Supplementary information

A comparative study of the degradation efficiency of chlorinated organic compounds by bimetallic zero-valent iron nanoparticles

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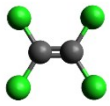
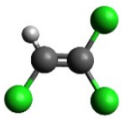
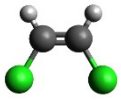
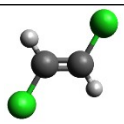
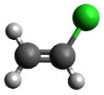
SI Content:

Text S1: Chemical oxygen demand (COD), NH_4^+, and Fe^{2+} were determined using the commercial kits LCK414, LCK305 and LCK320 (Hach-Lange), respectively. Chlorides, nitrates and sulfates were determined by Thermo Scientific™ Dionex™ ICS-2100 with Regent-Free™ IC (RFIC™) system, equipped with the conductivity detector.

Table S1 Physical and chemical properties of chlorinated solvents.

VOCs	Molecular formula and 3D model	Molecular weight (g/mol)	Density at 25 °C (g/L)	Boiling point (°C)	Melting point (°C)	Water solubility (mg/L)	Approximate half-lives (yr)	Max. contaminant concentration (µg/L) in drinking water*
PCE	CCl_4 	165.8	1.62	121	-19	150	0.7	5
TCE	C_2HCl_3 	131.4	1.46	87	-85	1100	0.7	5
DCE	$C_2H_2Cl_2$ *cis*-1,2 	96.9	1.21	54	-65	3500	1.1	70
	trans-1,2					6260	-	100

								
VC	C_2H_3Cl 	62.5	0.91	-13	-153	2700	0.55	2

*(USA regulation)

Table S2: Pseudo-first-order kinetic constants (k_{obs}) calculated for PCE degradation by various nZVI/X (nZVI/X 1 g/L).

Nanoparticles	Initial concentration[1] (mg/L)	Final concentration[2] (mg/L)	nZVI/X (g/L)	k_{obs} (h^{-1})
Blank	24	18.9	1	-
nZVI	24	17.87	1	-
nZVI/Pd	24	0.28	1	0.184 ± 0.006
nZVI/Ni	24	0	1	0.245 ± 0.017
nZVI/Ag	24	5.29	1	0.065 ± 0.018
nZVI/Cu	24	16.5	1	0.016 ± 0.001

[1]Initial concentration detected by GC/MS, [2]final concentration detected after 24 h (0 = below the detection limit)

Table S3: Comparison of the price of metal precursors used in this work (Sigma-Aldrich 16/09/2021).

Compound	g	Price (USD)	USD/g	Purity
Potassium tetrachloropalladate(II)	10	768.7	76.8	98%
Nickel(II) chloride	250	354	1.4	98%
Silver nitrate	500	1630	3.26	≥99%
Copper(II) chloride	1000	143.9	0.14	97%

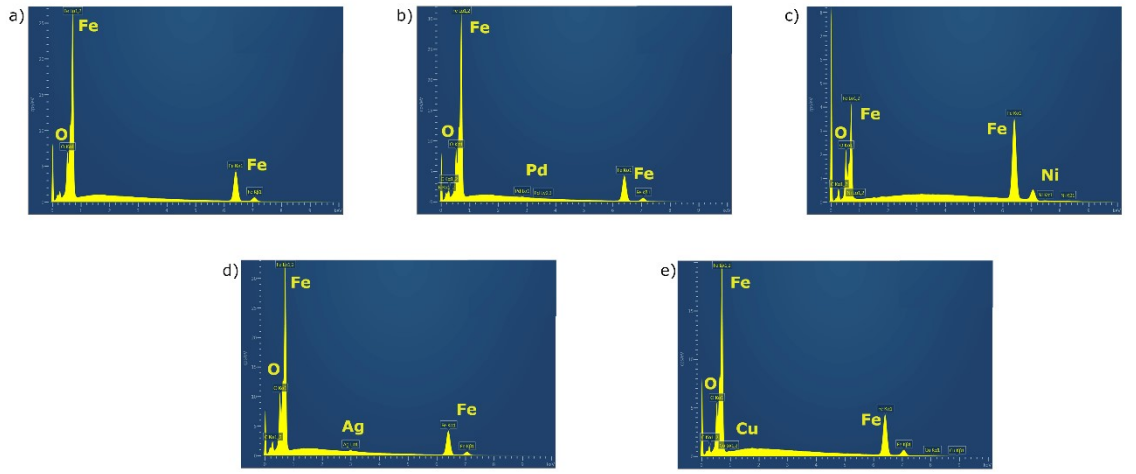


Figure S1 EDS of a) nZVI, b) nZVI/Pd, c) nZVI/Ni, d) nZVI/Ag and e) nZVI/Cu.

