

# III. Chemical, Metallurgical, and Materials Engineering

## 1 Engineering research fronts

### 1.1 Trends in Top 11 engineering research fronts

The Top 11 engineering research fronts as assessed by the Field Group of Chemical, Metallurgical, and Materials Engineering are shown in Tables 1.1.1 and 1.1.2. “Design and process optimization of low-carbon and energy-saving metallurgical reactors”, “integrated monolithic electrodes for highly efficient electrochemical energy storage”, and “efficient preparation and catalytic mechanism of super-dispersed single-atom alloy catalysts” were recommended by experts directly. The other fronts were chosen by a panel of experts using core-paper statistics provided by Clarivate. Topics on “electrocatalysis, monoatomic catalysis and intrinsically safe battery” are still hot topics, with more than 200.00 citations per paper (Table 1.1.1). However, the annual number of core papers for all topics is decreasing (Table 1.1.2).

#### (1) Renewable energy-driven bioconversion of carbon dioxide to chemicals, fuels, and materials

Biological carbon dioxide (CO<sub>2</sub>) sequestration, which is a clean and highly efficient technique, is indispensable for realizing carbon peak and carbon neutrality goals. Renewable energy-driven bioconversion of CO<sub>2</sub> takes full advantage of biological CO<sub>2</sub> sequestration. In this technique, renewable energy, such as light or electricity, is used as a substitute for chemical energy to provide energy and reducing equivalents for biological carbon sequestration pathways that produce chemicals, fuels, and materials. To date, relevant research has focused on *in vitro* multi-enzyme-based CO<sub>2</sub> sequestration and whole cell-based CO<sub>2</sub> sequestration

Table 1.1.1 Top 11 engineering research fronts in chemical, metallurgical, and materials engineering

No.	Engineering research front	Core papers	Citations	Citations per paper	Mean year
1	Renewable energy-driven bioconversion of carbon dioxide to chemicals, fuels, and materials	92	13 644	148.30	2018.9
2	Chaotic nonlinear enhancement technology of metallurgical flow field	120	9 337	77.81	2018.9
3	High-performance electrocatalysts and electrolysis systems for CO <sub>2</sub> conversion and utilization	107	25 965	242.66	2018.8
4	<i>In situ</i> molecular/atomic scale characterization of heterogeneous catalysts under reaction conditions	76	9 481	124.75	2018.7
5	Design and process optimization of low-carbon and energy-saving metallurgical reactors	82	3 788	46.20	2018.5
6	Rational design and fabrication of special alloys for cryogenic environments	148	13 642	92.18	2018.7
7	Integrated monolithic electrodes for highly efficient electrochemical energy storage	109	14 356	131.71	2018.4
8	Research on high-strength high-toughness and low-density steel	59	3 246	55.02	2018.4
9	Efficient preparation and catalytic mechanism of super-dispersed single-atom alloy catalysts	61	13 127	215.20	2019.0
10	Selective confined mass transport membrane for ion separation	81	9 394	115.98	2019.0
11	Intrinsically safe battery systems for renewable energy storage	131	31 898	243.50	2018.6



Table 1.1.2 Annual number of core papers published for each of the Top 11 engineering research fronts in chemical, metallurgical, and materials engineering

No.	Engineering research front	2017	2018	2019	2020	2021	2022
1	Renewable energy-driven bioconversion of carbon dioxide to chemicals, fuels, and materials	16	21	26	17	12	0
2	Chaotic nonlinear enhancement technology of metallurgical flow field	26	25	30	21	15	3
3	High-performance electrocatalysts and electrolysis systems for CO <sub>2</sub> conversion and utilization	20	26	29	22	8	2
4	<i>In situ</i> molecular/atomic scale characterization of heterogeneous catalysts under reaction conditions	20	18	17	12	6	3
5	Design and process optimization of low-carbon and energy-saving metallurgical reactors	23	28	13	9	7	2
6	Rational design and fabrication of special alloys for cryogenic environments	43	25	37	23	16	4
7	Integrated monolithic electrodes for highly efficient electrochemical energy storage	37	21	28	16	7	0
8	Research on high-strength high-toughness and low-density steel	23	10	13	6	7	0
9	Efficient preparation and catalytic mechanism of super-dispersed single-atom alloy catalysts	8	13	17	14	9	0
10	Selective confined mass transport membrane for ion separation	10	20	22	22	6	1
11	Intrinsically safe battery systems for renewable energy storage	33	32	30	28	8	0

driven by light/electricity. The main goals have been ① the construction of new biological carbon sequestration pathways, ② the design and preparation of new biocompatible photo- or electrocatalytic materials, and ③ the adaptation of biocatalytic modules and photocatalytic modules. Bioconversion of CO<sub>2</sub> driven by renewable energy is a green process with a green raw material and green product. However, the overall energy efficiency of this technology is unsatisfactory, and there are still some bottlenecks in industrial applications. For future advances, the following directions are suggested: *in situ* characterization techniques for clarification of energy exchange mechanisms between biocatalysts and artificial catalysts to deepen the understanding of the coupling processes; core technologies for the rational design of enzymes and microbial cell factories to produce high-quality biocatalysts with high efficiency and adaptability and to further increase productivity; and advanced reactors and separation media to establish an integrated equipment and technology system for raw material supply, process intensification, and product separation engineering.

