Supporting Information

of

Dynamic remobilization of treated Cd from Fe-based nano-particles (nZVI, S-nZVI and nFeS) in oxic/anoxic aqueous environments

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Content

Table S 1 Changes of the XPS Fe 2p peaks of the samples before and after aging.

Material	Situation	Species	Binding energy	FWHM
nZVI	before aging	Fe(II)	709.89	3.42
		Fe(III)	719.89	3.37
		satellite	723.22	3.37
		Fe(II)	726.37	3.37
		Fe(III)	729.99	3.37
		satellite	736.87	3.62
	oxic aging	Fe(II)	710.1	3.1
		Fe(III)	713.24	3.59
		satellite	718.11	3.5
		Fe(II)	723.25	3.5
		Fe(III)	725.99	3.51
		satellite	731.91	3.39
	anoxic aging	Fe^0	706.29	2.28
		Fe(II)	709.32	3.5
		Fe(III)	712.63	3.5
		satellite	719.41	3.52
		Fe(II)	722.88	4
		Fe(III)	726.75	3.96
		satellite	730.88	3.5
S-nZVI	before aging	Fe(II)	711.5	2.7
		Fe(III)	713.46	3.6
		satellite	719.7	3.83
		Fe(II)	723.44	3.36
		Fe(III)	725.5	4.03
		satellite	731.85	3.36
	oxic aging	Fe(II)	709.79	3.17
		Fe(III)	712.5	3.36
		satellite	718.9	3.36
		Fe(II)	723.12	3.36
		Fe(III)	726.03	3.36
		satellite	730.05	3.36
	anoxic aging	Fe^0	705.59	1.23
		Fe(II)	709.07	3.44
		Fe(III)	712.61	4.04
		satellite	718.59	1.43
		Fe(II)	722.59	3.06
		Fe(III)	726.85	3.5
nFeS	before aging	Fe(II)	710.73	4.53

	Fe(III)	713.2	5.5
	satellite	718.6	6
	Fe(II)	723.19	2
	Fe(III)	725	5.5
	satellite	730.1	3.51
oxic aging	Fe(II)	709.73	2.79
	Fe(III)	712.31	3.36
	satellite	718.87	3.36
	Fe(II)	723.32	3.36
	Fe(III)	726.44	3.36
	satellite	731.98	3.76
anoxic aging	Fe^0	705.82	1.56
	Fe(II)	708.62	3.5
	Fe(III)	711.35	3.5
	satellite	718.96	3.5
	Fe(II)	722.52	3.5
	Fe(III)	726.34	3.5
	satellite	730.44	3.36

Table S 2 Changes of the XPS S 2p peaks of the samples before and after aging.

Material	**Situation**	**Species**	**Binding energy**	**FWHM**
S-nZVI	before aging	S^{2-}	160.45	1.28
		S_2^{2-}	161.7	1.33
		SO_4^{2-}	167.53	2.58
	oxic aging	S^{2-}	160.14	0.89
		S_2^{2-}	161.39	1.93
		SO_4^{2-}	167.66	2.35
	anoxic aging	S^{2-}	160.04	1.07
		S_2^{2-}	161.2	2.04
		SO_4^{2-}	167.34	1.34
nFeS	before aging	S^{2-}	160.06	1
		S_2^{2-}	161.22	1.54
		SO_4^{2-}	167.64	2.28
	oxic aging	S^{2-}	160.06	1.02
		S_2^{2-}	161.27	1.42
		SO_4^{2-}	167.42	2.19
	anoxic aging	S^{2-}	160.15	1.09
		S_2^{2-}	161.37	1.34
		SO_4^{2-}	167.99	2.48

Table S 3 Changes of the XPS Cd 3d peaks of the samples before and after aging.