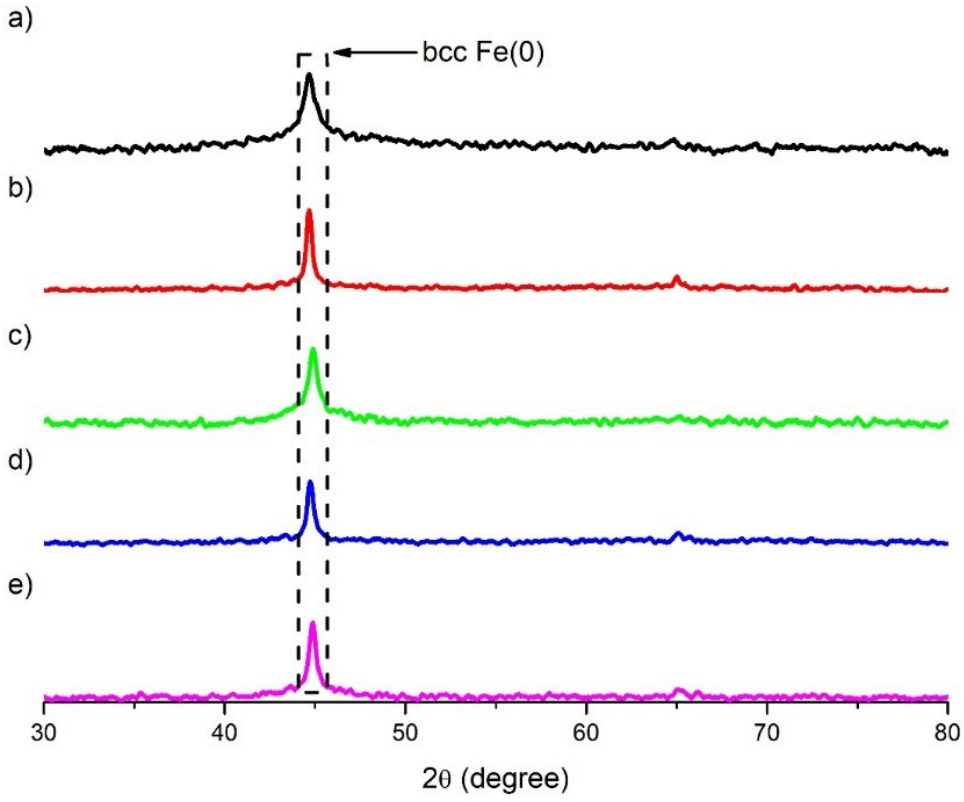
