarios	Precautionary need			
	Workers, general **[WG]**	Workers, worst case **[WWC]**	Consumers **[C]**	Environment **[E]**
Remediation: magnetite, liquid [**ML**] *Particles*: IONP (magnetite) *Medium*: IONP in suspension Remediation: magnetite, dry [**MD**] *Particles*: IONP (magnetite) *Medium*: IONP as dry powder	Precautionary need for workers in general *Workers*: all persons getting potentially into contact with the IONP during production Assumptions refer to normal production process	Precautionary need for workers in the worst case *Workers*: all persons getting potentially into contact with the IONP during production Assumptions refer to worst case	Precautionary need for consumers *Consumers*: all persons getting potentially into contact with the IONP during use at remediation site	Precautionary need for the environment
Remediation: nZVI, liquid [**ZVL**] *Particles*: nZVI *Medium*: nZVI in suspension Remediation: nZVI, dry [**ZVD**] *Particles*: nZVI *Medium*: nZVI as dry powder	Precautionary need for workers in general *Workers*: all persons getting potentially into contact with the nZVI during production Assumptions refer to normal production process	Precautionary need for workers in the worst case *Workers*: all persons getting potentially into contact with the nZVI during production Assumptions refer to worst case	Precautionary need for consumers *Consumers*: all persons getting potentially into contact with the nZVI during use at remediation site	Precautionary need for the environment

Table S3: Hydrodynamic diameter (Hd), pH and zetapotential (Zp) of the PVP-coated IONP stock solution and the used samples in medium. Stock: IONP [1 g Fe/L] in water Sample: IONP [100 mg Fe/L] in medium Blank: pure medium. See Table S1 for media abbreviations.

Medium	Day	Sample / Stock			Blank		
		Hd	pH	Zp	Hd	pH	Zp
H_2O Stock	0	26.5 ± 2.3	5.2	1.17 ± 2.06			
	1	23.4 ± 1.5	5.6	0.8 ± 0.97			
	3	25.7 ± 3.1	5.8	1.74 ± 0.83			
	6	23.6 ± 1.1	5.7	-2.25 ± 2.34			
H_2O Sample	0	22.9 ± 2.1	5.2	0.13 ± 0.36		5.6	-0.28 ± 0.28
	1	23.6 ± 3.1	5.1	2.3 ± 1.31		5.8	-0.68 ± 0.3
	3	26.7 ± 3.7	5.1	6.25 ± 4.64		5.6	-0.62 ± 0.28
	6	29.8 ± 4.8	5.0	3.2 ± 3.6		5.8	-0.03 ± 0.14
Elendt M7	0	46.6 ± 2	7.4	-0.96 ± 1.13		7.6	-0.16 ± 0.18
	1	82.3 ± 3.4	7.4	-1.01 ± 0.84		7.7	-0.59 ± 1.07
	3	132.5 ± 15.6	7.4	-1.41 ± 0.34		7.6	-0.35 ± 1.35
	6	232.7 ± 50.4	7.5	-1.2 ± 0.68		7.6	-0.88 ± 0.75
DMEM-FCS	0	28.5 ± 5.1	7.9	-5.42 ± 1.57	25.4 ± 4.3	7.8	-6.76 ± 1.44
	1	32.5 ± 3.2	8.2	-7.12 ± 0.98	29.3 ± 0.6	8.0	-7.89 ± 1.09
	3	33.8 ± 1.5	8.2	-7.99 ± 0.52	26.6 ± 7.5	8.0	-7.05 ± 1.67
	6	36.5 ± 1.9	8.2	-7.2 ± 0.97	35.1 ± 7.9	8.1	-7.8 ± 0.59
AchE	0	21.5 ± 2.7	8.0	-0.36 ± 0.3		8.0	-0.33 ± 0.41
	1	23.7 ± 2.2	8.0	-0.49 ± 0.42		8.0	0.07 ± 0.92
GR	0	23.5 ± 2.8	7.6	0.18 ± 0.55		7.6	-0.75 ± 1.84
	1	26.6 ± 3.7	7.6	-0.14 ± 1.71		7.6	-2.68 ± 2.15
AS	0	28.3 ± 1.2	7.6	-0.92 ± 0.39		7.6	-1.39 ± 1.24
	1	36.5 ± 2.4	7.7	3.69 ± 1.36		7.6	-1.46 ± 2.6
DSM	0	27.2 ± 1.4	6.9	-1.36 ± 1.77		6.9	0 ± 0.74
	1	26.3 ± 1.6	6.9	-0.77 ± 0.81		6.9	-0.53 ± 0.71

Table S4: List of physical constants for DLVO theory calculations (according to Lide et al. 1997.)

