Supplementary Information for

Microbial–mineral–organic matter framework links environment and soil sulfur cycling

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Supplementary Information file includes:

Supplementary Methods and Discussion

1. Supplementary Methods

1.1. Bibliometric analysis methods

At present, bibliometric analysis has become a significant technique for conducting extensive literature reviews in the scientific field[1]. The synergy between scientific knowledge graph technology and bibliometric analysis facilitates the elucidation of provenance, structural evolution, and interconnections of knowledge[2]. VOSviewer and Biblioshiny are the primary tools for knowledge graphing and visualization analysis[3]. The former has demonstrated proficiency in the analysis of multidimensional co-occurrence networks, encompassing authors, keywords, and citations. Conversely, the latter utilizes the R language for quantitative analysis and the identification of research themes. Both tools are compatible with standardized data formats and can perform multidimensional index analysis on countries, institutions, authors, publications, and similar entities. This study employs VOSviewer and Biblioshiny to conduct bibliometric analysis in the field of soil sulfur biogeochemical cycles. A comprehensive data extraction process was conducted from 3,946 publications, followed by systematic clustering and analysis of collaboration information among authors, institutions, and countries. Additionally, association information among key keywords was examined, and the results were visually represented through network diagrams[4]. The data analysis methods and framework utilized in this study are schematically delineated in Fig. S1. The main objectives of the strategy were to identify dominant themes and innovative research avenues, to provide quantitative evidence of the advancement of knowledge in related fields, and to outline future research programs[5].

1.2. Data collection and processing

In this study, we chose Web of Science (WoS) for bibliometric analysis, which uses the keyword search to identify the data source[6]. The analysis of data is based on SCI-Expanded in the WoS core collection database of the Institute of Scientific Information.

The retrieval term is TI = soil* AND TS = (“sulfur” OR “sulph*” OR “sulfide” OR “sulfo*” OR “sulfate*” OR “sulphate*” OR “SO_4^{2-}” OR “FeS” OR “FeS_2” OR “AVS” OR “organic sulfur” OR “organic sulphur” OR “organic S” OR “inorganic sulfur” OR “inorganic sulphur” OR “inorganic S” OR “sulfur Isotop*” OR “sulphur Isotop*” OR “sulfide isotop*” OR “S isotop*”) AND (“microorganism*” OR “soil microorganism*” OR “soil microbe*” OR “soil microbial” OR “soil microbial communit*” OR “SRB” OR “SOB” OR “soil microbial biomass” OR “functional gene*” OR “function gene*” OR “functional genomic*” OR “gene*” OR “functional microorganism*” OR “functional microbe*” OR “functional microbial” OR “functional bacteria” OR “function microorganism*” OR “soil mineral-organic matter” OR “mineral-organic matter” OR “biogeochemical cycl*” OR “biogeochemistry cycl*” OR “biogeochemistry” OR “biogeochemical circulation” OR “environmental effect*” OR “environmental impact*” OR “environmental influence” OR “environment effect*”). The asterisk is used to retrieve all potential derivatives of the words, while the quote marks are used to obtain accurate and exact formulations. TS represents the theme subject search in the WoS database search. Using keywords, the TS retrieval technique based on Boolean logic can quickly and simply find a large amount of literature data related to the topic[7]. After the screening, comparison, and weighing, 3,946 bibliography catalogs were finally obtained from 1998 to 2025. The dataset fields included authors, institutions, author keywords, year of publication, journals, and references[8]. Additionally, the extracted data underwent a series of processing steps aimed at removing duplicates, eliminating items of minimal significance, and combining synonyms[9]. Furthermore, the present study employed mapping tools such as Adobe Illustrator and Microsoft PowerPoint to effectively illustrate the processes and mechanisms of sulfur transformations. These transformations were examined within the core framework of "microbial-mineral-organic interactions", microbial-supported sulfur transformations networks, and human-induced sulfur loading. The environmental impacts of the soil sulfur cycle were also investigated.

2. Supplementary Discussion

2.1. Bibliometric mapping of research hotspots and knowledge structure in soil sulfur cycling

This review systematically characterizes the evolving knowledge structure and research trajectories of soil sulfur cycling research from a bibliometric perspective (Fig. S2). Framed around the conceptual lens of the "microbial–mineral–organic matter interface", the analysis highlights the increasing integration of molecular, ecological, and environmental perspectives across the field. Network analysis resolves five principal research clusters, spanning fundamental biogeochemical mechanisms to environmental applications, thereby clarifying both the major contemporary hotspots and the emerging frontiers likely to shape future research directions (Fig. S3).

Cluster 1, which focuses on central processes in soil sulfur biogeochemistry, represents a conceptual core of the field. It emphasizes the mechanistic basis and ecological consequences of sulfur cycling under variable redox and pH conditions, including sulfur transformation pathways, mineral-associated reactions, and system-level biogeochemical feedbacks[10,11]. Cluster 2 centers on microbial ecology, soil health, and rhizosphere interactions, highlighting the important role of microbial diversity, community assembly, and functional networks in regulating sulfur transformations and sustaining ecosystem functions and services[12,13]. Clusters 3 and 4 extend the scope of soil sulfur cycling research toward its intersection with environmental contamination and remediation, addressing topics such as heavy metal mobility, sulfur-driven redox chemistry, pollutant transformation, and advances in bioremediation and stabilization technologies[14,15]. Cluster 5 focuses on sulfur-related feedbacks on soil acidification, nutrient cycling, and broader environmental stress responses, thus linking sulfur dynamics to wider ecosystem vulnerability and resilience under changing environmental conditions[16].

Taken together, these clusters illustrate the integrative, cross-scale, and multi-dimensional nature of contemporary soil sulfur cycling research. More importantly, they indicate that current progress in the field increasingly depends on linking mechanistic understanding of sulfur transformations with microbial regulation, mineral reactivity, and environmental impacts within a common analytical framework. In this context, the interface-centric perspective provides a particularly useful basis for organizing diverse lines of evidence and for interpreting how sulfur cycling interacts with soil ecosystem feedbacks under anthropogenic disturbance and global change (Table S1).

2.2. Temporal research trends, collaboration patterns, and future directions in soil sulfur cycling

Temporal keyword heatmap analysis (Fig. S3) indicates a marked shift in research priorities over recent decades, reflecting a transition from classical sulfur geochemistry toward more integrative themes, including pollution remediation, microbial ecology, and sustainable soil management. Emerging topics—such as antibiotic resistance genes, sulfur-associated contaminant dynamics, and the application of remediation materials such as biochar—highlight both the expanding scope of the field and the practical relevance of interface-based interpretations of sulfur cycling. These temporal patterns suggest that soil sulfur research is increasingly moving beyond descriptive geochemistry toward a more process-oriented and application-relevant framework that links microbial activity, mineral reactivity, and environmental outcomes.