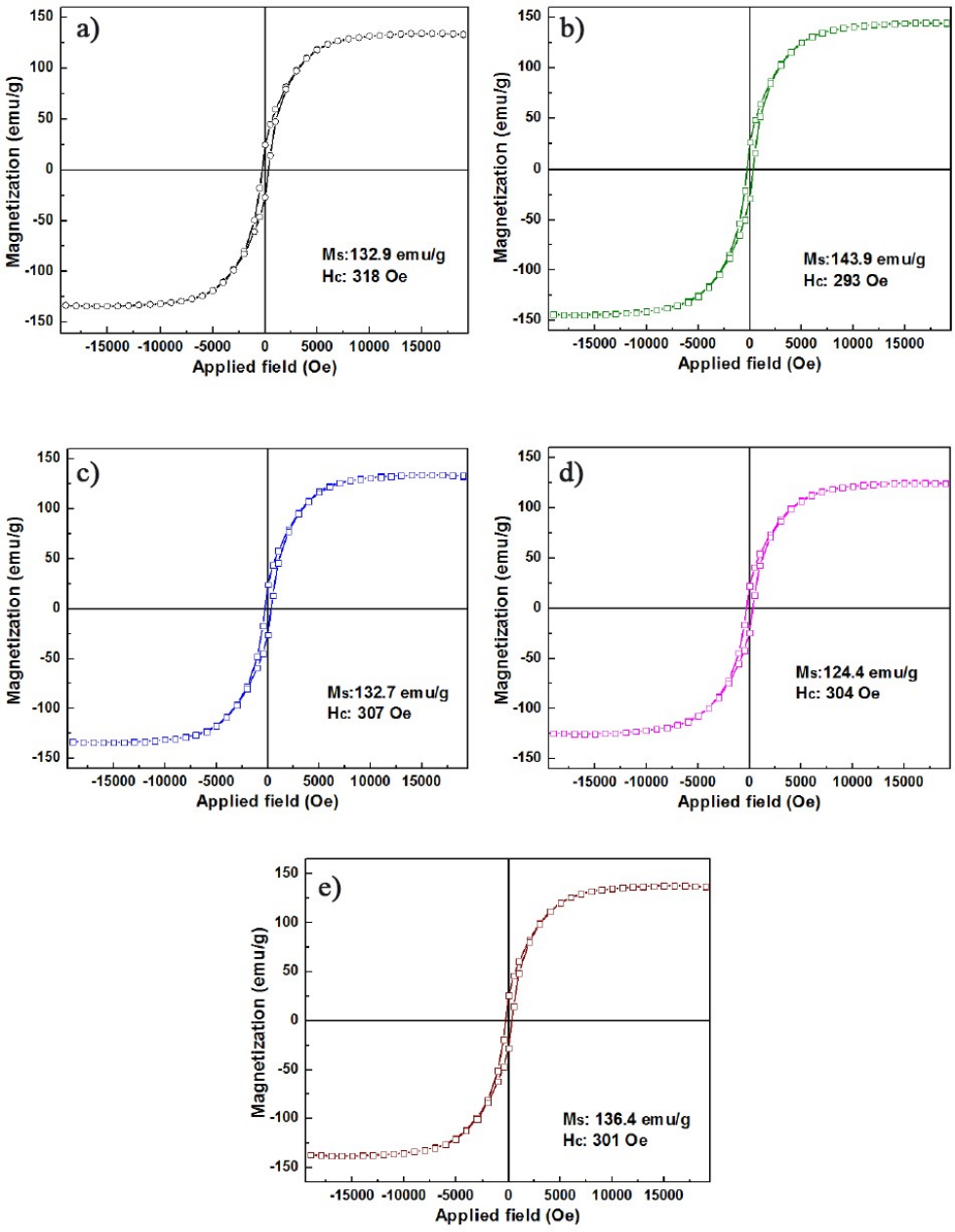