### (2) Chaotic nonlinear enhancement technology of metallurgical flow field

In metallurgical processes, the interplay of flow, heat/mass transfer, and reaction involves intricate nonlinear dynamic mechanisms and multi-scale spatiotemporal characteristics. These features pose formidable challenges for the design, optimization, and operation of metallurgical reactors. Chaotic nonlinear enhancement of metallurgical flow field integrates knowledge from fluid dynamics, chaos theory, and nonlinear science. This aims to uncover the coupling and scale-up theory governing the interplay of flow, heat/mass transfer, and reaction in metallurgical reactor processes. Inherent connections between chaotic characteristics of the fluid phase, destabilization of intermediate steady flow structures, and enhancement through chemical chaos are elucidated. By constructing a correlation model between chaotic flow and temperature field-flow uniformity, the relationship between chaotic flow and temperature field-flow uniformity is precisely delineated. Leveraging the coupling mechanism between chaotic mixing characteristics, field uniformity, and the formation, transport, and conversion of multi-scale flow structures, this technology enhances heat and mass transfer efficiency by modulating the chaotic behavior of bubble clusters. This technique offers a fresh regulatory approach for topological coupling of complex multiphase flow patterns in metallurgical furnaces, and

effectively addresses the challenge of accurately describing the cooperative nature of the flow field-temperature field during the enhancement process and intensified heat transfer via bubble cluster agitation. This theory is promising for further development of extreme and unconventional metallurgy, large-scale equipment, and intelligent metallurgy.

### (3) High-performance electrocatalysts and electrolysis systems for CO<sub>2</sub> conversion and utilization

In the overall energy and environmental system, green and efficient conversion and utilization of CO<sub>2</sub> is important for realizing efficient conversion of low-carbon energy. Among the available methods, CO<sub>2</sub> capture, utilization, and storage technology has gradually become the key technology to cope with climate change and achieve the goals of carbon peak and carbon neutrality. Currently, green electricity provided by renewable energy sources such as solar energy and wind energy drives the catalytic conversion of CO<sub>2</sub>. This solves the problem of excessive CO<sub>2</sub> emissions and realizes the direct conversion of intermittent electric energy into chemical energy, which is important for achieving carbon balance and optimizing energy consumption. The research on CO<sub>2</sub> electrocatalytic conversion has focused on the following aspects: ① the use of *in situ* spectroscopy to monitor key intermediates in the CO<sub>2</sub> reduction reaction (CO<sub>2</sub>RR), and construction of the reaction network in the catalytic conversion process of CO<sub>2</sub> using theoretical calculations; ② design and development of high-performance electrocatalysts, regulation and optimization of the catalyst structure, and study of the structure–activity relationship between the catalyst and CO<sub>2</sub>RR performance; and ③ design and optimization of the electrode structure and adjustment of the entire electrolytic reactor to control the operation of the reaction system and use its modular characteristics to achieve regulation and optimization so that each index meets the requirements of industrial application. Further development of CO<sub>2</sub>RR requires improvement of the long-term continuous operation stability of the electrocatalyst and expansion of the scale of the CO<sub>2</sub> electrolyzer. Additionally, the target for practical application, the economics of the product, market supply, and demand need to be determined. The final product separation and recovery costs of excess CO<sub>2</sub> feedstock gas and electrolyte also require further design management.

### (4) *In situ* molecular/atomic scale characterization of heterogeneous catalysts under reaction conditions

The structure and surface/interface properties of a catalyst are directly related to the catalytic performance and provide direct evidence for modeling. The active sites of catalysts and coordination environment change dynamically during catalytic reactions, and their spatiotemporal evolution provides vital information for the rational design of heterogeneous catalysts. The characterization of these surface/interface structures and chemistry, especially *in situ* characterizations under relevant reaction conditions, is important for elucidating the mechanisms. State-of-the-art *in situ* characterization techniques for heterogeneous catalysts at the molecular/atomic scale under various reaction conditions include *in situ* electron/scanning probe microscopy, *in situ* infrared/Raman spectroscopy, and X-ray photoelectron/absorption spectroscopy. Research has focused on ① revealing the structural active sites of specific reactions through *in situ* atomic-scale observation of dynamic structure changes of heterogeneous catalysts for rational design of atom-precise new catalysts; ② revealing the chemisorption and dissociation of molecules at the catalyst surface and determining the intermediates and their spatiotemporal distributions to elucidate the entire reaction route; and ③ combining multiple characterization methods and model catalysts to relate structural and chemical active sites for critical chemical reactions.

