

Enhanced oxidative and adsorptive removal of arsenite by heterogeneous interfacial reaction of sulfidated nanoscale zerovalent iron

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Tab. S1 Pseudo-first-order and Pseudo-second-order kinetic model parameters

Materials	Pseudo-first-order			Pseudo-second-order		
	$k_1(\text{min}^{-1})$	$q_e(\text{mg/g})$	R^2	$k_2(\text{g}\cdot\text{mg}^{-1}\cdot\text{min}^{-1})$	$q_e(\text{mg/g})$	R^2
nZVI	0.06091	5.804015	0.8741	0.020048	16.90617	0.99911
S-nZVI ^{0.01}	0.07425	1.312272	0.67052	0.108089	17.2117	0.99993
S-nZVI ^{0.1}	0.05308	0.579112	0.54526	0.280152	19.28268	0.99999
S-nZVI ^{0.5}	0.04738	2.654855	0.65549	0.060466	17.18508	0.99992

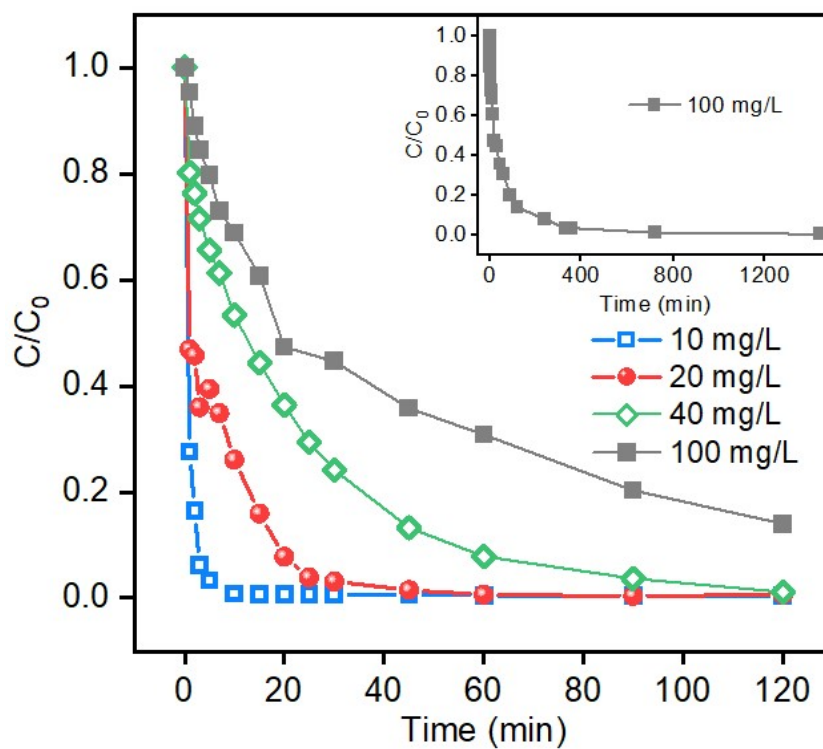


Fig.S1 As(III) removal by S-nZVI under different initial As(III) concentration.

The insert figure in the top right-hand corner is the reaction time of 24 h.

Reaction conditions: the S-nZVI dose is $0.5 \text{ g} \cdot \text{L}^{-1}$; $[\text{As(III)}]_{\text{initial}} = 10 \text{ mg} \cdot \text{L}^{-1}$; the

$\text{pH}_{\text{initial}}$ is 5.