Institutional and international collaboration analyses (Fig. S4) further show that the Chinese Academy of Sciences occupies a prominent position within the current research network, while global partnerships have expanded substantially in recent years, with growing contributions from emerging research economies (Table S2, Table S3). This pattern indicates that soil sulfur cycling research is becoming increasingly internationalized and collaborative, which is particularly important for addressing questions that span contrasting soil types, climatic conditions, and management regimes. At the author level, collaboration network analysis (Fig. S5) suggests that several scholars—including Peter Osterholm, Jizhong Zhou, Jing Wang, and Jianming Xu—occupy influential positions within the co-authorship network and have contributed substantially to the continuity and development of the field. The sustained publication activity of these and other highly connected authors, together with the expansion of collaborative ties, indicates an active and evolving research community with growing capacity for interdisciplinary integration.

Taken together, the bibliometric patterns summarized here highlight both the active hotspots and the emerging frontiers of soil sulfur cycling research. When interpreted through the lens of microbial–mineral–organic matter interactions, these trends suggest that future progress will increasingly depend on integrating mechanistic insight with broader ecological and environmental applications. In particular, continued advances in high-throughput molecular techniques, multi-omics, advanced imaging, and predictive modeling will be essential for resolving the complex networks and feedbacks that underpin sulfur cycling across scales[17,18]. At the same time, sustained international collaboration and interdisciplinary integration will be critical for addressing global environmental change, protecting soil health, and maintaining the ecosystem services supported by sulfur-regulated processes[19,20].

Looking forward, future research may benefit from greater emphasis on the development and testing of engineered microbial consortia, novel composite amendments, and precision fertilization strategies for mitigating sulfur-related soil degradation and restoring ecosystem function[21,22]. In parallel, strengthening international collaboration and interdisciplinary coordination will be important for harmonizing monitoring protocols, expanding data sharing, improving AI-assisted model development, and leveraging complementary expertise across soil science, microbial ecology, and environmental science[23,24] (Fig. S6). Collectively, these directions point toward a more predictive, application-oriented, and globally coordinated research agenda for soil sulfur cycling.

Supplementary figures and tables

Figure captions

Fig. S1. Workflow of the bibliometric analysis used in this study.

The bibliometric framework focused on studies of the soil sulfur cycle in relation to the microbial–mineral–organic matter interaction framework. Records were retrieved from the Web of Science Core Collection and analysed using VOSviewer and Biblioshiny to examine research trends, keyword networks, thematic evolution, institution distribution, authors' productivity, and country-level collaboration.

Fig. S2. Trends in the number of publications in different countries from 1998 to 2025.

The number of publications increased markedly over time, particularly after the mid-2010s, with China and the USA contributing the largest shares in recent years. This pattern indicates growing global interest and increasing international participation in soil sulfur cycling research.

Fig. S3. (a) Cluster analysis of the author keywords' co-occurrence of biogeochemical cycling and environmental effects of soil sulfur; (b) Author keywords frequency distribution and author keywords cumulative frequency distribution heatmap.

Co-occurrence network of author keywords showing five major thematic clusters in soil sulfur research, spanning biogeochemical processes, microbial ecology, environmental contamination, remediation, and acidification-related responses. Node size indicates keyword frequency, and link strength reflects co-occurrence intensity. Heatmaps showing the temporal distribution and cumulative frequency of representative author keywords from 1998 to 2025, illustrating the evolution of research emphasis and the emergence of major thematic hotspots over time.

Fig. S4. (a) Analysis of cooperation networks between institutions of biogeochemical cycling and environmental effects of soil sulfur; (b) Analysis of cooperation networks between countries; (c) Network map of cooperation between countries (NP: the number of papers).

Institutional collaboration network showing major contributing organizations and their interconnections in soil sulfur research. Country-level collaboration network illustrating the international structure of research partnerships. Global distribution of publication output by country, with color intensity indicating the number of papers. Together, these panels highlight the central roles of major institutions and countries and the increasingly international character of research on soil sulfur biogeochemical cycling and its environmental effects.

Fig. S5. (a) Network analysis of collaboration between authors of biogeochemical cycling and environmental effects of soil sulfur (color shades indicate the average publication year of the author); (b) Top 30 authors in terms of quantity and quality of publications (NP: the number of papers; TCPY: total citations per year).

Collaboration network showing major author groups and their connections in soil sulfur research, with color gradients indicating the average publication year of each author. Temporal distribution of publication output and citation impact for the top 30 authors, illustrating patterns of research productivity and academic influence over time.

Fig. S6. A concise flowchart for constructing AI models for soil sulfur cycle research.

Schematic workflow for AI model development in soil sulfur cycle research, including data collection, preprocessing, feature engineering, model selection, training, evaluation, interpretation, and deployment. The framework highlights a stepwise pipeline for integrating multi-source data and building interpretable, application-oriented predictive models.

Table captions

Table S1. Top 30 keywords with high occurrences of biogeochemical cycling and environmental effects of soil sulfur.

Table S2. Top 20 countries with high cooperation of biogeochemical cycling and environmental effects of soil sulfur.

Table S3. Top 20 research institutions with high cooperation of biogeochemical cycling and environmental effects of soil sulfur.

Table S4. Framework-informed research questions: linking reactive interfaces and cross-scale dynamics in soil sulfur cycling.

Table S5. Measurable proxies and model-compatible variables for operationalizing the microbial–mineral–organic matter framework in soil sulfur cycling.