### (5) Design and process optimization of low-carbon and energy-saving metallurgical reactors

In the process of size amplification, structure adjustment, and process optimization of super-large or special smelting equipment, a lack of a theoretical basis often leads to equipment amplification distortion, operation instability under changeable working conditions, and amplification mismatch between the theoretical model and practical equipment. This can lead to high energy consumption of the metallurgical reactor and smelting process. The operation process involves complex concentration-melt-rich oxygen jets, electric–magnetic–flow–heat–particles–components multi-fields, cooperative coupling between microscopic response, mesoscopic motion, and macroscopic operation, and requires size amplification in the design of low carbon smelting equipment and fine optimization for processes of dynamic test and simulation methods. Future research should focus on developing new methods for quantitative visual characterization of the flow field in a cold simulated multiphase system. For the cold state test model of large equipment using similarity theory, visual analysis techniques such as high-speed dynamic recording

of flow field characteristics and PIV (particle image velocimetry), quantitative measurement techniques such as image analytical processing, mixing time determination, and chaos mathematical analysis can be used to realize quantitative characterization of the mixing degree of the nonlinear flow field. Furthermore, studies should look at the multi-field coupling mechanism of electric–magnetic–flow–heat–particles–components in gas–liquid–solid multiphase systems, including various transfer processes and metallurgical chemical reaction rules in actual metallurgical reactors. The results could be used to simulate and analyze the cooperative coupling laws of single and multiple associated reactors to optimize and improve the existing process and develop new carbon energy-conserving metallurgical processes and reactors.

#### (6) Rational design and fabrication of special alloys for cryogenic environments

Governments around the world are focusing on innovation and development of equipment in clean energy, aerospace, and other areas. Key components in the equipment often experience cryogenic environments, such as superconducting coils of magnetic confinement fusion reactors ( $\sim 4$  K), aerospace liquid oxygen/liquid hydrogen engines ( $\sim 20$  K), and wind tunnels with high Reynolds numbers ( $\sim 77$  K). This results in the need for exceptionally stringent requirements for the involved special alloys. Currently, special alloys in cryogenic environments face various challenges including inferior performance, ambiguous regulation mechanisms for their microstructures and properties, and immature preparation processes. These challenges largely limit improvements in aircraft manufacturing technology and the utilization of clean energy. There are many scientific problems that need to be solved in the rational design and preparation of special alloys for cryogenic environments. First, precise control of phase stability is required during cryogenic service. This mainly includes the mechanism of the austenite stacking fault energy in special alloys under cryogenic conditions, the effective control of phase stability, and the role of their interactions in different cryogenic properties, which in turn guides the alloy composition design and fabrication process. Second, systematic study is required for the multiphase microstructure evolution behavior and the strengthening and toughening mechanism during the integrated processing of melting–forging/rolling–heat treatment–welding for cryogenic special alloys. This includes the principle of forward/reverse phase transformation, alloy element partitioning, precipitation control, and cryogenic deformation. The microstructure–property relationships need to be determined among typical processing routes, multiphase microstructure components, and mechanical properties. Third, in complex cryogenic environments, it is necessary to study the failure modes and mechanisms under multi-field coupled service conditions with highly corrosive media over wide temperature ranges and under cyclic loading. This should include the mutual matching mechanism of multiple mechanical and physical properties at low temperatures, cryogenic failure behaviors under the coupling of thermal fatigue, wear, and corrosion, and the relationship between service performance and failure mechanisms. The results could be used to provide guidance for alloy design and fabrication process optimization of the cryogenic special alloys.

#### (7) Integrated monolithic electrodes for highly efficient electrochemical energy storage

Lithium-ion batteries occupy the majority of the market in the field of electrochemical energy storage. However, their present energy densities and power densities still need to be improved to meet growing social development. It is important to develop a new generation of lithium batteries with high specific energy, high power density, high stability, long life spans, high safety, and low cost. The key to achieving this goal is to have a clear understanding of the electrochemical energy storage mechanism of each involved active electrode material, and to carry out system design at the level of cell components and the overall electrode architecture. Therefore, research has focused on the design and fabrication of integrated monolithic electrodes with various compositions and structures. The developed electrodes will have excellent ion–electron mixed conductivities and could eliminate the use of inactive components such as binders. They will also have a suitable pore structure to maintain high structural stability during the charge–discharge process. To date, the research in this area has focused on the following aspects: advanced electrode structure design, simple electrode fabrication strategies, design and selection of current collectors and loading of active components, increasing the loading mass of active materials in area and volume, improving the conductivity of the overall electrode, matching of cathodes and anodes (construction of a full cell), development of flexible or thick electrodes, and determining the working or electrochemical reaction mechanism of the electrode. The structural design and simple fabrication of integrated monolithic electrodes with high active material loads are technical bottlenecks that need to be solved in this field.

