

Reporting Summary

Nature Portfolio wishes to improve the reproducibility of the work that we publish. This form provides structure for consistency and transparency in reporting. For further information on Nature Portfolio policies, see our [Editorial Policies](#) and the [Editorial Policy Checklist](#).

Statistics

For all statistical analyses, confirm that the following items are present in the figure legend, table legend, main text, or Methods section.

n/a	Confirmed
☐	☒ The exact sample size (<i>n</i>) for each experimental group/condition, given as a discrete number and unit of measurement
☐	☒ A statement on whether measurements were taken from distinct samples or whether the same sample was measured repeatedly
☒	☐ The statistical test(s) used AND whether they are one- or two-sided <i>Only common tests should be described solely by name; describe more complex techniques in the Methods section.</i>
☐	☒ A description of all covariates tested
☐	☒ A description of any assumptions or corrections, such as tests of normality and adjustment for multiple comparisons
☐	☒ A full description of the statistical parameters including central tendency (e.g. means) or other basic estimates (e.g. regression coefficient) AND variation (e.g. standard deviation) or associated estimates of uncertainty (e.g. confidence intervals)
☒	☐ For null hypothesis testing, the test statistic (e.g. <i>F</i> , <i>t</i> , <i>r</i>) with confidence intervals, effect sizes, degrees of freedom and <i>P</i> value noted <i>Give P values as exact values whenever suitable.</i>
☒	☐ For Bayesian analysis, information on the choice of priors and Markov chain Monte Carlo settings
☐	☒ For hierarchical and complex designs, identification of the appropriate level for tests and full reporting of outcomes
☒	☐ Estimates of effect sizes (e.g. Cohen's <i>d</i> , Pearson's <i>r</i>), indicating how they were calculated

Our web collection on [statistics for biologists](#) contains articles on many of the points above.

Software and code

Policy information about [availability of computer code](#)

Data collection	Data were acquired using commercial instruments (Rigaku D/max-2200PC, Thermo Scientific K-Alpha, Nicolet iS20, IONTOF TOF.SIMS 5, FEI Talos F200X, ASAP 2460, Agilent 9790, CHI-760e,Agilent 1260 Infinity ?, Agilent 1290-6545, ICS-1100, Agilent 7900, Bruker EMXplus-6/1, LabRAM HR Evolution, Agilent 7890B, Bruker 400M) with manufacturer-provided software for instrument control. DFT calculations were performed using VASP 6.3.2 (commercially available). No custom code was used for data collection.
Data analysis	Data were analyzed using commercial software, including MDI Jade 6.5, XPSPeak 4.1, OMNIC 9.2, DigitalMicrograph 3.2, ZSimpWin 3.6, Qualitative Analysis B.07.00, MestReNova 14.0, VASP 6.4.1, VESTA 3.5. No custom code was used for data analysis.

For manuscripts utilizing custom algorithms or software that are central to the research but not yet described in published literature, software must be made available to editors and reviewers. We strongly encourage code deposition in a community repository (e.g. GitHub). See the Nature Portfolio [guidelines for submitting code & software](#) for further information.

Data

Policy information about [availability of data](#)

All manuscripts must include a [data availability statement](#). This statement should provide the following information, where applicable:

- Accession codes, unique identifiers, or web links for publicly available datasets
- A description of any restrictions on data availability
- For clinical datasets or third party data, please ensure that the statement adheres to our [policy](#)

The data that support the findings of this study are available in the paper and Supplementary Information. The DFT optimized structures used for electronic structure calculations are provided in the Supplementary Data 1. Source data are provided with this paper.

Research involving human participants, their data, or biological material

Policy information about studies with [human participants or human data](#). See also policy information about [sex, gender \(identity/presentation\), and sexual orientation](#) and [race, ethnicity and racism](#).

Reporting on sex and gender

This study does not involve human participants, human data, or biological samples from human subjects. Therefore, no sex- or gender-based analyses were performed or required.

Reporting on race, ethnicity, or other socially relevant groupings

This study does not involve human participants or socially relevant grouping variables. No such classifications were used in the experimental design or data analysis.

Population characteristics

The research was conducted using chemical reagents and environmental water samples; no human research participants were enrolled.

Recruitment

No human participants were recruited for this study.

Ethics oversight

As this research does not involve human participants, human data, or animal experiments, no ethical approval was required. The groundwater samples used were collected from an industrial site for chemical analysis only, and no human or biological data were collected.

Note that full information on the approval of the study protocol must also be provided in the manuscript.

Field-specific reporting

Please select the one below that is the best fit for your research. If you are not sure, read the appropriate sections before making your selection.

