Supplementary Material

Correlation between the structural-activity of sulfidated nanoscale zerovalent iron and its enhanced reactivity for Cr(VI) reduction

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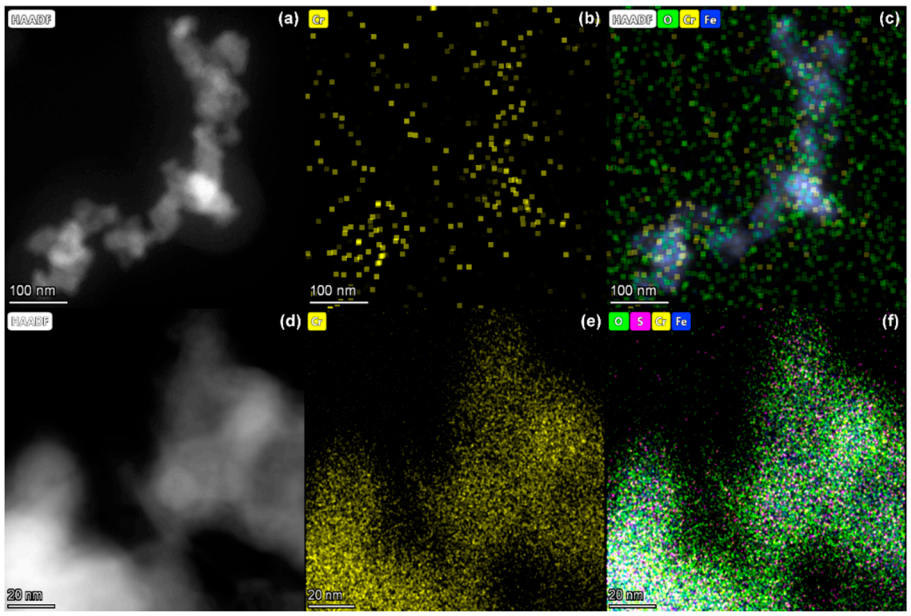


Figure S1. TEM−EDS elemental mappings of nZVI (a-c) and S-nZVI^{one}-0.32 (d-f) after their reaction with Cr(VI) in the batch systems: HAADF images (a, d), Cr mappings (b, e), color overlays (c, f). Reaction conditions: [nZVI or S-nZVI] = 0.1 g/L, S/Fe molar ratio = 0.32, $[Cr(VI)]_0$ = 8.0 mg/L, $[Na_2SO_4]$ = 0.2 mM, pH_{ini} = 5.0, reaction time = 90 min, T = 25ºC.

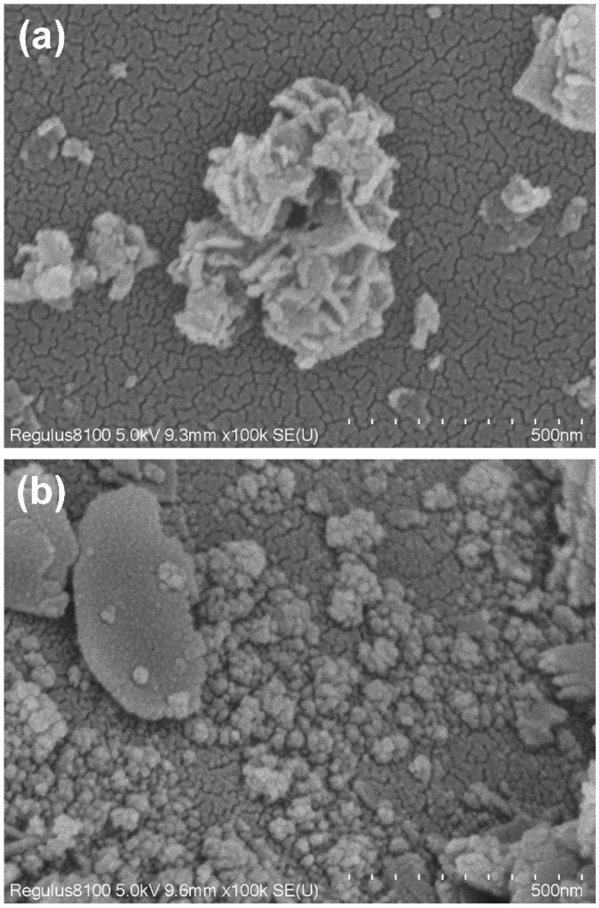


Figure S2. SEM images of nZVI (a) and S-nZVI^{one}-0.32 (b) after reaction with Cr(VI) in the column systems. Reaction conditions: $[nZVI \text{ or } S\text{-}nZVI]_{Input}$ = 0.2 g/L, $[Cr(VI)]_0$ = 10.0 mg/L, Quartz sand mesh=30-50 mesh, $[Na_2SO_4]$ = 0.2 mM, pH_{ini} = 5.0, T = 25°C.

Table S1. Parameters of zero-order and first-order models for fitting the removal kinetics of Cr(VI) by nZVI-based materials.

Materials	Zero-order kinetic model			First-order kinetic model		
	$k_{obs\text{-}Cr}$ (mg L^{-1} min^{-1})	R^2	Stand. error of estimate	$k_{obs\text{-}Cr}$ (min^{-1})	R^2	Stand. error of estimate
nZVI	0.0037	0.7119	0.0138	0.0039	0.7148	0.0137
S-nZVI^{one}-0.08	0.0166	0.7408	0.0578	0.0220	0.7646	0.0551
S-nZVI^{one}-0.16	0.0201	0.7517	0.0681	0.0285	0.7802	0.0641
S-nZVI^{one}-0.32	0.0220	0.5682	0.1131	0.0382	0.6157	0.1067
S-nZVI^{two}-0.08	0.0118	0.6873	0.0469	0.0144	0.7014	0.0458
S-nZVI^{two}-0.16	0.0150	0.6024	0.0717	0.0205	0.6273	0.0694
S-nZVI^{two}-0.32	0.0129	0.6326	0.0579	0.0164	0.6520	0.0564

Table S2. Parameters for the correlation analysis of the reactivity and structural-activity of S-nZVI.

Systems	Slope	Stand. error of slope	R	Stand. error of estimate
$k_{obs\text{-}Cr}$ vs $k_{obs\text{-}Sed.}$	-2.7341	1.1348	0.7330	0.0086
$k_{obs\text{-}Cr}$ vs lg$R$	-0.0207	0.0059	0.8419	0.0068