

Supporting Information

Complete degradation of 2,4-dichlorophenol in sequential sulfidated nanoscale zero-valent iron/peroxydisulfate system: Dechlorination, mineralization and mechanism

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Text S1 GC-MS method

The intermediate product samples of 2,4-DCP degradation process were analyzed by Gas chromatography-mass spectrometry (GC-MS) through liquid-liquid extraction pretreatment. 30 mL of samples and 10 mL of dichloromethane were mixed in a liquid separation funnel, and the pH of the mixed solutions was adjusted to 2.0, 7.0 and 12.0 by H₂SO₄ and HCl, respectively. After three oscillations of extraction, the underlying liquid is collected for subsequent use. The collected solution was evaporated and concentrated to 5 mL and filtered by 0.22 μm organic filter. The obtained solution was diluted and transferred to 2 mL injection bottle for testing. HP5 capillary column (30 m×0.25 mm×0.25 μm) was used for the chromatography. 2 μL of samples was injected within 2 min without diffluent. The scanning mass range was 60-400 amu, and the carrier gas flow rate was 1.0 mL·min⁻¹, and the solvent delay time was 7 min. The heating procedure of column temperature is as follows: Initial temperature 40°C, maintaining for 8 min; The temperature was raised to 260°C at a gradient of 20°C per minute and maintained for 20 min. The inlet temperature is 260°C, the ion source temperature is 230°C, and the electron energy is 70 eV. Due to the different charge-mass ratio of each chemical substance, the time of ion peak is different, and the corresponding chemical substance can be obtained by referring to the database comparison.

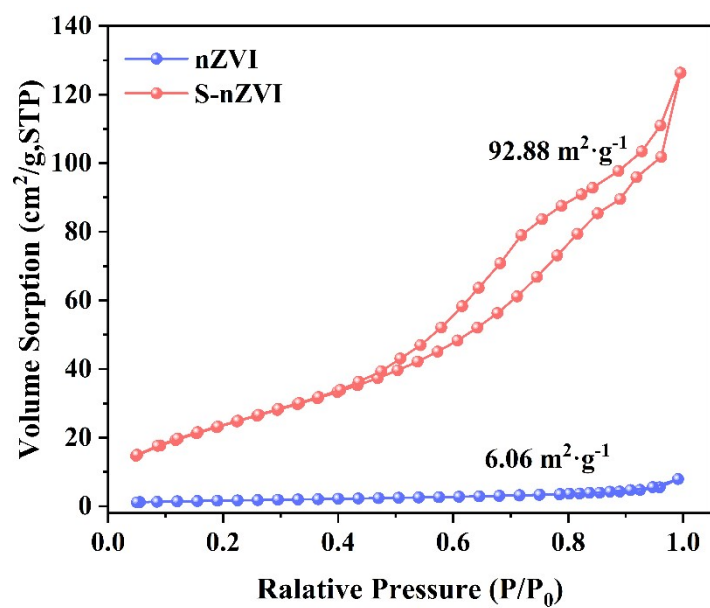


Figure S1. The N₂ adsorption-desorption isotherms of nZVI and S-nZVI.