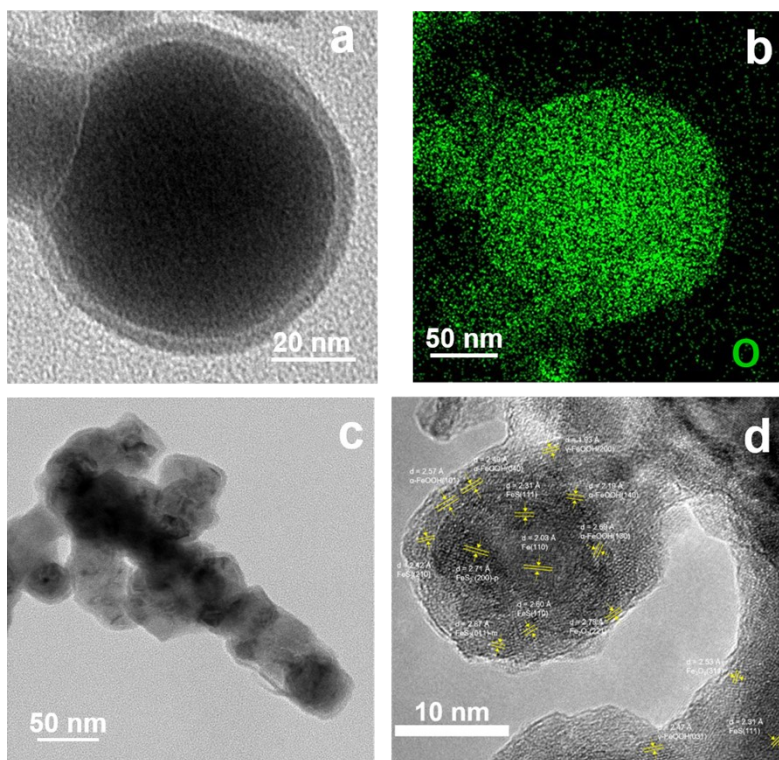


Fig.S2 (a) TEM image of nZVI; ADF image (b) O mapping of S-nZVI; (c) TEM image of S-nZVI; (d) SAED pattern of S-nZVI.

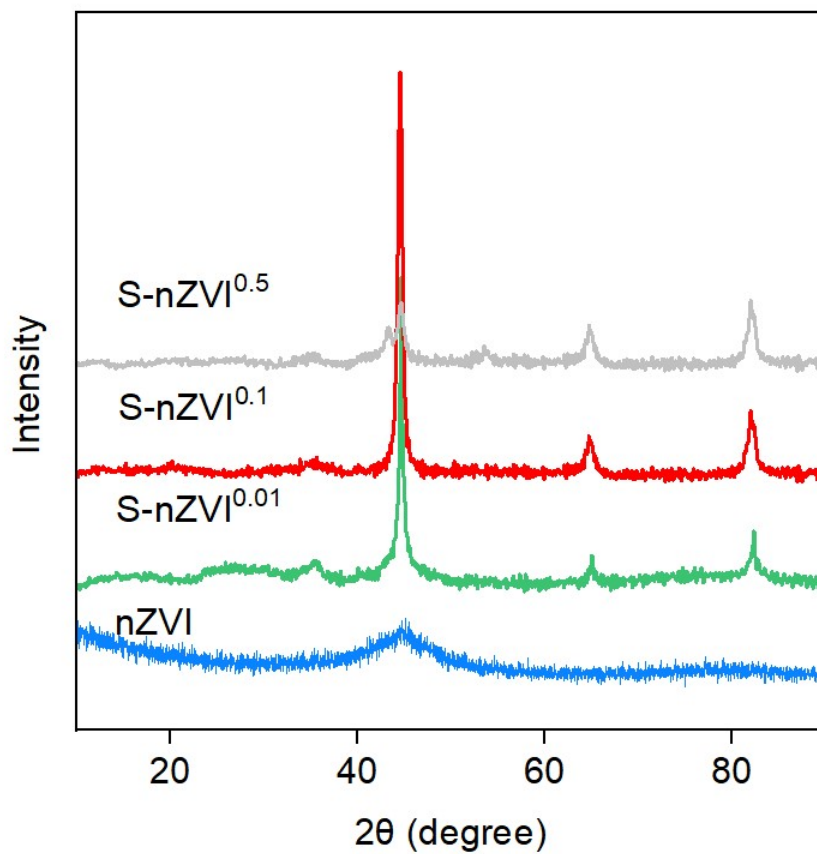


Fig.S3 XRD patterns of S-nZVI at different S/Fe.