Fig. S1

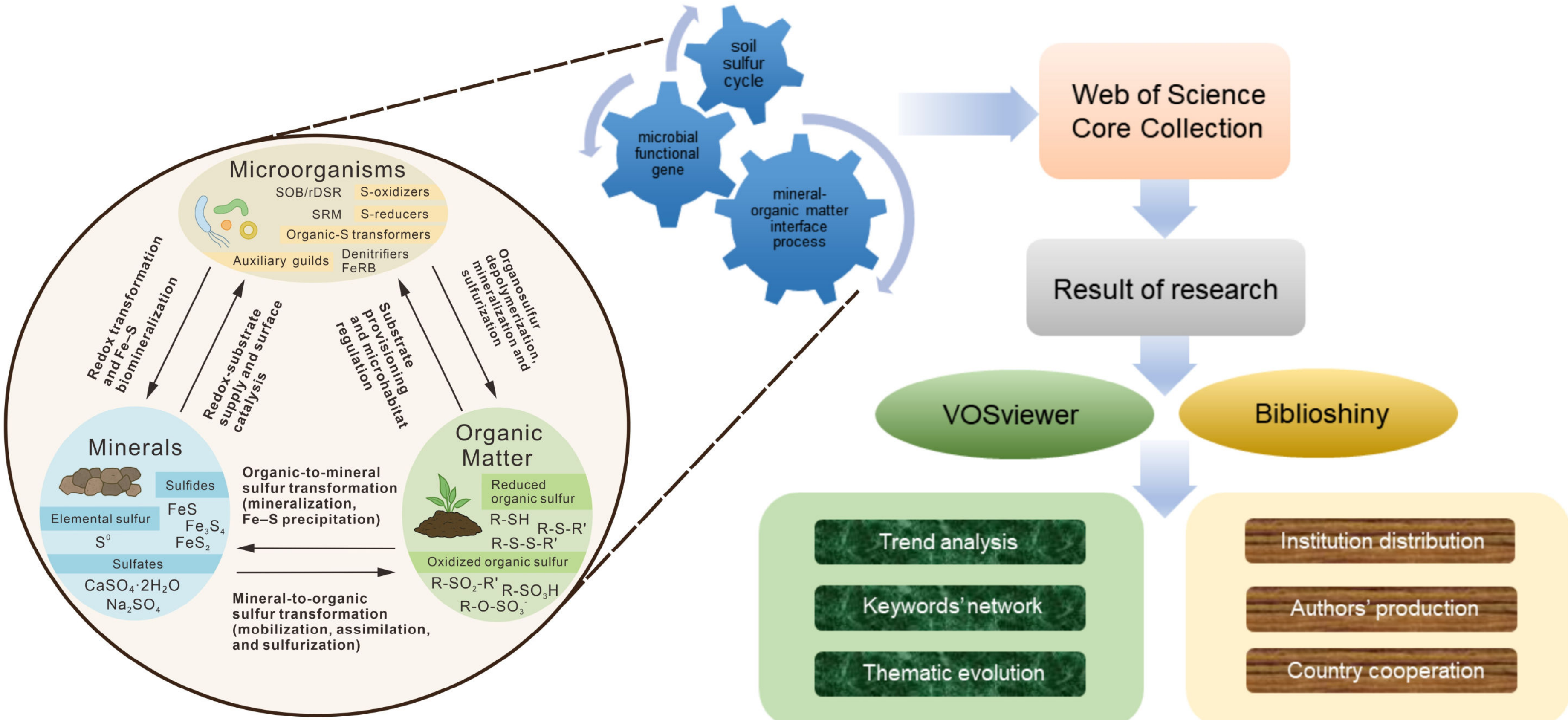
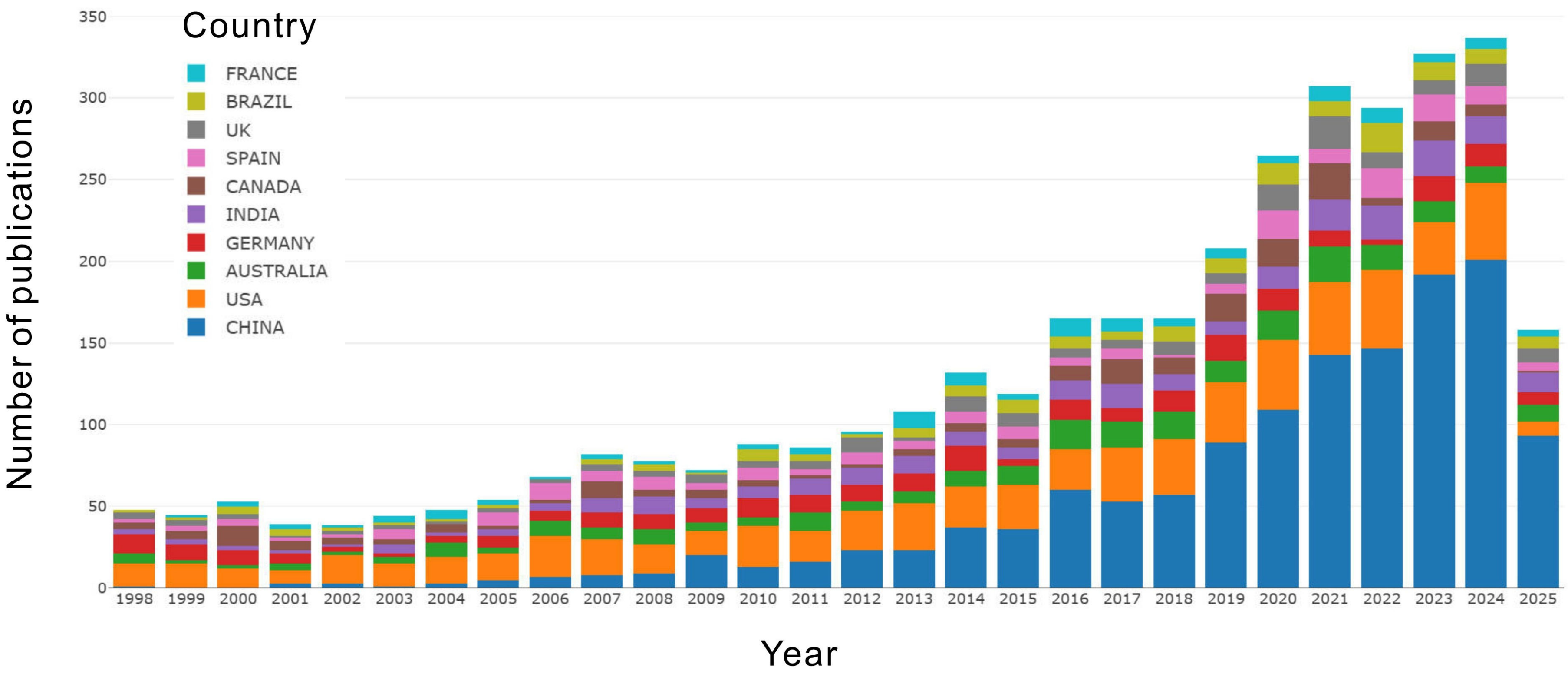

Microorganisms
SOB/rDSR
S-oxidizers
SRM
S-reducers
Organic-S transformers
Auxiliary guilds
Denitrifiers
FeRB
Redox transformation and Fe–S biomineralization
Redox-substrate supply and surface catalysis
Substrate provisioning and microhabitat regulation
Organosulfur depolymerization, mineralization and sulfurization
Minerals
Sulfides
Elemental sulfur
FeS
Fe_3S_4
S^0
FeS_2
Sulfates
$CaSO_4 \cdot 2H_2O$
Na_2SO_4
Organic-to-mineral sulfur transformation (mineralization, Fe–S precipitation)
Mineral-to-organic sulfur transformation (mobilization, assimilation, and sulfurization)
Organic Matter
Reduced organic sulfur
R-SH
R-S-R'
R-S-S-R'
Oxidized organic sulfur
$R-SO_2-R'$
$R-SO_3H$
$R-O-SO_3^-$
soil sulfur cycle
microbial functional gene
mineral-organic matter interface process
Web of Science Core Collection
Result of research
VOSviewer
Biblioshiny
Trend analysis
Keywords' network
Thematic evolution
Institution distribution
Authors' production
Country cooperation

Fig. S2


Country
FRANCE
BRAZIL
UK
SPAIN
CANADA
INDIA
GERMANY
AUSTRALIA
USA
CHINA
Number of publications
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50
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200
250
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Year