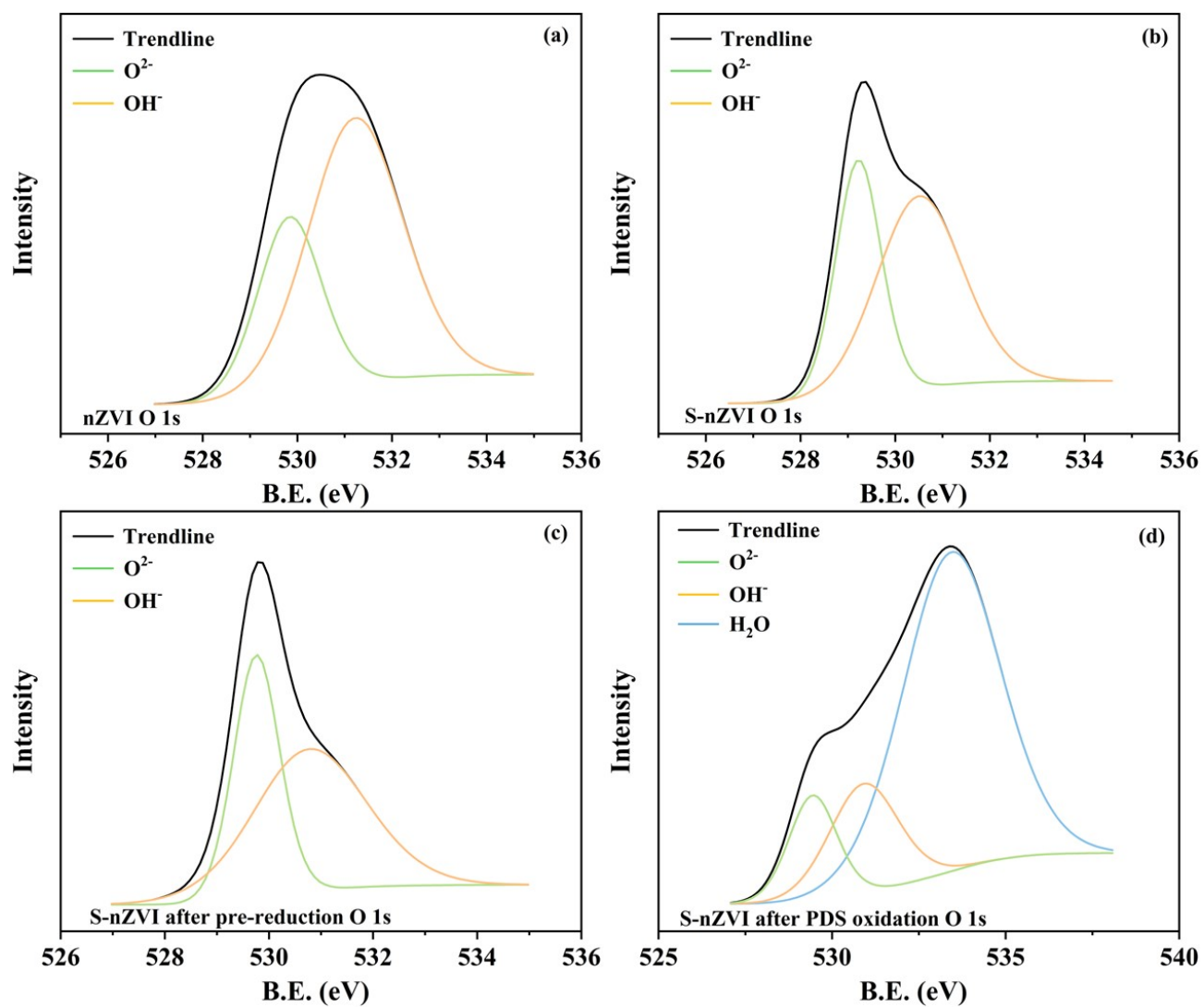


Figure S2. O (1s) high resolution of nZVI (a), S-nZVI (b), S-nZVI after pre-reduction (c), S-nZVI after PDS oxidation (d).

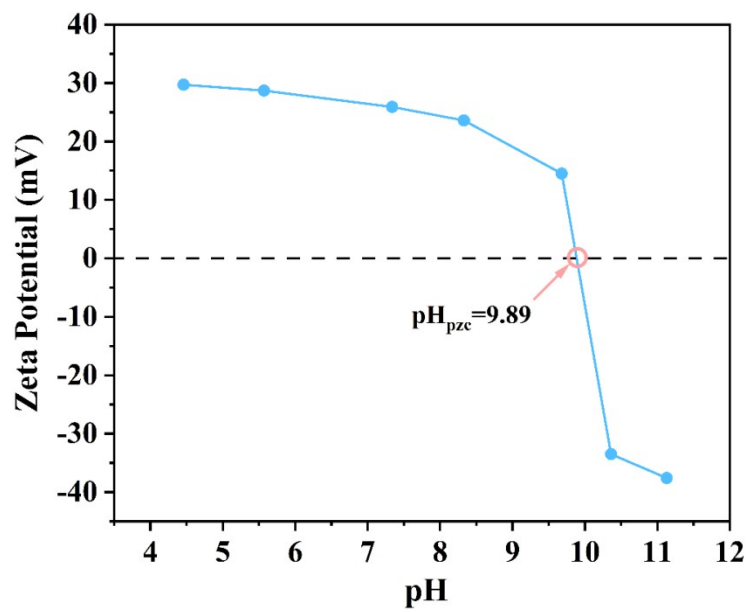


Figure S3. The Zeta potential of S-nZVI.