#### (8) Research on high-strength high-toughness and low-density steel

Low-density steel, also known as lightweight alloy steel, is a lightweight material that reduces the density of the alloy by adding lightweight elements such as Al, Mn, and C. Research has shown that adding Al at a mass fraction of 1% can reduce the density of the steel by 1.3%. Low-density steel has broad application prospects in lightweight and safe service in vehicles, ships, aerospace and military fields. At the beginning of the 21st century, a study by the Max Planck Society in Germany showed that Fe–Mn–Al–C high-strength, high-toughness, and low-density steel had excellent potential for mass reduction, which was a driver for research on the use of low-density steel in automobiles. In 2015, POSCO in Republic of Korea trialed industrial production of rolling low-density steel, and in 2022, Xingcheng Special Steel in China trialed industrial production of high-strength, high-toughness, and low-density steel plates. Additionally, companies such as JFE and Nippon Steel in Japan, ThyssenKrupp in Germany, and Baowu and Ansteel in China have conducted research on and trialed production of low-density steel. However, further development and application of high-strength, high-toughness and low-density steel are restricted, due to factors such as manufacturing costs, surface quality and application technology. To date, research on high-strength, high-toughness, and low-density steel has focused on Fe–Mn–Al–C low-density steel. The main research directions include single ferrite steel, ferrite-based dual-phase steel, austenite-based dual-phase steel, and austenitic steel. There are still many scientific issues that need to be studied for the composition design, microstructure control, and service performance of Fe–Mn–Al–C low-density steel.

#### (9) Efficient preparation and catalytic mechanism of super-dispersed single-atom alloy catalysts

Single-atom alloy catalysts (SAACs) are usually prepared by dispersing a single atom of an active metal (typically a precious metal) in a second metal support (commonly a non-precious metal). SAACs have attracted attention in recent years because they have high utilization efficiency of noble metal atoms, high catalytic activity, and high selectivity. Since Sykes and colleagues proposed the concept of SAACs [Pd<sub>1</sub>/Cu(111)] in 2012, scientists worldwide have explored various preparation methods of SAACs and gradually applied them to catalytic reactions such as fuel cells, electrolytic water, selective hydrogenation, and CO oxidation. To date, research on SAACs has focused on three aspects. First, exploring facile and efficient strategies to prepare SAACs with high atom pairing ratios and to precisely adjust the interactions between the active site and surrounding atoms. Second, revealing the structure–activity relationship between single-atom alloy structures and catalytic performance and the catalytic mechanism at the atomic level using *in situ* fine structure analysis and theoretical calculations. This could be used to provide a theoretical basis for the rational design of functional SAACs. Third, developing macro-preparation process for SAACs with adjustable noble metal loading, which will bridge the gap between fundamental research and industrial application. Because of their low noble metal loading and excellent catalytic activity, selectivity, and stability, super-dispersed SAACs will be key for the development of industrial catalysis.

#### (10) Selective confined mass transport membrane for ion separation

Ion-selective separation is an important area of membrane separation technology. This technique has been applied to lithium extraction from salt lakes, saltwater purification, high-salinity wastewater resource recovery, and flow batteries. The performance of traditional polymer membrane materials is restricted by the trade-off effect, where flux and selectivity cannot be improved simultaneously. Confined mass transfer membranes, which can be constructed using artificially engineered channels at the sub-nanometer scale, have unique mass transfer characteristics and are promising for use in this area. Currently, research on selective ion-transport membranes is divided into two areas. The first involves the fundamental exploration of separation mechanisms to explore the factors influencing mass transfer dynamics and selectivity at the microscale, such as the channel geometric structure and interfacial physicochemical properties. The results from this could aid in membrane design. The second involves the design of membrane materials to achieve ultrafast mass transfer using materials with different sizes, functional groups, and interfacial charges, such as COFs and MOFs. Future research will look at *in situ* visualization of confined channels to establish an effective connection between ideal mass transfer models and the actual performance of separation membranes. This will be achieved through the manufacture of confined transport membranes with high mass transfer rates and selectivity, the transition from laboratory-scale specifications to large-scale production, and realization of industrial development.