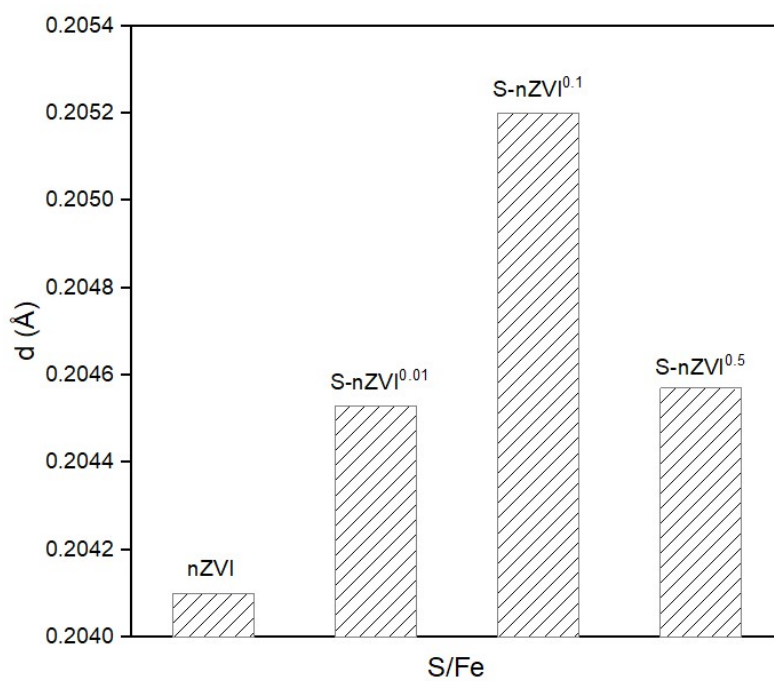


Fig. S4 Crystal plane spacing of Fe (110) in S-nZVI.