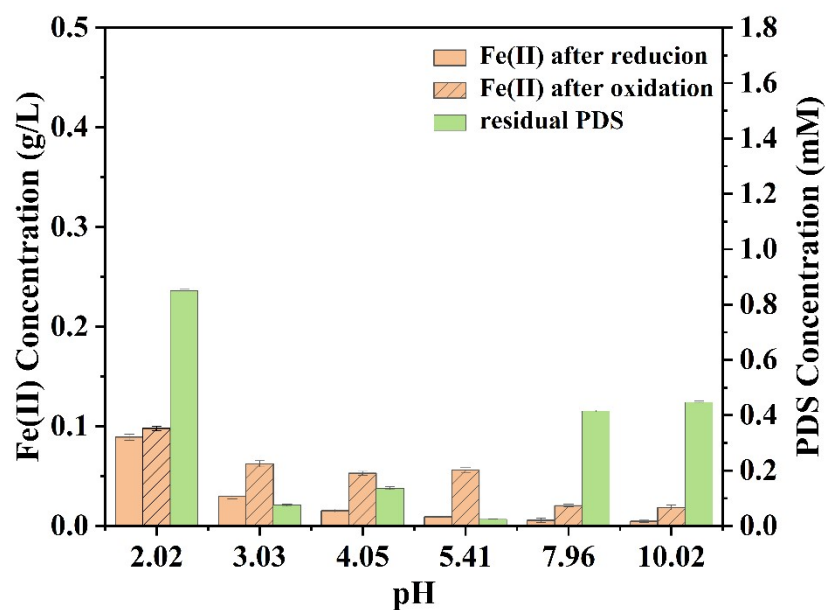


Figure S4. Residual PDS concentration and Fe(II) concentration after reduction and oxidation under different pH value. (Reaction conditions: S-nZVI dosage= $2.5 \text{ g}\cdot\text{L}^{-1}$, $[\text{PDS}] = 1.8 \text{ mM}$, $[\text{2,4-DCP}] = 10 \text{ mg}\cdot\text{L}^{-1}$)