Material	Situation	Species	Binding energy	FWHM
nZVI	before aging	Cd(II)	404.39	1.54
		Cd(II)	411.1	1.53
	oxic aging	Cd(II)	403.81	1.01
		Cd(II)	410.54	1
	anoxic aging	Cd(II)	403.81	1.06
		Cd(II)	410.55	1.05
S-nZVI	before aging	Cd(II)	410.91	1.35
		Cd(II)	404.17	1.35
	oxic aging	Cd(II)	411.35	1.61
		Cd(II)	404.6	1.61
	anoxic aging	Cd(II)	411.35	1.64
		Cd(II)	404.62	1.67
nFeS	before aging	Cd(II)	410.6	1.08
		Cd(II)	403.86	1.08
	oxic aging	Cd(II)	410.48	1.09
		Cd(II)	403.75	1.09
	anoxic aging	Cd(II)	410.5	1.04
		Cd(II)	403.78	1.04

Table S 4 Changes of the XPS O 1s peaks of the samples before and after aging.

Material	Situation	Species	Binding energy	FWHM
nZVI	before aging	-OH	531.31	2.87
	oxic aging	O^{2-}	529.86	1.14
		-OH	531.47	2.35
	anoxic aging	O^{2-}	528.71	1.07
		-OH	530.06	1.95
S-nZVI	before aging	-OH	530.94	1.67
	oxic aging	O^{2-}	528.58	1.77
		-OH	530.54	2.57
	anoxic aging	-OH	531.67	2.29
nFeS	before aging	O^{2-}	528.7	1.11
		-OH	530.58	1.92
	oxic aging	O^{2-}	529.69	0.9
		-OH	531.21	2.79
	anoxic aging	O^{2-}	528.61	1.12
		-OH	530.44	2.4

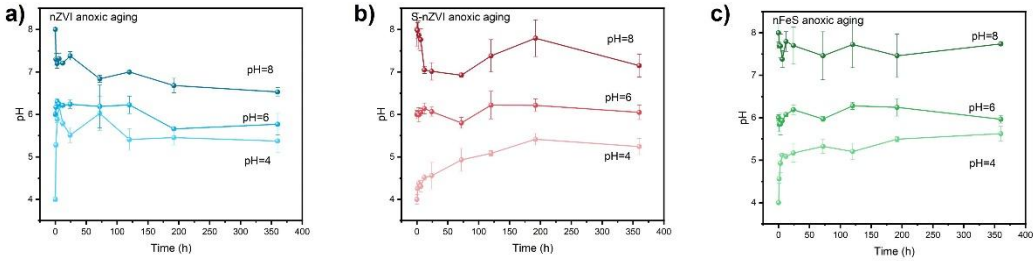

Fig. S 1 Kinetics of pH under anoxic aging by a) nZVI, b) S-nZVI and c) nFeS.

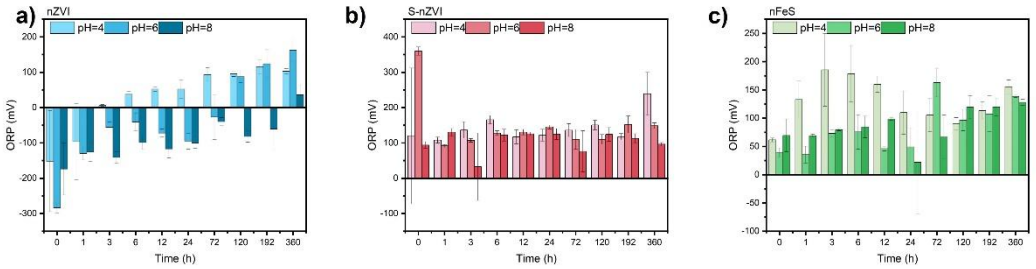

Fig. S 2 Evolution ORP of a) nZVI, b) S-nZVI and c) nFeS under anoxic aging.