Name	Symbol	Value	Unit
Boltzmann constant	k_B	$1.38066 \cdot 10^{-23}$	J/K
Elementary charge	e_0	$1.60218 \cdot 10^{-19}$	As
Avogadro number	N_A	$6.02214 \cdot 10^{23}$	1/mol
Permittivity of the vacuum	ε_0	$8.85419 \cdot 10^{-12}$	F/m
Permeability of free space	μ_0	$1.25664 \cdot 10^{-6}$	N/A^2

Table S5: List of parameters for DLVO theory calculations

Name	Symbol	Value	Unit	Source
Temperature	T	298.15	K	Temperature during dynamic light scattering (DLS) measurements
Radius of the particles	r	various	m	
Separation distance between particles (surface to surface)	h	various	m	
Separation distance between particles (centre to centre)	s	various	m	
Relative dielectric constant	ε_r	78.36		Water, 298.15 K (Lide et al. 1997)
Surface potential	ζ	various	V	According to Table S6
Inverse Debye length	κ	various	1/m	
Ionic strength of the solution	I	various	mol/m^3	According to Table S6
Hamaker constant for Fe_3O_4 / H_2O / Fe_3O_4	A	33	zJ (1 zJ = 10^{-21} J)	(Fauré 2011)
Saturation magnetization (volume)	M_s	various	$emu/cm^3 = 10^3 A/m$	
Thickness of polymer layer	L	various	m	
Segment length of PVP	l	0.269	nm	estimated by Hyperchem 7.5
Surface density of adsorbed chains	σ_p	1	nm^{-2}	(Lim et al. 2009) , estimated
Number of segments in polymer chains	N_p	43	-	See ESI text

Density of Fe_3O_4	ρ	5.17	g/cm^3	at 298.15 K (Lide et al. 1997)
Density of PVP	ρ	1.23	g/cm^3	MSDS (ScienceLab.com)
Saturation magnetization of Fe_3O_4 (bulk) (mass)	M_s	92	emu/g = Am^2/kg	at 300 K Utech et al. (2010)
Thickness of non magnetic oxide layer	l_m	1.0	nm	Kim et al. (2009)

Table S6: Experimental database for extended DLVO theory calculations. The data were compiled from Tables S1 and S3. The calculations were done for primary particles (data of IONP in water: d_H = 23 nm, r = 7.5 nm, L = 4 nm). Influence of media on possibly further agglomeration was considered due to different zeta potential and ionic strength in media.

Medium	**Zeta potential [mV]**	**Ionic strength/ [mol/ m³]**
Water	0.1	10^{-4}
Elendt M7	-1.0	8.3
DMEM	-5.4	167.8
AchE	-0.4	28.6
GR	0.2	207.9
AS	-0.9	52.3
DSM	-1.4	205.9

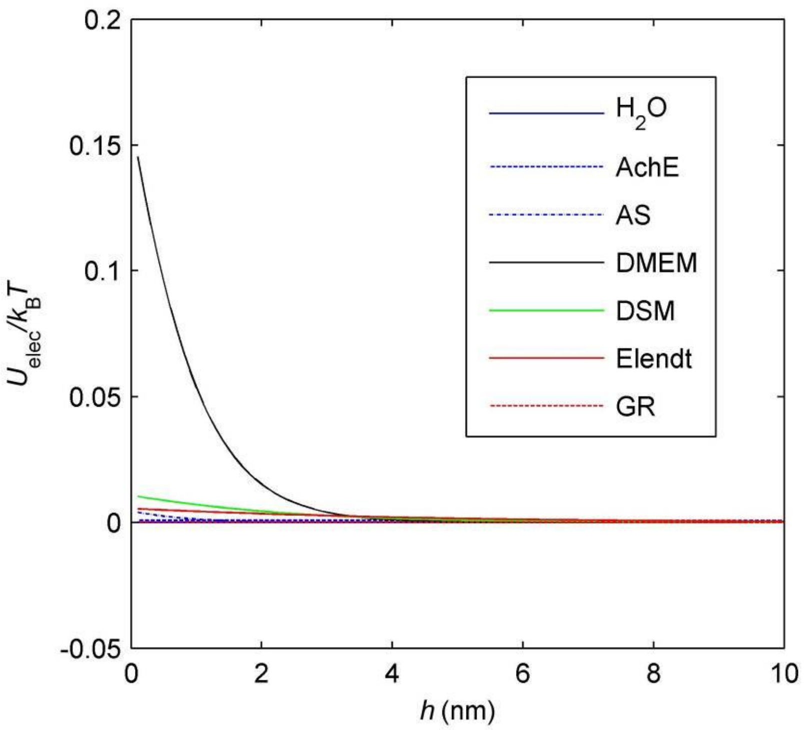

Figure S1: Electrostatic repulsion U_{elec} of PVP-coated IONP in the test media as a function of the surface to surface distance *h* between the magnetite cores. Differences in U_{elec} resulting from the changes in ionic strength of the media and the zeta potential change are minute compared to the other interactions U_{vdW}, U_{steric} and U_{magn} (see also Figure 5 and data in Table S6).