Fig. S3

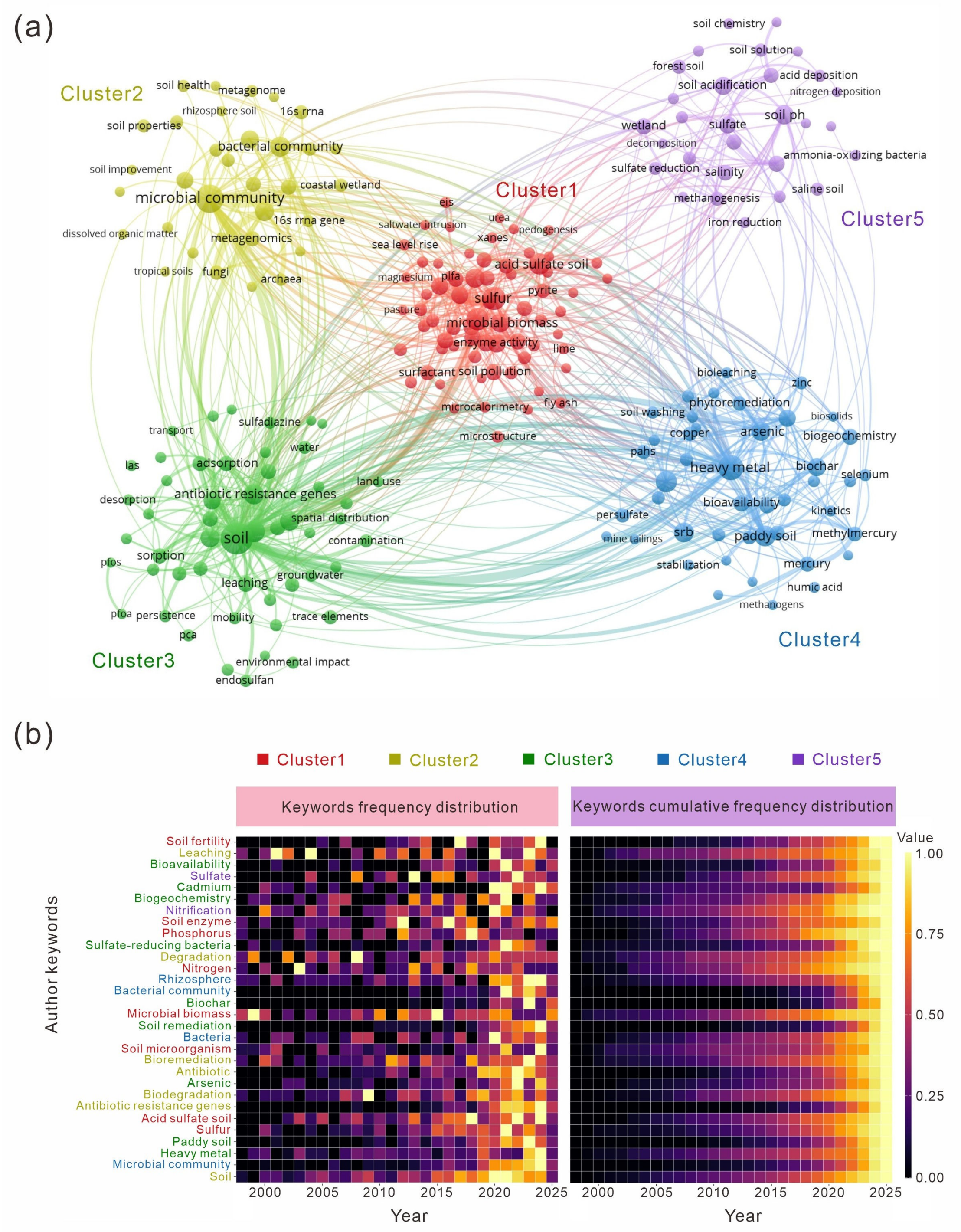
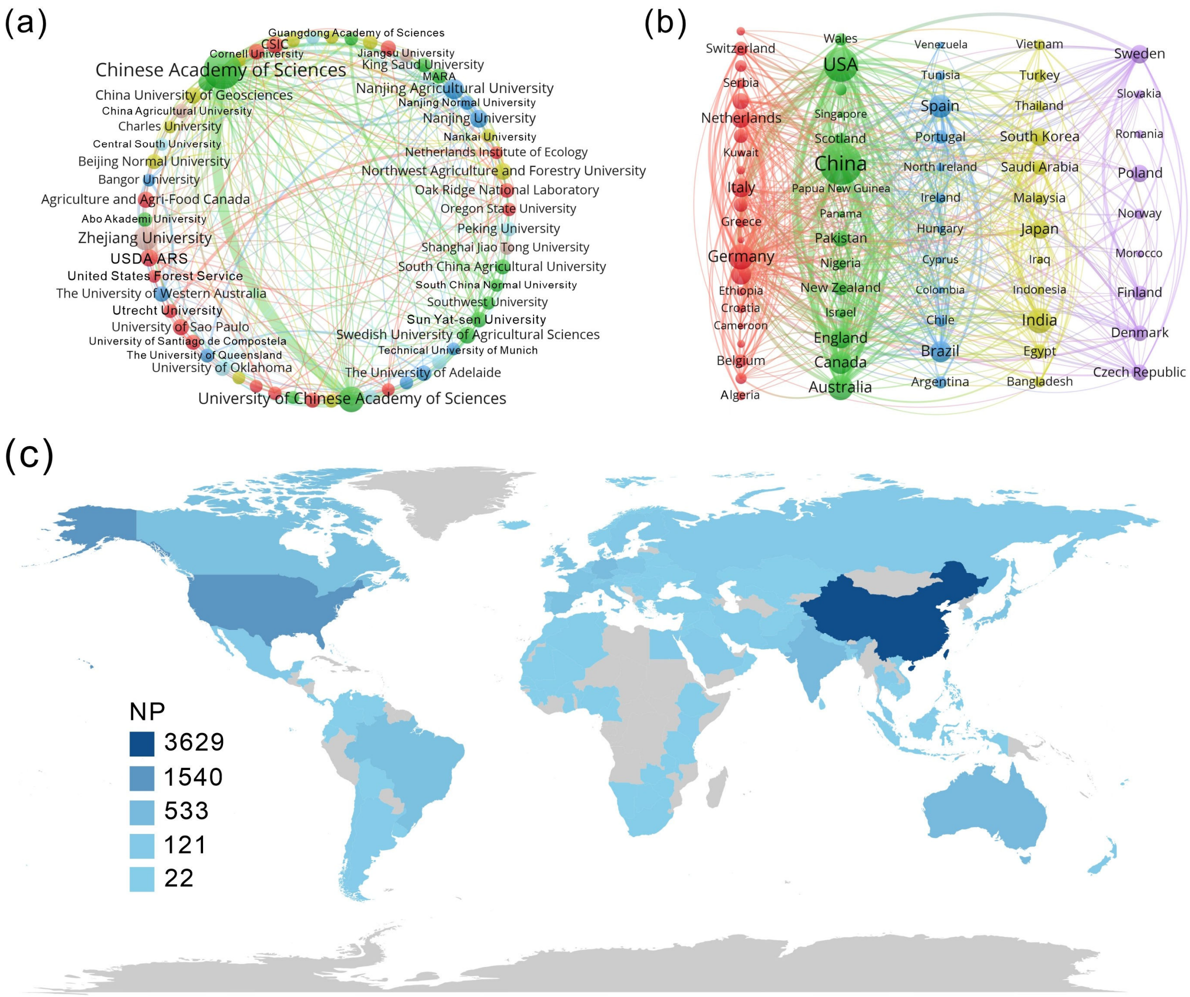