Figure S2 XRD patterns of a) nZVI, b) nZVI/Pd, c) nZVI/Ni, d) nZVI/Ag and e) nZVI/Cu.



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66 **Figure S3** Vibrating-sample magnetometer hysteresis loops for a) nZVI, b) nZVI/Pd, c)

67 nZVI/Ni, d) nZVI/Ag and e) NZVI/Cu.

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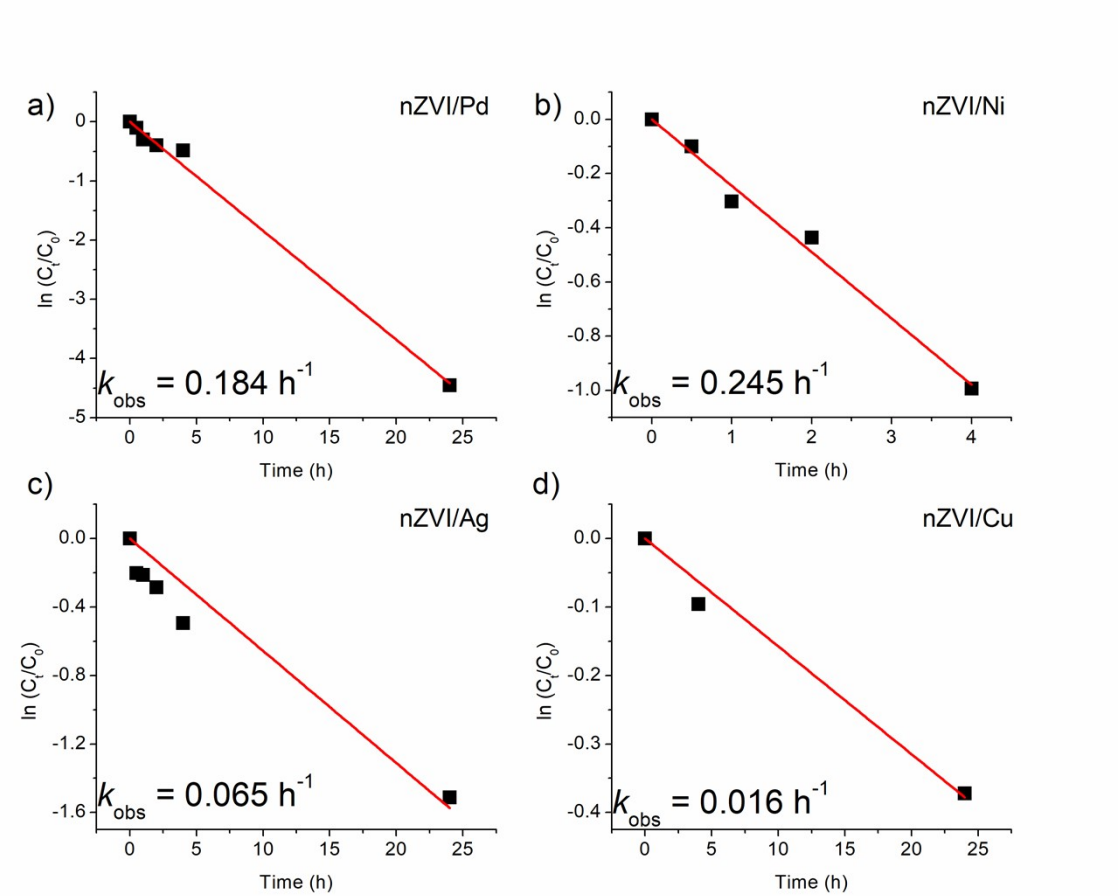

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73 **Figure S4** Pseudo-first-order model for PCE reduction in synthetic water by a) nZVI/Pd, b)

74 nZVI/Ni, c) nZVI/Ag and d) nZVI/Cu.