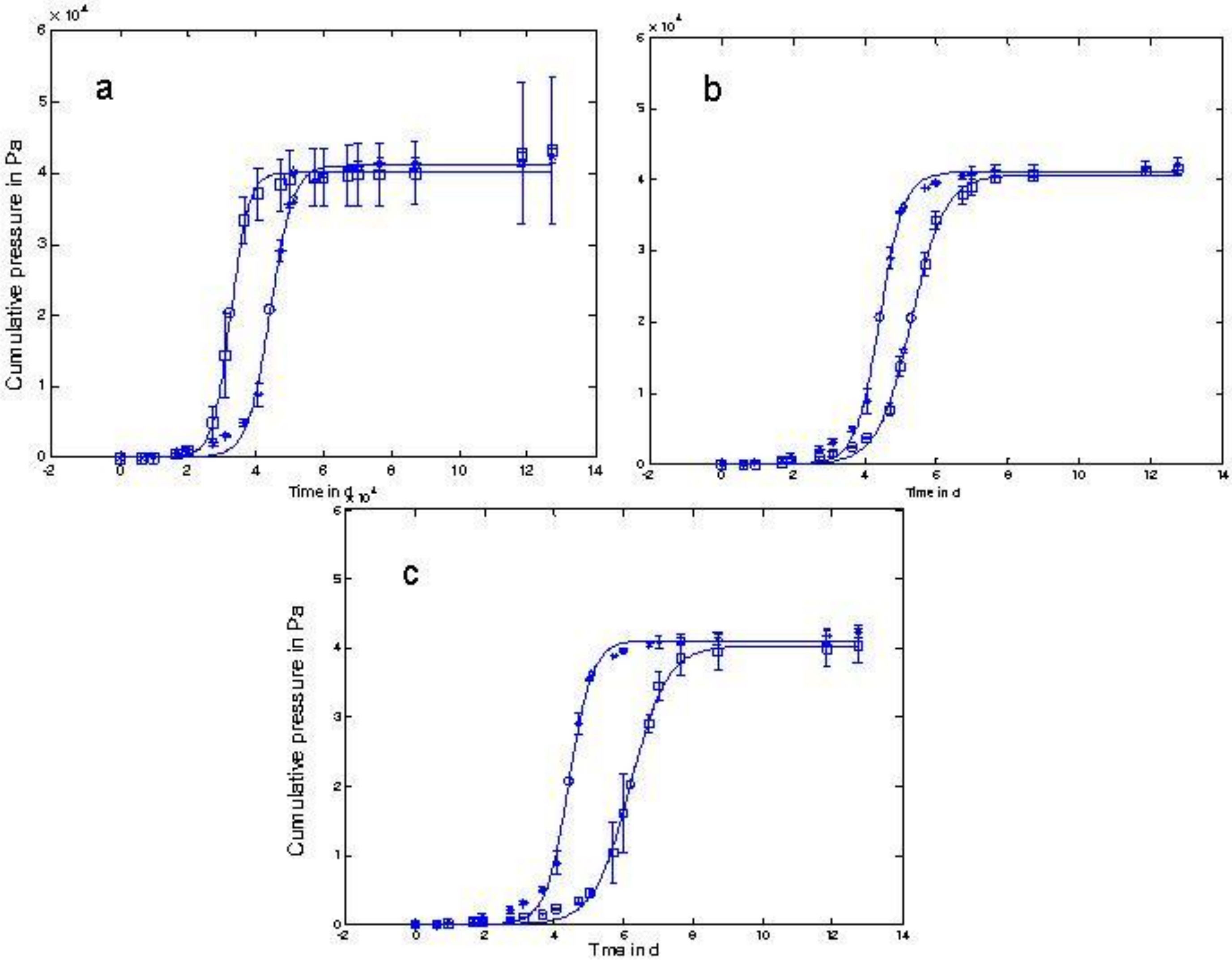

Figure S2: Fitted bacterial growth curves shown as the cumulative pressure development over the incubation time of the sewage sludge samples in days. Each data point represents the mean ± SD of three independent replicates. Open squares: PVP-FeNP treated samples, asterisks: untreated controls. The sewage sludge samples were incubated with three different PVP-coated IONP concentrations: a.) 1.5 mg Fe/mg TS, b.) 0.16 mg Fe/mg TS and c.) 0.01 mg Fe/mg TS.