☐ Life sciences

☐ Behavioural & social sciences

☒ Ecological, evolutionary & environmental sciences

For a reference copy of the document with all sections, see [nature.com/documents/nr-reporting-summary-flat.pdf](https://www.nature.com/documents/nr-reporting-summary-flat.pdf)

Ecological, evolutionary & environmental sciences study design

All studies must disclose on these points even when the disclosure is negative.

Study description

This study investigates the hydrodehalogenation performance of mechanochemically activated zero-valent iron via interfacial hydride transfer. Batch degradation experiments were conducted using florfenicol (FF) and several chlorinated hydrocarbons. Quantitative data include pseudo-first-order rate constants, surface-area-normalized rate constants, electron efficiency, and kinetic isotope effects. Each treatment was performed in triplicate (n=3). Treatment factors include material type, water source, and pollutant type. The experimental design is completely randomized with repeated measurements over time.

Research sample

The research samples consist of chemically synthesized ZVI materials and aqueous pollutant solutions; no biological organisms, populations, or field specimens were involved. A groundwater sample collected from an industrial site in Taizhou, Zhejiang, China, was used as a real environmental matrix to validate material performance, selected for its representative co-contamination profile (chlorinated solvents, As, and Cr(VI)). The target pollutants (FF, TCE, PCE, CF, etc.) were chosen based on their environmental prevalence and structural representativeness.

Sampling strategy

For laboratory batch experiments, no statistical sample-size calculation was performed. Sample sizes of n=3 independent replicates per condition were chosen based on standard practices in environmental chemistry kinetics studies, which provide sufficient data points for reliable pseudo-first-order kinetic fitting and acceptable standard deviations. For the real groundwater, a single grab sample was used; this is representative of the site conditions (Supplementary Table 10) and was used without treatment to validate material performance, rather than for statistical comparison.

Data collection

Data were collected by the co-authors (L.G., S.W., Z.Z., and F.G.) using standard analytical instruments. Concentrations of FF and its degradation products were determined by HPLC (Agilent 1260) and UPLC-Q-TOF MS/MS (Agilent 1290/6545). Chlorinated

hydrocarbons were analyzed by GC (Agilent 7890B). Material characterizations (XRD, XPS, FTIR, TOF-SIMS, Raman, HRTEM, BET, etc.) were performed by trained personnel following manufacturer protocols.

Timing and spatial scale	Laboratory degradation experiments were conducted at a constant temperature (25 ± 2 °C) with sampling at predetermined time intervals (ranging from hours to days depending on the reaction kinetics). For FF degradation, samples were collected at 0, 1, 3, 5, 7, 10, 15, 20, 30, and 40 days. For chlorinated hydrocarbons, sampling times were shorter (0, 1, 2, 4, 6, 8, 12, 24, and 48 h). The continuous-flow column experiment ran for 10 days with daily effluent sampling. All experiments were performed in the laboratory at Zhejiang University of Technology and Shanghai Jiao Tong University. No field data collection beyond the single groundwater grab sample was performed.
Data exclusions	No data were excluded from the analyses. All collected data points were included in the kinetic fitting and statistical evaluations.
Reproducibility	All batch experiments were performed with at least three independent replicates (n=3). All attempts to repeat the experiments were successful, as indicated by the small standard deviations reported in the kinetic data.
Randomization	Randomization was not relevant to this study because the experimental units are inanimate chemical materials and solutions, not biological organisms or human participants. All samples were treated identically except for the intentionally varied parameters (material type, water source, pollutant type). Covariates such as temperature, pH, and material dosage were controlled and kept constant across all groups to ensure fair comparisons.
Blinding	Blinding was not relevant to this study.

Did the study involve field work? ☐ Yes ☒ No

Reporting for specific materials, systems and methods

We require information from authors about some types of materials, experimental systems and methods used in many studies. Here, indicate whether each material, system or method listed is relevant to your study. If you are not sure if a list item applies to your research, read the appropriate section before selecting a response.

Materials & experimental systems

n/a	Involved in the study
☒	☐ Antibodies
☒	☐ Eukaryotic cell lines
☒	☐ Palaeontology and archaeology
☒	☐ Animals and other organisms
☒	☐ Clinical data
☒	☐ Dual use research of concern
☒	☐ Plants

Methods

n/a	Involved in the study
☒	☐ ChIP-seq
☒	☐ Flow cytometry
☒	☐ MRI-based neuroimaging

Plants

Seed stocks	No seed stocks or plant materials were used in this study.
Novel plant genotypes	No novel plant genotypes were generated or analyzed.
Authentication	No plant genotype authentication was performed as no plant materials were involved.