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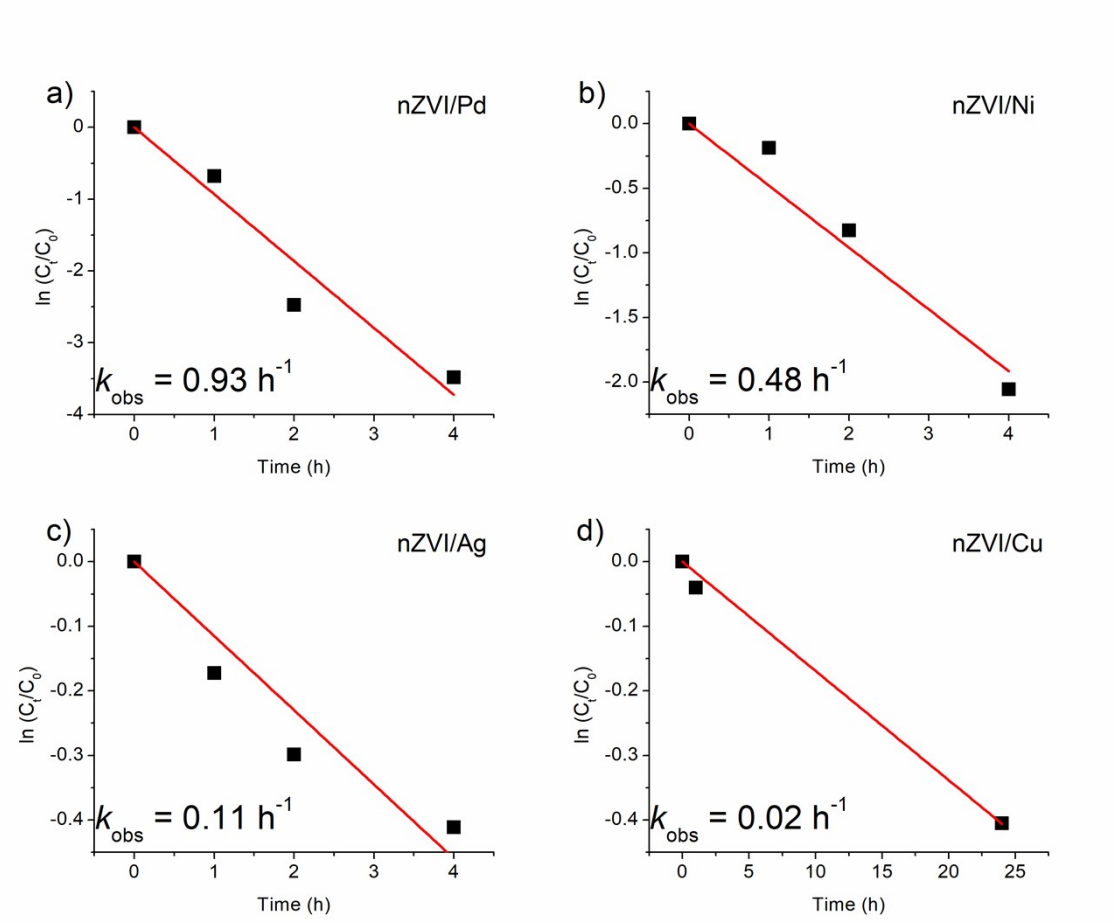

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77 **Figure S5** Pseudo-first-order model for PCE reduction in real groundwater by a) nZVI/Pd, b)

78 nZVI/Ni, c) nZVI/Ag and d) nZVI/Cu.

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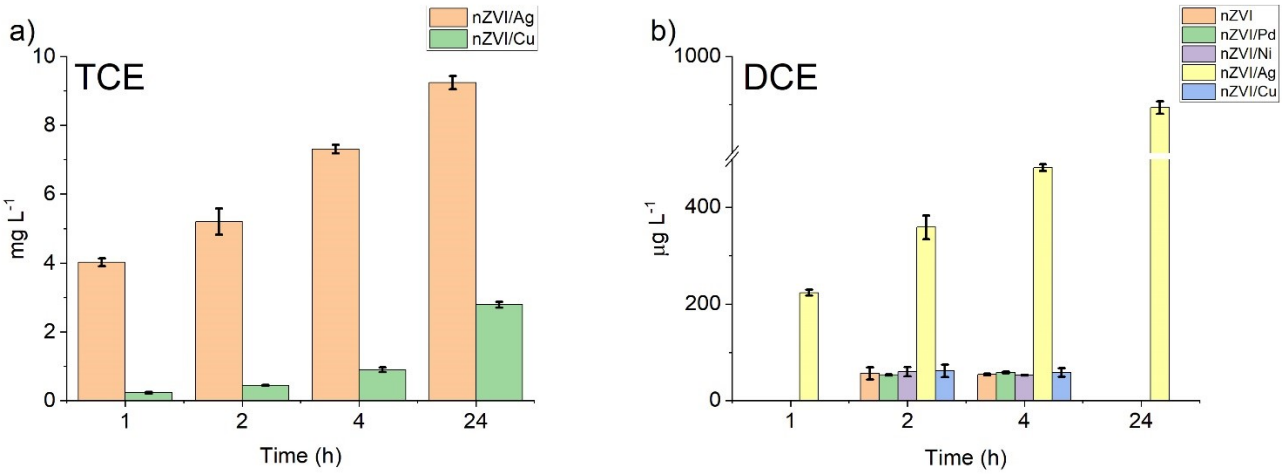

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Figure S6 a) TCE and b) DCE determination during the PCE degradation. nZVI, nZVI/Pd and nZVI/Ni do not show TCE formation during the test.