### (11) Intrinsically safe battery systems for renewable energy storage

Large-scale energy storage stations have strict requirements for battery safety. An intrinsically safe battery is one with an inner safety mechanism, which can improve the safety performance in the internal structure, and materials that can effectively prevent and control dangerous situations such as thermal runaway, explosion, and leakage. Current research in the field of intrinsically safe batteries is creating new breakthroughs. Scientists are committed to developing new materials and optimizing the battery structure to improve the intrinsic safety performance and electrochemical performance of batteries, for example, by the addition of flame retardants to effectively inhibit the combustion of electrolytes, development of intrinsic flame-retardant polymer electrolytes to improve the safety of solid-state batteries, and suppression of lithium dendrite to improve the safety of lithium metal anodes. Research on intrinsically safe batteries has focused on the following aspects: improving the electrochemical stability to prevent side reactions, electrolyte decomposition, or instability of electrode materials during charging and discharging; improving the thermal safety of batteries in high-temperature environments by developing non-flammable (or flame-retarding) battery materials and upgrading the battery thermal management system to prevent overheating from causing battery runaway, combustion, or explosion; improving the mechanical stability of the battery by addressing external impact and internal stress of the battery to avoid safety hazards such as battery rupture or an internal short circuit; and replacing the traditional organic electrolytes with solid electrolytes or aqueous electrolytes to improve the safety and stability of the battery and solve the problems of combustion and leakage of organic electrolytes.

## 1.2 Interpretations for three key engineering research fronts

### 1.2.1 Renewable energy-driven bioconversion of carbon dioxide to chemicals, fuels, and materials

Many countries and regions have development strategies for green biorefineries. The 14th Five-Year Plan in China highlights that deep integration of the energy and manufacturing industries with biotechnology will be required to establish a green, low-carbon, and non-toxic circular economy. The Bold Goals for U.S. Biotechnology and Biomanufacturing plan is to achieve gigaton-level CO<sub>2</sub> fixation through bioconversion within the next 9 years at a cost of less than \$100 per metric ton. The use of renewable energy to drive the process of bioconversion of CO<sub>2</sub> to chemicals, fuels, and materials reduces carbon emissions, which is a focus for biorefineries. This will lower human dependence on fossil energy to trigger a change in industrial patterns and facilitate the transition to a green economy. Since third-generation biorefineries were proposed in 2020, research on biological carbon sequestration coupled with photocatalysis and electrocatalysis has developed rapidly to achieve carbon peak and carbon neutrality goals. Various pathways and mechanisms have been developed. Biocatalysts can directly take up electrons provided by photo- and electrocatalysts for CO<sub>2</sub> sequestration, and use formic acid, acetic acid, methanol, and other primary products of CO<sub>2</sub> reduction for fermentation. Enzyme engineering and synthetic biology has rapidly progressed and expanded the product spectrum of biological carbon sequestration driven by renewable energy. A series of products, including raw material chemicals such as L-lactic acid, dihydroxyacetone, glycolic acid, and biodegradable plastics such as PLA and PHA, can be produced with CO<sub>2</sub> as the only carbon source. However, compared with traditional methods conducted under high temperature and pressure, there is an efficiency bottleneck for the use of renewable energy to drive biological carbon sequestration. The main solutions to this are development of highly active enzymes and strains and rational design of efficient biological pathways for carbon sequestration; improvement of the utilization of renewable energy and development of photo- and electrocatalysts with bioaffinity and low toxicity; and optimization of the thermodynamic and kinetic adaptation of artificial modules and biocatalytic modules, or decoupling of these modules to ensure optimum efficiency.

The main countries with the greatest output of core papers in recent years on “bioconversion of carbon dioxide to chemicals, fuels, and materials driven by renewable energy” are shown in Table 1.2.1, and the main institutions are shown in Table 1.2.2. The main contributor to these core papers is China (41.3% of the total), followed by the USA, India, Republic of Korea, and Germany (all > 10% of the total). The main institutions in China are Chinese Academy of Sciences and Tianjin University. Figures 1.2.1 and 1.2.2 show the collaboration network among major countries and among major institutions. Scientists have established extensive global collaborations in this field. China’s largest collaborator is the USA. Among the cited core papers, China accounted for 52.02% of

the total (Table 1.2.3 and 1.2.4). Among the top ten major producing institutions of the citing papers, all, except for King Abdulaziz University, were Chinese universities or institutes. These institutions included Chinese Academy of Sciences, Jiangsu University, and Tsinghua University.