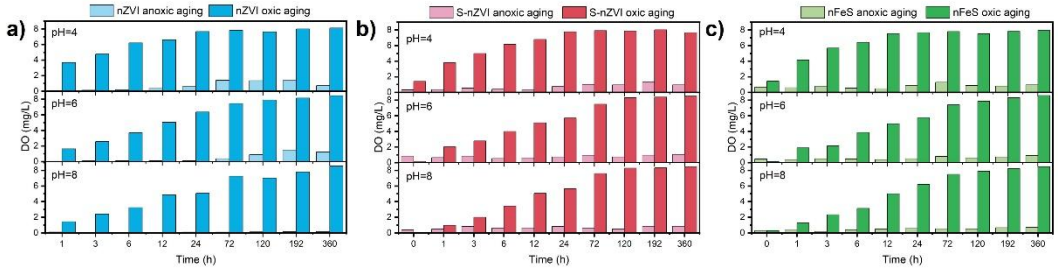

Fig. S 3 Dissolved oxygen content of a) nZVI, b) S-nZVI and c) nFeS.

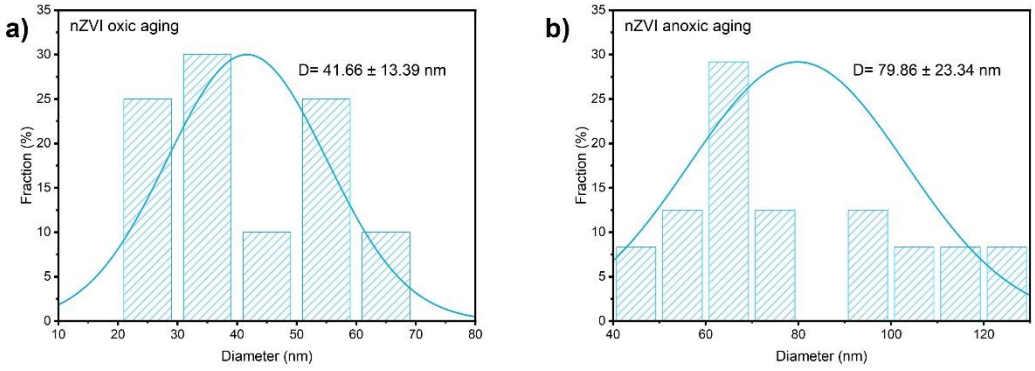

Fig. S 4 Particle size distribution of nZVI under a) oxic and b)anoxic aging.

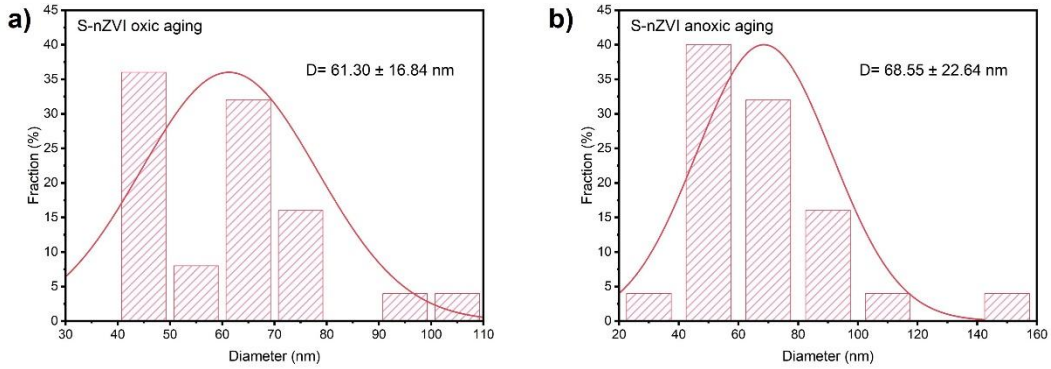

Fig. S 5 Particle size distribution of S-nZVI under **a)** oxic and **b)** anoxic aging.