(a)
Cluster1
Cluster2
Cluster3
Cluster4
Cluster5
(b)
Keywords frequency distribution
Keywords cumulative frequency distribution
Author keywords
Soil fertility
Leaching
Bioavailability
Sulfate
Cadmium
Biogeochemistry
Nitrification
Soil enzyme
Phosphorus
Sulfate-reducing bacteria
Degradation
Nitrogen
Rhizosphere
Bacterial community
Biochar
Microbial biomass
Soil remediation
Bacteria
Soil microorganism
Bioremediation
Antibiotic
Arsenic
Biodegradation
Antibiotic resistance genes
Acid sulfate soil
Sulfur
Paddy soil
Heavy metal
Microbial community
Soil
Year
Value
1.00
0.75
0.50
0.25
0.00

Fig. S4


(a)
Chinese Academy of Sciences
University of Chinese Academy of Sciences
Zhejiang University
USDA ARS
Nanjing Agricultural University
Northwest Agriculture and Forestry University
(b)
USA
China
Germany
Italy
Netherlands
Spain
Japan
India
Brazil
Australia
Canada
England
Sweden
(c)
NP
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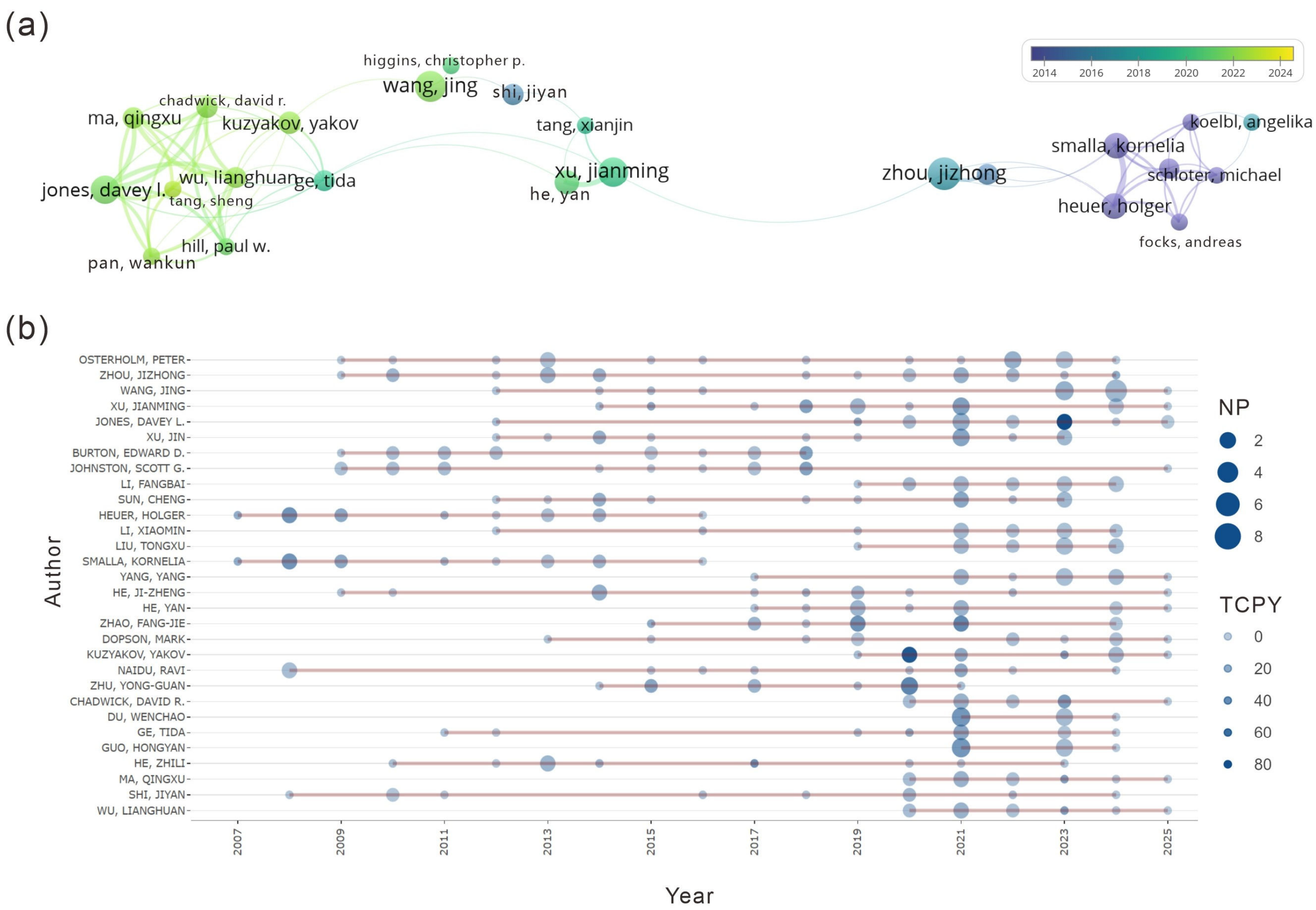
1540
533
121
22

Fig. S5



(a)
higgins, christopher p.
wang, jing
shi, jiyan
chadwick, david r.
ma, qingxu
kuzyakov, yakov
tang, xianjin
xu, jianming
jones, davey l.
wu, lianghuan
ge, tida
tang, sheng
he, yan
hill, paul w.
pan, wankun
zhou, jizhong
smalla, kornelia
koelbl, angelika
schloter, michael
heuer, holger
focks, andreas
2014
2016
2018
2020
2022
2024
(b)
Author
OSTERHOLM, PETER
ZHOU, JIZHONG
WANG, JING
XU, JIANMING
JONES, DAVEY L.
XU, JIN
BURTON, EDWARD D.
JOHNSTON, SCOTT G.
LI, FANGBAI
SUN, CHENG
HEUER, HOLGER
LI, XIAOMIN
LIU, TONGXU
SMALLA, KORNELIA
YANG, YANG
HE, JI-ZHENG
HE, YAN
ZHAO, FANG-JIE
DOPSON, MARK
KUZYAKOV, YAKOV
NAIDU, RAVI
ZHU, YONG-GUAN
CHADWICK, DAVID R.
DU, WENCHAO
GE, TIDA
GUO, HONGYAN
HE, ZHILI
MA, QINGXU
SHI, JIYAN
WU, LIANGHUAN
2007
2009
2011
2013
2015
2017
2019
2021
2023
2025
Year
NP
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4
6
8
TCPY
0
20
40
60
80