Renewable energy-driven bioconversion of CO<sub>2</sub> to chemicals, fuels, and materials has developed rapidly in recent years. A roadmap for the engineering research front of “renewable energy-driven bioconversion of carbon dioxide to chemicals, fuels, and materials” is shown in Figure 1.2.3. The key problem with coupling artificial devices that transform renewable energy with biocatalysts is the coupling mechanism. In future studies, it is important to develop techniques to identify the interaction mechanism between artificial devices and biological components. This will promote the development of new and efficient systems and new models. Biocatalysts are central to this process. Progress in the development of robust and efficient industrial enzymes and industrial strains will determine the industrialization process for biological carbon sequestration driven by renewable energy. This will speed

Table 1.2.1 Countries with the greatest output of core papers on “renewable energy-driven bioconversion of carbon dioxide to chemicals, fuels, and materials”

No.	Country	Core papers	Percentage of core papers/%	Citations	Citations per paper	Mean year
1	China	38	41.30	5 087	133.87	2019.0
2	USA	24	26.09	3 911	162.96	2018.7
3	India	16	17.39	2 676	167.25	2019.3
4	Republic of Korea	10	10.87	1 708	170.80	2018.4
5	Germany	10	10.87	1 114	111.40	2019.2
6	Australia	9	9.78	1 480	164.44	2019.0
7	UK	8	8.70	922	115.25	2019.0
8	Saudi Arabia	5	5.43	871	174.20	2019.0
9	Israel	4	4.35	635	158.75	2019.0
10	Canada	4	4.35	538	134.50	2018.0

Table 1.2.2 Institutions with the greatest output of core papers on “renewable energy-driven bioconversion of carbon dioxide to chemicals, fuels, and materials”

No.	Institution	Core papers	Percentage of core papers/%	Citations	Citations per paper	Mean year
1	Shoolini University	5	5.43	707	141.40	2020.0
2	Chinese Academy of Sciences	5	5.43	536	107.20	2019.4
3	Harvard University	4	4.35	780	195.00	2018.5
4	University of California, Berkeley	4	4.35	635	158.75	2019.0
5	University of Cambridge	4	4.35	520	130.00	2018.8
6	Lawrence Berkeley National Laboratory	3	3.26	538	179.33	2018.7
7	Korea Advanced Institute of Science and Technology	3	3.26	459	153.00	2018.0
8	Konkuk University	3	3.26	361	120.33	2018.3
9	Tianjin University	3	3.26	360	120.00	2018.7
10	Virginia Polytechnic Institute and State University	3	3.26	290	96.67	2019.0





Figure 1.2.1 Collaboration network among major countries in the engineering research front of “renewable energy-driven bioconversion of carbon dioxide to chemicals, fuels, and materials”

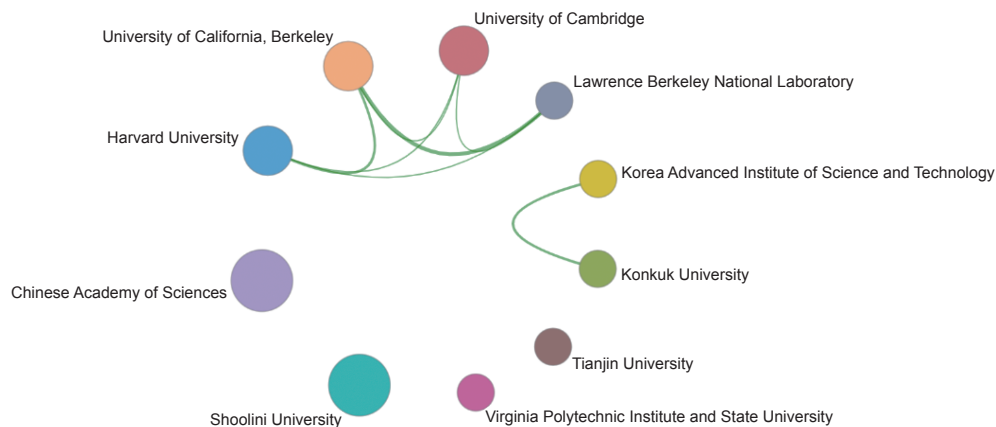


Figure 1.2.2 Collaboration network among major institutions in the engineering research front of “renewable energy-driven bioconversion of carbon dioxide to chemicals, fuels, and materials”

Table 1.2.3 Countries with the greatest output of citing papers on “renewable energy-driven bioconversion of carbon dioxide to chemicals, fuels, and materials”

No.	Country	Citing papers	Percentage of citing papers/%	Mean year
1	China	6 308	52.02	2021.0
2	USA	1 196	9.86	2020.7
3	India	1 130	9.32	2021.1
4	Republic of Korea	695	5.73	2020.8
5	Australia	481	3.97	2020.8
6	Germany	476	3.93	2020.8
7	Saudi Arabia	423	3.49	2021.1
8	UK	408	3.36	2020.9
9	Iran	355	2.93	2020.8
10	Spain	333	2.75	2020.8