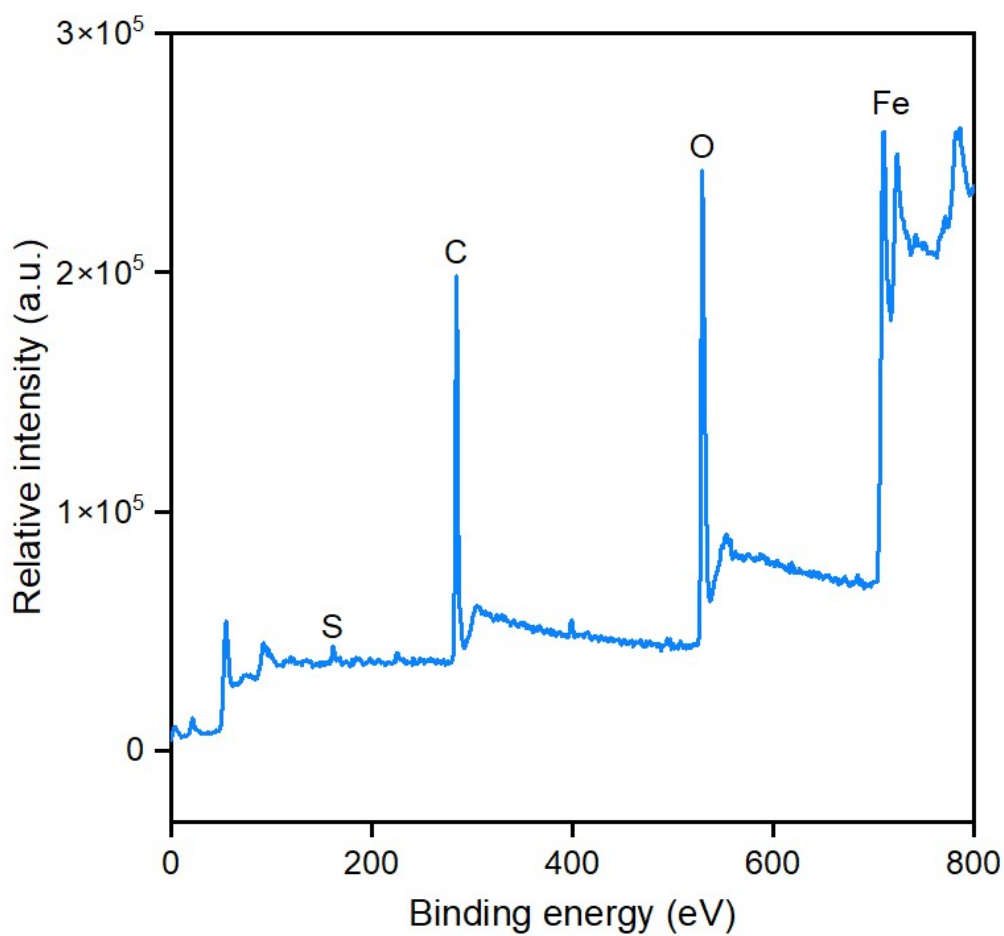


Fig.S5 XPS survey spectra for S-nZVI.

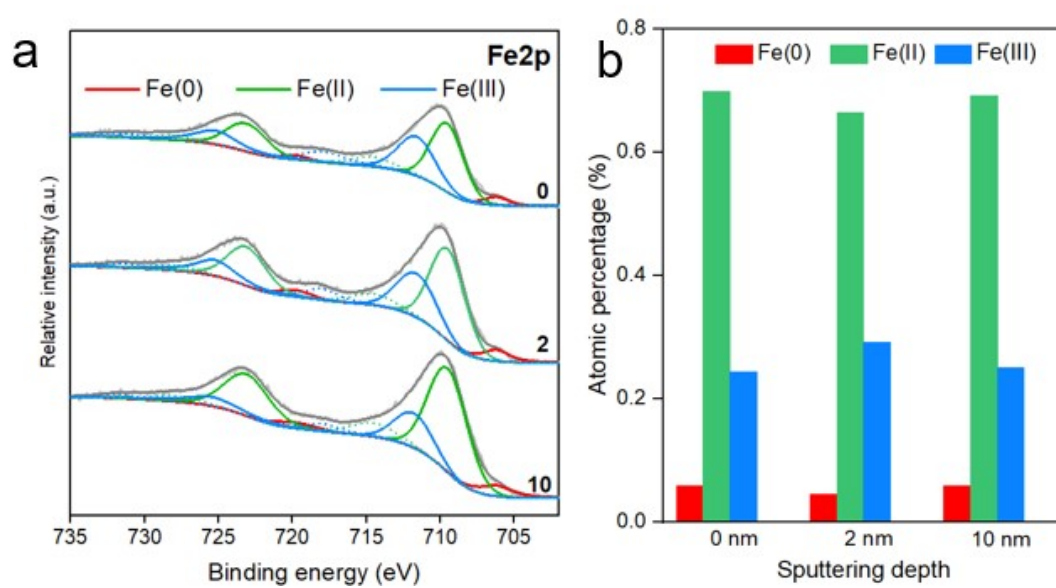


Fig.S6 XPS spectra peaks for S-nZVI. (a) Fe2p, (b) Fe species distribution.