Fig. S6

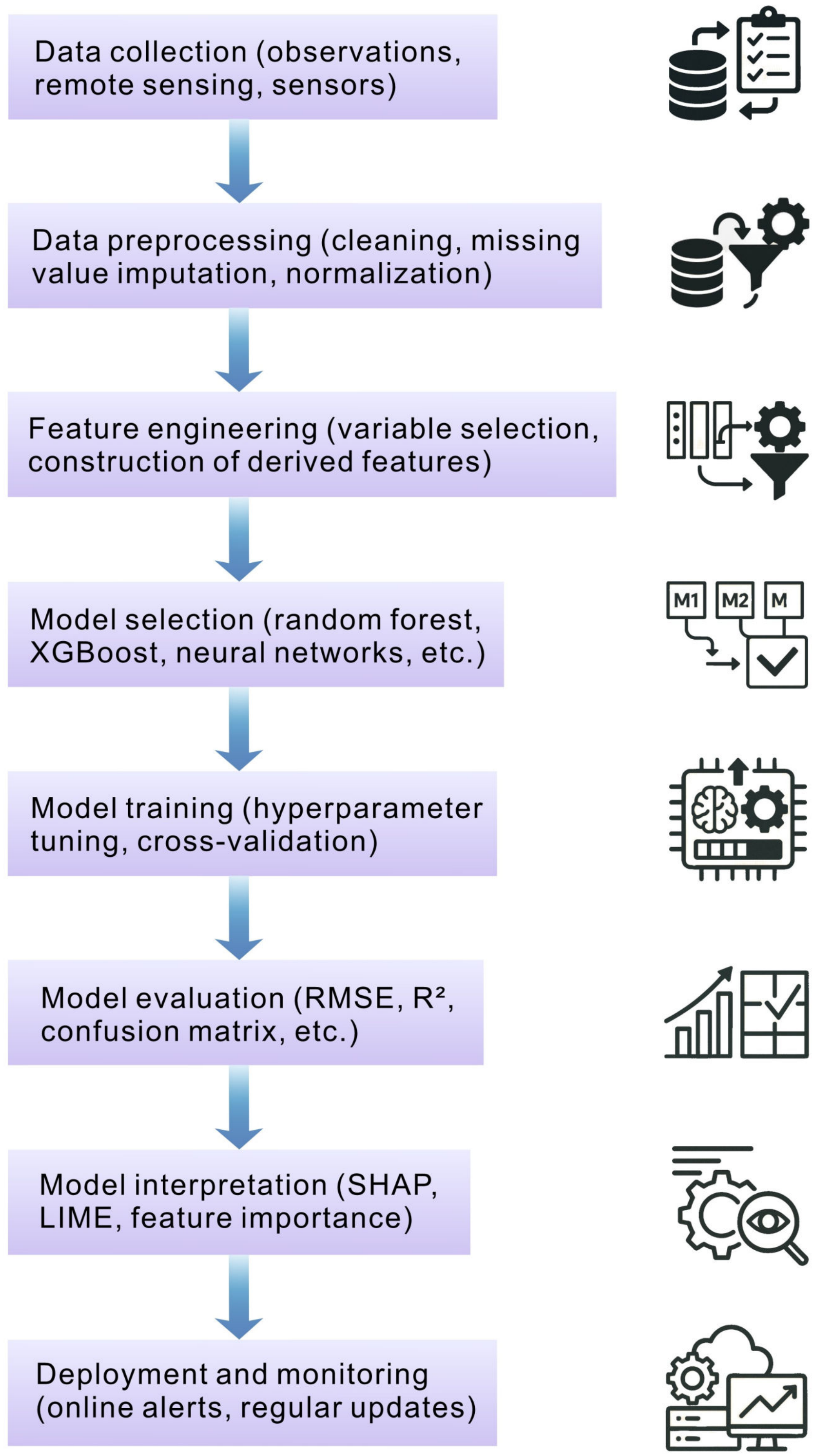
Data collection (observations, remote sensing, sensors)
Data preprocessing (cleaning, missing value imputation, normalization)
Feature engineering (variable selection, construction of derived features)
Model selection (random forest, XGBoost, neural networks, etc.)
M1
M2
M
Model training (hyperparameter tuning, cross-validation)
Model evaluation (RMSE, R², confusion matrix, etc.)
Model interpretation (SHAP, LIME, feature importance)
Deployment and monitoring (online alerts, regular updates)

Table S1

Rank	Keyword	Cluster	TL	TLS	O	APY
1	soil	2	174	558	296	2015.20
2	microbial community	4	140	301	203	2019.67
3	heavy metal	3	110	259	148	2015.29
4	sulfur	1	105	241	110	2015.48
5	soil microorganism	1	96	172	93	2016.56
6	antibiotic	2	78	198	90	2018.41
7	acid sulfate soil	1	63	124	85	2014.01
8	paddy soil	3	66	133	80	2019.50
9	soil remediation	3	59	105	77	2020.26
10	antibiotic resistance genes	2	45	110	71	2020.77
11	srb	3	49	80	70	2017.70
12	bacterial community	4	60	98	69	2020.96
13	bacteria	4	63	127	64	2015.72
14	biodegradation	2	48	83	61	2015.00
15	microbial biomass	1	61	113	59	2012.88
16	arsenic	3	53	110	59	2018.02
17	soil organic matter	1	64	108	55	2014.78
18	soil ph	5	70	106	55	2012.75
19	bioremediation	2	58	89	55	2014.67
20	enzyme activity	1	51	84	53	2016.06
21	soil acidification	5	48	78	49	2011.53
22	biochar	3	66	96	47	2021.74
23	rhizosphere	4	54	80	46	2015.80
24	sulfate	5	58	91	44	2015.00
25	nitrogen	1	52	118	43	2013.00
26	degradation	2	47	81	42	2012.98
27	microbiome	4	54	66	42	2021.98

28	cadmium	3	52	108	41	2017.66
29	phosphorus	1	54	105	40	2013.95
30	soil enzyme	1	51	77	39	2015.28

TL: total link. TLS: total link strength. O: occurrences. APY: average publication year.

Table S2

Rank	Institution	NP	C	TL	TLS	TC	CPP	APY
1	Chinese Academy of Sciences	350	China	76	359	12002	34.29	2018.53
2	University of Chinese Academy of Sciences	121	China	42	179	4073	33.66	2020.31
3	Zhejiang University	99	China	36	84	3331	33.65	2019.05
4	Nanjing Agricultural University	59	China	31	64	2619	44.39	2019.97
5	Nanjing University	44	China	19	55	1335	30.34	2020.09
6	Chinese Academy of Agricultural Sciences	42	China	25	42	759	18.07	2020.79
7	USDA ARS	42	America	16	27	1751	41.69	2009.38
8	CSIC	38	Spain	11	14	1256	33.05	2013.84
9	Swedish University of Agricultural Sciences	37	Sweden	20	23	1841	49.76	2012.43
10	Northwest Agriculture and Forestry University	36	China	18	25	1190	33.06	2020.39
11	Agriculture and Agri-Food Canada	35	Canada	6	14	920	26.29	2008.69
12	China University of Geosciences	34	China	17	26	996	29.29	2017.65
13	University of Sao Paulo	33	Brazil	9	13	831	25.18	2017.24
14	Cornell University	32	America	15	15	2362	73.81	2011.41
15	University of Oklahoma	31	America	26	53	1011	32.61	2016.81

16	The University of Adelaide	31	Australia	8	14	1438	46.39	2017.71
17	Sun Yat-sen University	30	China	19	36	746	24.87	2019.50
18	The University of Western Australia	30	Australia	17	36	1446	48.20	2015.90
19	South China Agricultural University	29	China	12	23	709	24.45	2021.45
20	Beijing Normal University	29	China	9	13	1536	52.97	2018.28

NP: the number of papers. C: country. TL: total link. TLS: total link strength. TC: total citations. CPP: citations per paper. APY: average publication year.