Table 1.2.4 Institutions with the greatest output of citing papers on “renewable energy-driven bioconversion of carbon dioxide to chemicals, fuels, and materials”

No.	Institution	Citing papers	Percentage of citing papers/%	Mean year
1	Chinese Academy of Sciences	793	33.47	2021.0
2	Jiangsu University	202	8.53	2020.9
3	Tsinghua University	193	8.15	2021.1
4	University of Science and Technology of China	185	7.81	2021.3
5	Tianjin University	178	7.51	2021.0
6	Zhengzhou University	174	7.34	2021.2
7	Hunan University	157	6.63	2021.0
8	King Abdulaziz University	132	5.57	2021.0
9	Fuzhou University	121	5.11	2020.8
10	Harbin Institute of Technology	120	5.07	2021.1

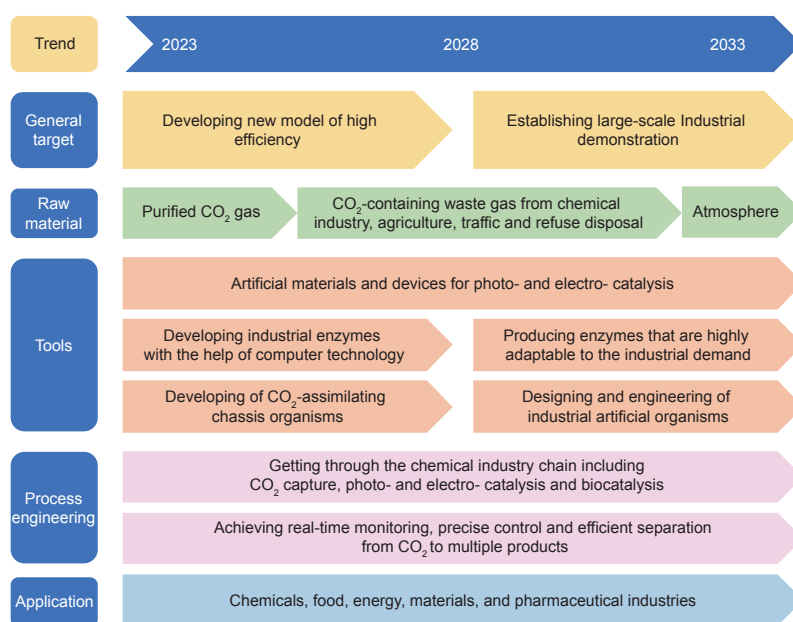


Figure 1.2.3 Roadmap of the engineering research front of “renewable energy-driven bioconversion of carbon dioxide to chemicals, fuels, and materials”

up considerably with application of computer technology, such as big data and artificial intelligence, and advanced physical and chemical technology to the screening, modification, and design of industrial enzymes and industrial strains. Technical autonomy of core enzymes and core strains will be achieved in the next few years. Research on advanced industrial reactors should be intensified to achieve real-time monitoring, precise regulation, and efficient separation of CO<sub>2</sub> from various fuels and chemicals according to production needs. This will result in establishment of targeted and efficient production routes.



### 1.2.2 Chaotic nonlinear enhancement technology of metallurgical flow field

Metallurgical reactors, which are used as reaction vessels in the metallurgical industry, play a pivotal role in industrial processes. These reactors provide a space for intricate multiphase mixing and reaction systems, encompassing the flow, mixing, reaction, heat transfer, and mass transfer of gas, solid, and liquid phases. They serve as a convergence point for micro-scale reactions and macroscopic processes. The metallurgical flow field, functioning as a conduit for energy and mass transfer, has a decisive influence over the synergy of these three domains and the overall system performance. Over the years, significant advancements in measurement and data acquisition techniques for metallurgical reaction systems have greatly enhanced the analytical capabilities of metallurgical flow fields under specific conditions. This progress has contributed to a deeper understanding of the intricate chemical processes involved. However, the design, optimization, and operation of these fields are still heavily reliant on empirical data. The chaotic nonlinear enhancement technology of metallurgical flow represents a cutting-edge research direction in the field of metallurgical science and engineering. This technology integrates knowledge from fluid dynamics, chaos theory, and nonlinear science. Its primary aim is to optimize the behavior of metallurgical flow fields to enhance production efficiency.