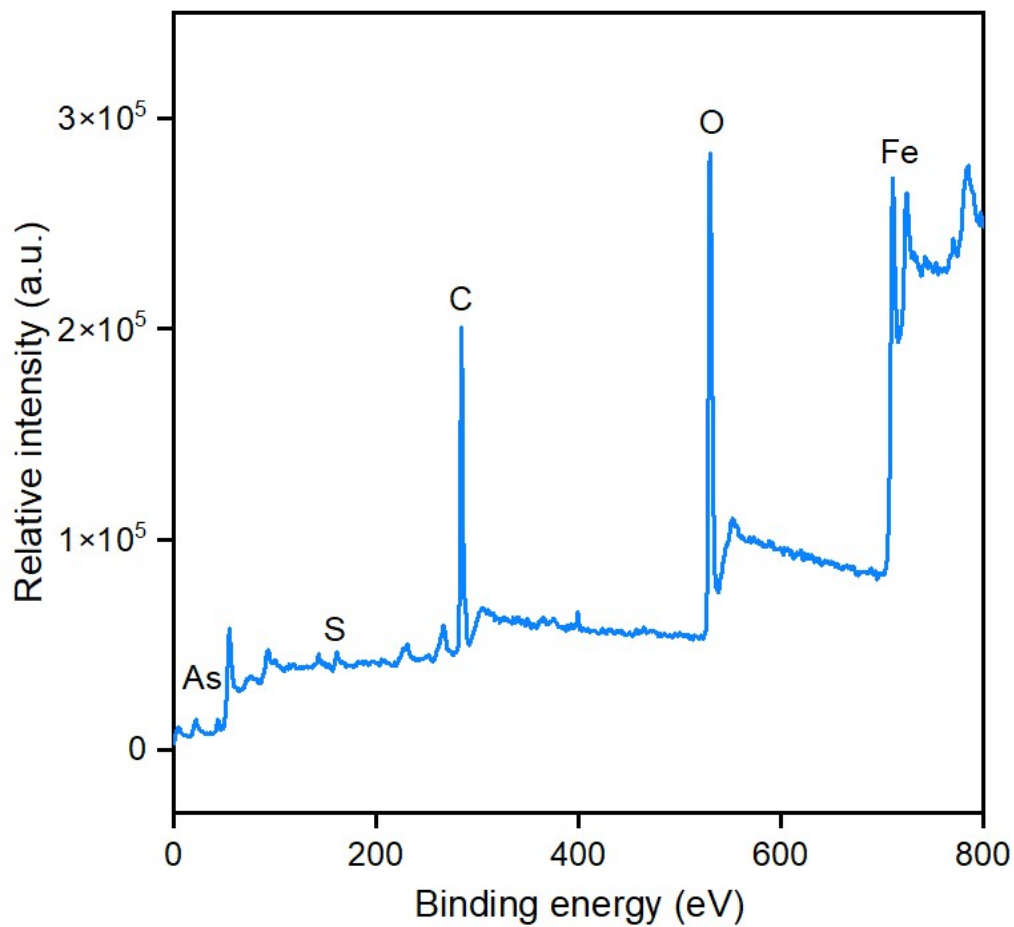


Fig.S7 XPS survey spectra for S-nZVI reacted with As(III). Reaction conditions: the S-nZVI dose is $5 \text{ g} \cdot \text{L}^{-1}$; $[\text{As(III)}]_{\text{initial}} = 100 \text{ mg} \cdot \text{L}^{-1}$; the $\text{pH}_{\text{initial}}$ is 5; and the reaction time is 24