Table S3

Rank	Country	Continent	NP	APY	TC	TL	TLS	CPP
1	China	Asia	1339	2019.93	37400	40	579	27.93
2	America	North America	693	2014.22	34006	45	462	49.07
3	Australia	Oceania	266	2015.00	10916	35	247	41.04
4	Germany	Europe	262	2012.77	17829	41	298	68.05
5	India	Asia	260	2015.75	6748	31	121	25.95
6	Canada	North America	199	2013.89	7289	33	170	36.63
7	Spain	Europe	191	2014.60	6057	38	155	31.71
8	Brazil	South America	157	2016.24	5209	26	114	33.18
9	England	Europe	135	2015.59	7317	40	192	54.20
10	France	Europe	127	2014.81	5505	34	143	43.35
11	Japan	Asia	112	2012.49	3503	26	75	31.28
12	Italy	Europe	107	2014.29	3285	31	90	30.70
13	Netherlands	Europe	102	2014.86	7304	39	136	71.61
14	Korea	Asia	102	2015.99	2944	24	100	28.86
15	Sweden	Europe	96	2014.35	3610	28	110	37.60
16	Poland	Europe	82	2017.84	1434	13	25	17.49
17	Pakistan	Asia	69	2019.57	2068	24	82	29.97
18	Russia	Asia	65	2017.18	1265	16	50	19.46
19	Czech republic	Europe	65	2016.60	2080	22	49	32.00
20	Denmark	Europe	59	2013.25	3224	25	67	54.64

NP: the number of papers. TL: total link. TLS: total link strength. TC: total citations. CPP: citations per paper. APY: average publication year.

Table S4

Research frontier	Core scientific question	Key interface-scale targets	Required evidence base	Recommended approaches	Expected outcomes
In situ quantification of reactive interfaces under realistic disturbance regimes	How can the spatiotemporal dynamics of reactive interfaces be quantified in situ under realistic disturbances (e.g., wetting–drying cycles, flooding–drainage transitions, fertilization, pollutant loading)?	Microscale redox gradients; turnover of organo–mineral coatings; sulfur speciation; "hotspots" of gene expression and activity	Co-registered measurements of redox status and terminal electron-acceptor availability; mineral-surface reactivity and reactive-site accessibility; organic matter functional chemistry and electron-shuttling capacity; microbial functional gene repertoires coupled with appropriate activity proxies	Interface-resolved observational platforms enabling spatiotemporal co-registration; integrated multi-evidence monitoring (redox status, mineral reactivity, organic matter electron-shuttling capacity, and omics-/activity-based indicators); disturbance-aware in situ/quasi in situ experimental designs	A unified spatiotemporal linkage among "interface state–sulfur speciation–functional expression/activity"; observational constraints for parameterizing interface-scale process representations
Thresholds and regime shifts under multi-driver perturbations	Where do thresholds occur such that modest changes in electron-acceptor availability,	Electron-acceptor competition (SO_4^{2-}/Fe(III)/NO_3^-); mineral reactivity;	Critical interface-state boundaries: expansion/contraction of redox microdomains; formation/disruption of organo–	Threshold/regime-shift diagnostics (state-space analyses; early-warning indicators where appropriate); perturbation-	Mechanistically grounded, testable predictions for critical thresholds; explanatory framework for

	mineral reactivity, or organic matter electron-shuttling capacity reorganize sulfur-cycling guilds and trigger abrupt shifts in net outcomes?	organic matter electron-shuttling capacity; sulfur-cycling guild structure	mineral coatings; switching in Fe–S precipitation/dissolution control on sulfide retention/release; integrative response metrics for CH_4, P, and metal outcomes	gradient experiments and scenario simulations; coupled-process attribution across S–C–P–metal linkages	abrupt net-outcome transitions (e.g., CH_4 suppression vs. stimulation, P mobilization vs. stabilization, and metal immobilization vs. release)
Transferable scaling rules from micro-interface networks to field- and landscape-scale fluxes	Which scaling relationships are transferable across soils versus system-specific? How do micro-interface reaction networks aggregate into field-scale sulfur budgets and manifest as ecosystem-integrated outcomes?	"Micro-interface rate laws" vs. "macroscale observations"; field-scale sulfur budgets/fluxes; ecosystem-integrated responses	Constraints for parameter/state inference: spectroscopic indicators of speciation and mineral association; omics constraints on functional potential/regulation; environmental state variables (Eh, moisture, solute fluxes)	Coupling reactive-transport modeling with data-assimilation frameworks; constraining parameter and state inference using spectroscopy- and omics-based observations; cross-scale benchmarking and transferability assessment	A credible "micro-to-macro" bridge; transferable scaling rules with uncertainty quantification; improved cross-system predictive skill supported by benchmarking

Reactive interfaces refer to dynamic microenvironments in which mineral surfaces, organic matter, and microbial activity co-localize and jointly regulate sulfur transformations through coupled redox reactions, sorption and ligand-exchange processes, and precipitation–dissolution pathways. Interface-state characterization denotes coordinated measurements of microscale redox environments and terminal electron-acceptor availability, mineral-surface reactivity and reactive-site accessibility, and the functional chemistry and electron-shuttling capacity of organic matter, ideally co-registered in space and time with functional gene repertoires and appropriate activity proxies. Functional potential is inferred from the abundance and composition of functional genes and should not be equated with in situ process rates. Transferability refers to the robustness of scaling relationships and model parameters across soil types, redox regimes, and disturbance gradients, evaluated through cross-system benchmarking.

Table S5

Framework component	Key process represented	Measurable variables or proxies	Model-compatible representation	Potential use in quantitative or comparative analysis
Interfacial physicochemical conditions	Local constraints on sulfur oxidation, sulfate reduction, and sulfur speciation	pH, Eh, dissolved O_2, EC, ionic strength, sulfate, sulfide, thiosulfate, Fe(II)/Fe(III), Mn(II)/Mn(IV), porewater chemistry	Continuous state variables; threshold variables; redox-class indicators; time-varying covariates	Identify redox windows for sulfur oxidation or reduction; compare process dominance across wetlands, croplands, urban soils, and acid sulfate soils
Mineral reactivity and sorption capacity	Sulfur retention, surface complexation, mineral buffering, sulfide precipitation, pyrite formation	Fe/Al/Mn oxides, poorly crystalline Fe, clay content, carbonate content, specific surface area, CEC, surface charge, zeta potential, sulfate adsorption capacity, AVS, CRS, FeS, FeS_2	Sorption coefficients; mineral-reactivity indices; partitioning parameters; geochemical constraints	Parameterize sulfur retention and release; constrain reactive-transport or mass-balance models; compare mineralogical controls among soil types
Organic matter chemistry and electron-donor supply	Organic sulfur turnover, microbial substrate supply, electron transfer, mineral–organic	SOC, DOC, dissolved organic matter composition, C/S ratio, labile carbon, microbial biomass C, thiols, sulfate esters, sulfonates, redox-active	Substrate-availability variables; electron-donor terms; organic-matter quality indices; mediation variables	Test how organic matter quality regulates sulfate reduction, sulfur mineralization, and mineral-associated sulfur stabilization