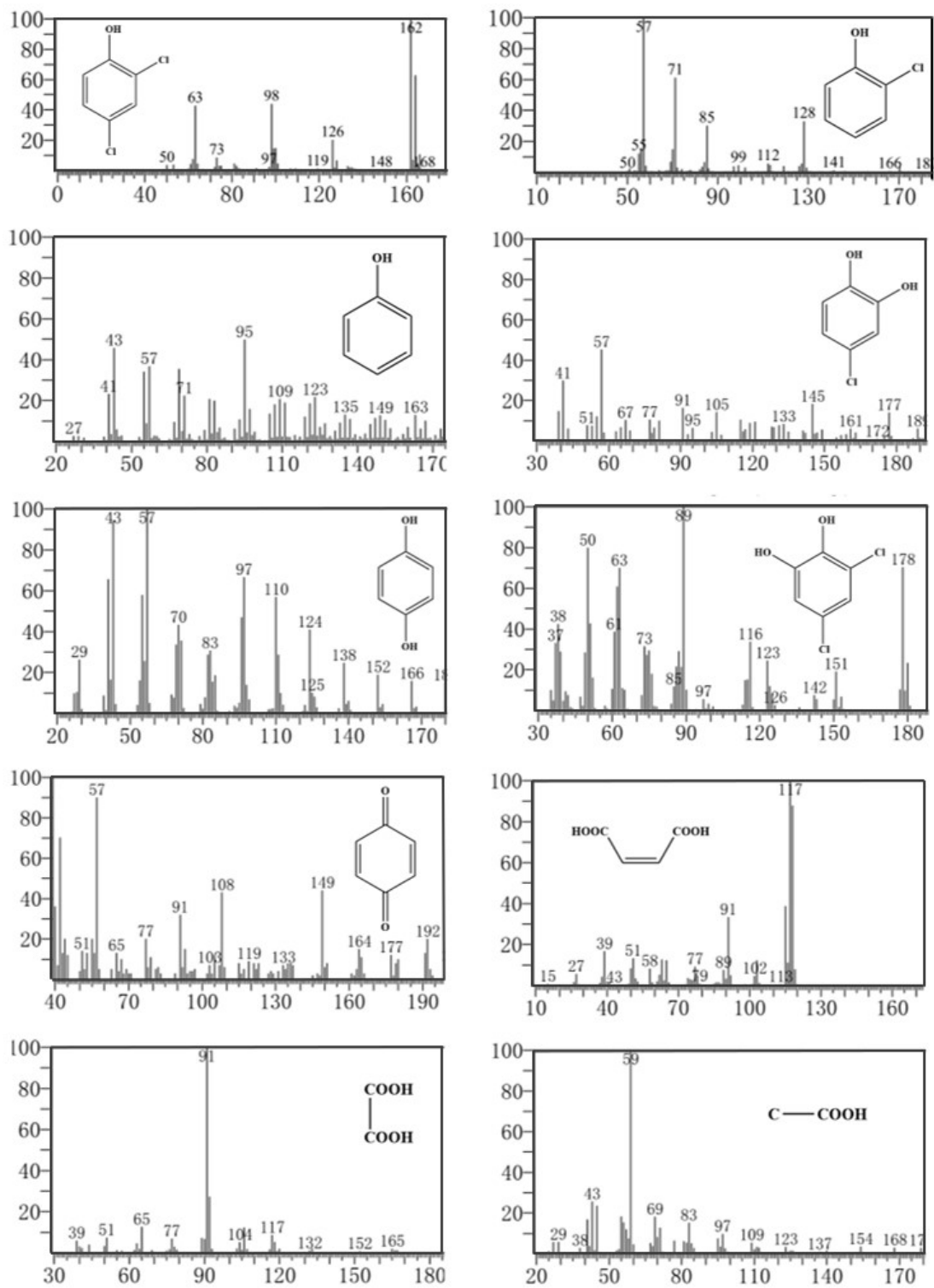


Figure S5. The mass spectra of the intermediates of 2,4-DCP.

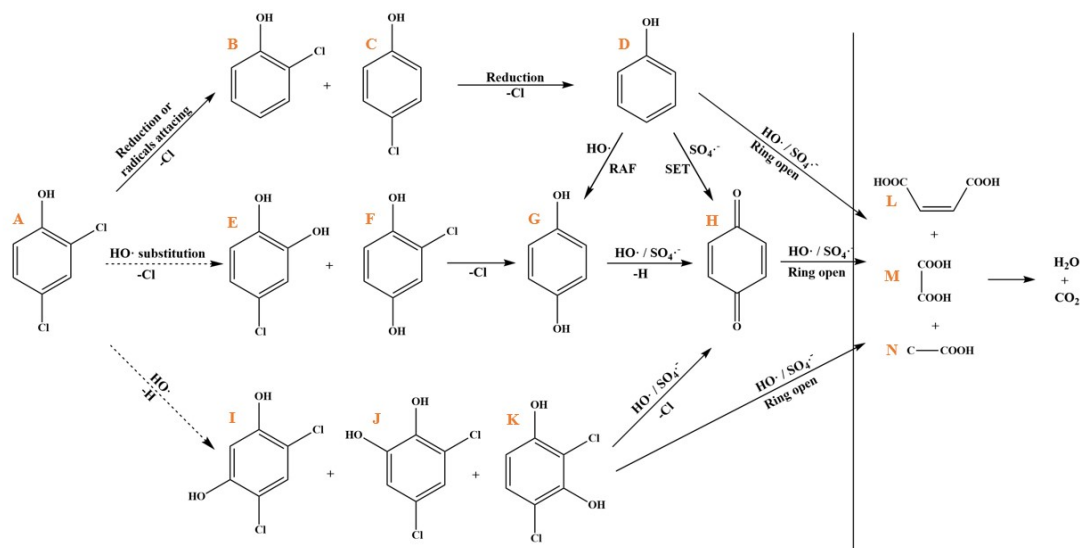


Figure S6. Degradation pathways of 2,4-DCP in sequential S-nZVI/PDS system.

Table S1. Preparation of S-nZVI with different Fe/S

Fe/S	40	60	80	100
FeCl ₃ ·6H ₂ O	3.3788 g	3.3788 g	3.3788 g	3.3788 g
Na ₂ S ₂ O ₄	0.2720 g	0.1814 g	0.1360 g	0.1088 g
NaBH ₄	1.8915 g	1.8915 g	1.8915 g	1.8915 g

Table S2. Water quality parameters of different water bodies.

Types	Milli-Q water	Tap water	Peach lake water
Initial pH	5.83	7.31	7.08
TOC (mg·L ⁻¹)	NA	5.75	19.06
Cl ⁻ (mg·L ⁻¹)	NA	13.63	10.91
SO ₄ ²⁻ (mg·L ⁻¹)	NA	28.47	16.37