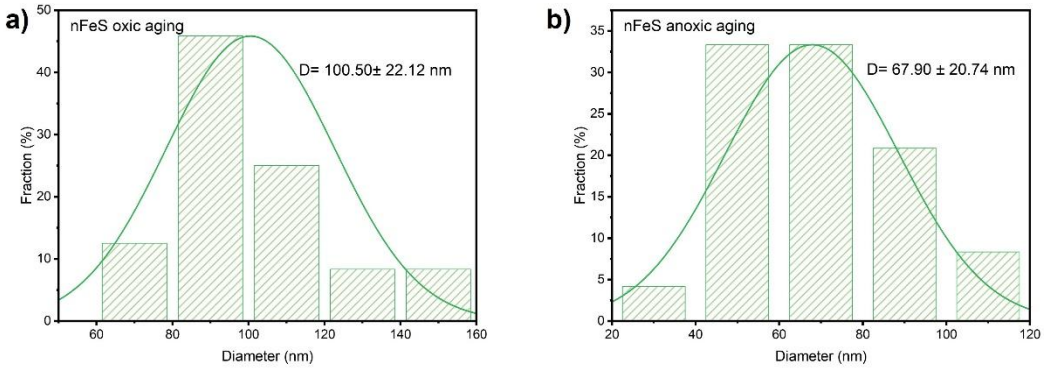

Fig. S 6 Particle size distribution of nFeS under a) oxic and b)anoxic aging.

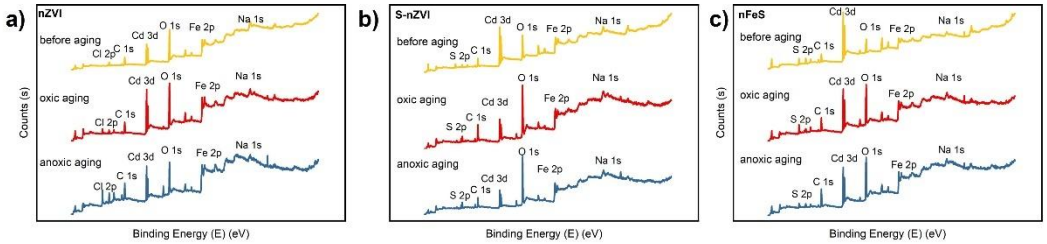

Fig. S 7 XPS spectra of a) nZVI, b) S-nZVI and c) nFeS.

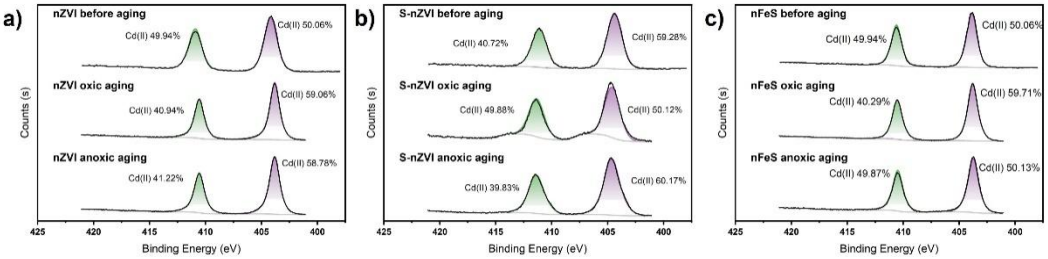

Fig. S 8 XPS spectra for Cd 3d of a) nZVI, b) S-nZVI and c) nFeS.

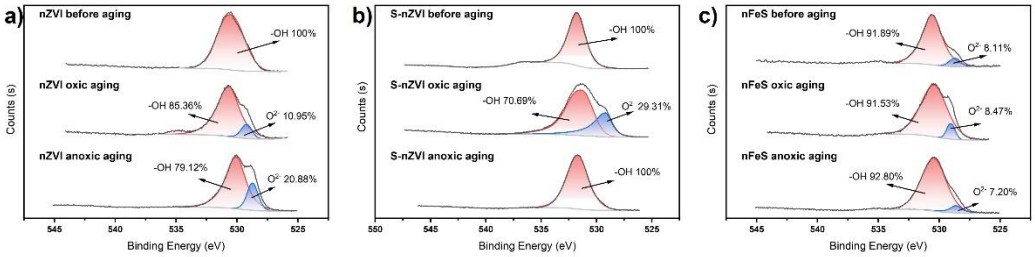

Fig. S 9 XPS spectra for O 1s of a) nZVI, b) S-nZVI and c) nFeS.