	association	moieties, electron-donating/accepting capacity		
Microbial functional potential and activity	Sulfur oxidation, sulfate reduction, organic sulfur mineralization, sulfur disproportionation, cross-guild coupling	Abundance or expression of *dsrAB*, *aprAB*, *sat*, *soxXYZABCD*, *sqr*, *fccAB*, *atsA*, *ssuD*; SRB/SOB abundance; metatranscriptomic activity; enzyme activity	Functional predictors; latent microbial-function variables; interaction terms with Eh, substrate, and mineral variables	Link microbial potential to geochemical constraints; distinguish potential from realized activity; evaluate microbial contributions across land-use or disturbance gradients
Redox gradients and hydrological microarchitecture	Formation and collapse of oxic–anoxic microzones; diffusion limitation; hotspot formation	Water-filled pore space, soil moisture, bulk density, aggregate stability, pore-size distribution, hydraulic conductivity, oxygen penetration depth, wetting–drying frequency	Connectivity indices; diffusion parameters; event-frequency variables; random effects or hierarchical grouping variables	Explain spatial heterogeneity in sulfur transformation; model wetting–drying effects; compare flooded, intermittently saturated, and well-drained soils
Sulfur pool composition and isotope constraints	Sulfur source attribution, pool exchange, transformation pathway identification	Total S, sulfate-S, sulfide-S, elemental S, organic S, AVS, CRS, pyrite-S, $\delta^{34}S$, $\delta^{18}O\text{-}SO_4$, isotope fractionation factors	Response variables; source-apportionment terms; turnover parameters; isotope constraints	Constrain mass balance; separate external inputs from internal cycling; validate inferred sulfur transformation pathways

Spatial co-localization of microbes, minerals, and sulfur species	Identification of reactive hotspots and interface-scale coupling	Co-localization of S species, Fe phases, organic coatings, microbial cells, extracellular polymeric substances, and functional genes	Hotspot density; spatial co-occurrence metrics; interface-occupancy indices	Quantify whether microbial functional signals are spatially coupled with reactive mineral–organic interfaces rather than inferred only from bulk samples
Ecosystem-scale outcomes	Propagation from interface-scale sulfur transformations to environmental effects	CH_4, CO_2, N_2O, H_2S emissions, metal mobility, P release, sulfate leaching, acidification, nutrient retention, microbial diversity loss	Model outputs; validation endpoints; management response variables	Test whether interface-scale indicators improve prediction of greenhouse-gas fluxes, nutrient loss, pollutant mobility, and soil health responses

Variables and proxies listed in this table provide an operational pathway for translating the microbial–mineral–organic matter interaction framework into quantitative and model-compatible analyses of soil sulfur cycling. They are representative rather than exhaustive and should be selected according to the target process, ecosystem type, redox regime, and spatial–temporal scale. These indicators may be used as predictors, state variables, interaction terms, constraints, latent variables, or validation endpoints in comparative statistics, structural equation models, reactive-transport models, mass-balance models, and hybrid AI–process models. Gene abundance indicates functional potential, whereas gene expression, enzyme activity, isotope tracing, and process-rate measurements provide stronger evidence for realized sulfur-cycling activity.

Supplementary References

1. Mukherjee D, Lim WM, Kumar S, Donthu N. Guidelines for advancing theory and practice through bibliometric research. *J Bus Res* **148**, 101-115 (2022).
2. Tosi MDL, dos Reis JC. SciKGraph: A knowledge graph approach to structure a scientific field. *J Informetr* **15**, 22 (2021).
3. van Eck NJ, Waltman L. Software survey: VOSviewer, a computer program for bibliometric mapping. *Scientometrics* **84**, 523-538 (2010).
4. Zhang TK*, et al.* Visualising the trends of biochar influencing soil physicochemical properties using bibliometric analysis 2010-2022. *Environ Dev Sustain* **27**, 2815-2839 (2025).
5. Aria M, Cuccurullo C, D'Aniello L, Misuraca M, Spano M. Comparative science mapping: a novel conceptual structure analysis with metadata. *Scientometrics* **129**, 7055-7081 (2024).
6. Perianes-Rodriguez A, Waltman L, van Eck NJ. Constructing bibliometric networks: A comparison between full and fractional counting. *J Informetr* **10**, 1178-1195 (2016).
7. Cahlik T. Comparison of the maps of science. *Scientometrics* **49**, 373-387 (2000).
8. Abdeljaoued E*, et al.* Bibliometric analysis of the evolution of biochar research trends and scientific production. *Clean Technol Environ Policy* **22**, 1967-1997 (2020).
9. Zhang TK, Tang Y, Li H, Hu W, Cheng JZ, Lee XQ. A bibliometric review of biochar for soil carbon sequestration and mitigation from 2001 to 2020. *Ecotox Environ Safe* **264**, 15 (2023).
10. Zhang ZY, Furman A. Soil redox dynamics under dynamic hydrologic regimes - A review. *Sci Total Environ* **763**, 17 (2021).
11. Fox PM*, et al.* Sulfur Biogeochemical Cycling and Redox Dynamics in a Shale-Dominated Mountainous Watershed. *J Geophys Res-Biogeosci* **127**, 18 (2022).
12. Santana MM, Dias T, Gonzalez JM, Cruz C. Transformation of organic and inorganic sulfur-adding perspectives to new players in soil and rhizosphere. *Soil Biol Biochem* **160**, 13 (2021).
13. Qian L*, et al.* Comprehensive profiles of sulfur cycling microbial communities along a mangrove sediment depth. *Sci Total Environ* **944**, 11 (2024).
14. Wang Z*, et al.* Mechanisms of S cooperating with Fe and Mn to regulate the conversion of Cd and Cu during soil redox process revealed by LDHs-DGT technology. *Sci Total Environ* **867**, 10 (2023).
15. Liu HQ*, et al.* Sulfate-reducing consortium HQ23 stabilizes metal(loid)s and activates biological N-fixation in mixed heavy metal-contaminated soil. *Sci Total Environ* **946**, 10 (2024).
16. Wang QQ*, et al.* Soil pH and phosphorus availability regulate sulphur cycling in an 82-year-old fertilised grassland. *Soil Biol Biochem* **194**, 10 (2024).
17. Védère C, Gonod LV, Nunan N, Chenu C. Opportunities and limits in imaging microorganisms and their activities in soil microhabitats. *Soil Biol Biochem* **174**, 22 (2022).
18. Li Z*, et al.* A framework for integrating genomics, microbial traits, and ecosystem biogeochemistry. *Nat Commun* **16**, 11 (2025).
19. Winowiecki LA*, et al.* Multistakeholder Engagement to Scale Soil Health Globally: The Coalition of Action 4 Soil Health. *Eur J Soil Sci* **76**, 8 (2025).
20. Cherubin MR*, et al.* Global blind spots in soil health research overlap with environmental vulnerability hotspots. *Commun Earth Environ* **6**, 10 (2025).
21. Ruan ZP*, et al.* Engineering natural microbiomes toward enhanced bioremediation by microbiome modeling. *Nat Commun* **15**, 19 (2024).

22. Vullaganti N, Ram BG, Sun X. Precision agriculture technologies for soil site-specific nutrient management: A comprehensive review. *Artif Intell Agric* **15**, 147-161 (2025).
23. Froger C*, et al.* Comparing LUCAS Soil and national systems: Towards a harmonized European Soil monitoring network. *Geoderma* **449**, 17 (2024).
24. Batjes NH, Calisto L, de Sousa LM. Providing quality-assessed and standardised soil data to support global mapping and modelling (WoSIS snapshot 2023). *Earth Syst Sci Data* **16**, 4735-4765 (2024).