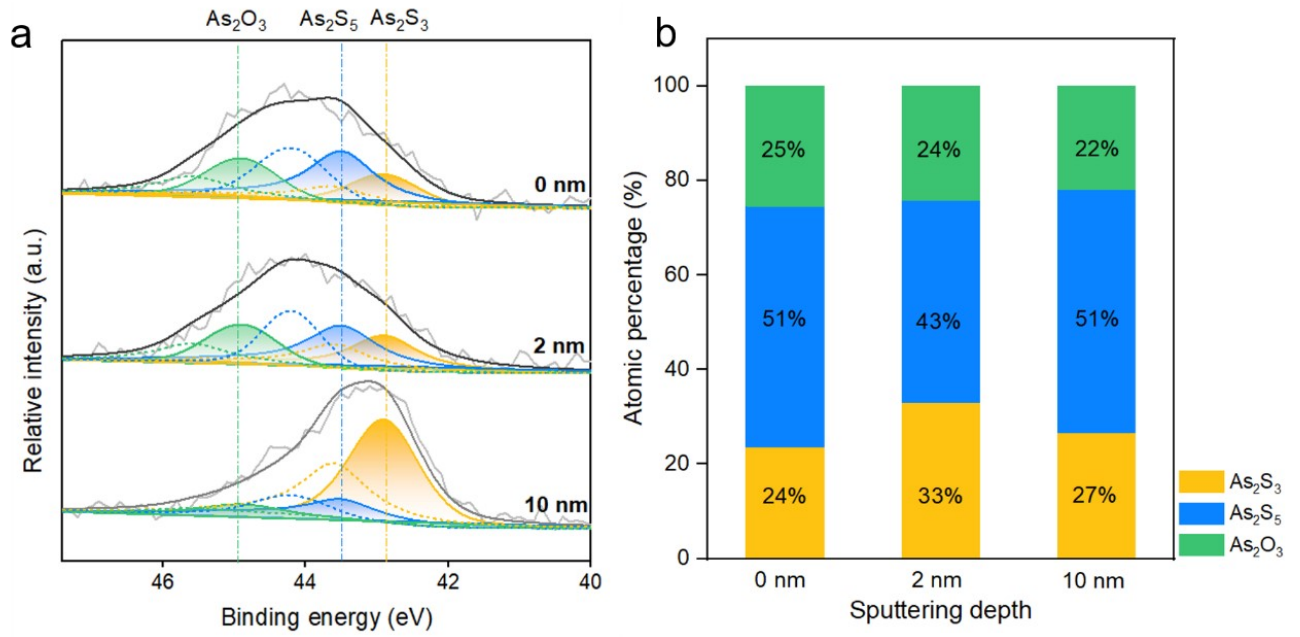


Fig. S8 HR-XPS spectra of As3d peaks for S-nZVI reacted with As(III) at sputtering depths of 0, 2, 10 nm. (a) As3d species distribution; (b) Relative percentage of As species. Reaction conditions: the S-nZVI dose is $5 \text{ g}\cdot\text{L}^{-1}$; $[As(III)]_{\text{initial}}=100 \text{ mg}\cdot\text{L}^{-1}$; the $\text{pH}_{\text{initial}}$ is 5; and the reaction time is 24 h.

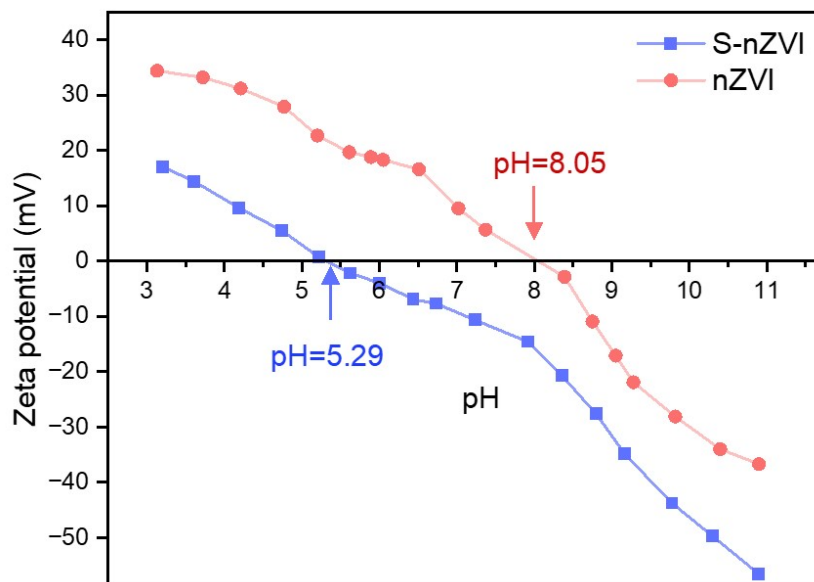


Fig. S9 Zeta potential of nZVI and S-nZVI.

Tab. S2 As species distribution of XPS spectra curve fitting for spent particles of S-nZVI / nZVI reacted with As(III)

Ion etching depth	Materials	As(V)	As(III)	As(0)
0 nm	S-nZVI	0.44855	0.55145	/
	nZVI	0.08228	0.57309	0.34463
2 nm	S-nZVI	0.3899	0.6101	/
	nZVI	0.10414	0.52084	0.37502
10 nm	S-nZVI	0.32224	0.67776	/
	nZVI	0.12545	0.50257	0.37198