Metallurgical multiphase flow is a typical nonlinear process that deviates from equilibrium. It encompasses numerous complex nonlinear dynamic mechanisms and exhibits spatiotemporal cross-scale coupling characteristics. This leads to a lack of synergy between mixing, heat/mass transfer, and chemical reaction processes in metallurgical reaction systems, which poses challenges for effective control, enhancement, and engineering upscaling. The core direction of this field focuses on the synergistic evolution of continuous and dispersed phase topological structures in multiphase systems within metallurgical reactors, the interaction of chaotic flow mixing characteristics with multi-physics fields, and their correlation with transfer performance. The research pathway for chaotic nonlinear enhancement of metallurgical flow is as follows. First, chaos theory is used to describe the multiphase nonlinear systems in metallurgical processes, and rapid inter-phase heat and mass transfer is achieved via chaotic enhancement to accelerate chemical reaction rates. Second, the synergistic coupling of multi-physics fields, including flow, temperature, and composition fields, is realized, which enables effective control of the flow distribution. Third, through the enhancement of the synergy and uniformity of flow-transfer-reaction processes, efficient and uniform mixing is achieved along with intensified heat and mass transfer. This forms the theoretical foundation for the enhancement of metallurgical processes and optimization of reactors.

The major contributors to the engineering research front on “chaotic nonlinear enhancement technology of metallurgical flow field” in recent years are detailed in Table 1.2.5 for countries and Table 1.2.6 for institutions. Among the countries, China holds the lead position, followed by Iran. Among the institutions, the Islamic Azad University ranks first, while China’s Xi’an Jiaotong University, Shanghai Jiao Tong University, and the Chinese Academy of Sciences also rank highly. The collaborative network among the main countries and institutions is illustrated in Figures 1.2.4 and 1.2.5. China occupies a central position in this collaborative network, forming partnerships with multiple countries, and notably has a prominent collaboration with Pakistan. Pakistan is an important node in the network as well, and cooperates with all countries except for the UK and Singapore. Collaborations between institutions are tightly interconnected within Asia, with the Islamic Azad University holding a central position in the collaborative network and partnering with multiple institutions. As indicated in Table 1.2.7, China has the highest number of core paper citations, with 2 490 citations accounting for 26.51% of the total. China is the leader for both the core paper count and cited core paper count, which highlights the advanced position of Chinese scholars in this field. This indicates that Chinese scholars are at the forefront of research in this domain and are keeping abreast of the dynamics in this cutting-edge field.

Chaotic nonlinear enhancement of metallurgical flow involves using chaotic nonlinear theory to study the mixing mechanism of multiphase flow in metallurgical processes and analyzing the formation, transport, and transformation of multi-scale flow structures. To date, because of limitations in experimental measurement techniques and the development of multi-scale simulation methods, research on chaotic flow in extreme and unconventional metallurgy and the scaling up of large-scale equipment remains limited. Moreover, this research direction involves the intersection of multiple disciplines, including

metallurgy, fluid dynamics, and physics. There are three future research directions (Figure 1.2.6). First, research on chaotic flow enhancement in extreme and unconventional metallurgical reaction fields by advancing chaotic flow enhancement under extreme and unconventional metallurgical process conditions, involving electric, magnetic, and thermal stress fields. This will break down interdisciplinary barriers and enhance the systematic and universal aspects of nonlinear chaotic theory. Second, research on mechanisms and criteria for amplifying chaotic flow in super-large metallurgical smelting equipment by overcoming the mechanisms and criteria for chaotic flow amplification in metallurgical flow fields and addressing issues arising from the lack of theoretical guidance in the amplification of super-large smelting equipment, including distortion, operational instability, and process mismatch. Third, research on metallurgical flow field chaos nonlinear enhancement technology using machine learning by constructing metallurgical flow field nonlinear enhancement models using machine learning to overcome the complex coupling mechanisms of various factors in metallurgical processes. This will strengthen the intelligent development of metallurgical systems through software and hardware using machine learning.

Table 1.2.5 Countries with the greatest output of core papers on “chaotic nonlinear enhancement technology of metallurgical flow field”

No.	Country	Core papers	Percentage of core papers/%	Citations	Citations per paper	Mean year
1	China	40	33.33	3 192	79.80	2019.0
2	Iran	26	21.67	2 411	92.73	2018.5
3	USA	20	16.67	1 632	81.60	2018.4
4	India	20	16.67	1 529	76.45	2019.8
5	Pakistan	16	13.33	992	62.00	2019.9
6	Saudi Arabia	13	10.83	1 099	84.54	2019.6
7	UK	8	6.67	872	109.00	2019.2
8	Vietnam	8	6.67	540	67.50	2019.9
9	Singapore	7	5.83	454	64.86	2018.7
10	The United Arab Emirates	6	5.00	393	65.50	2019.3

Table 1.2.6 Institutions with the greatest output of core papers on “chaotic nonlinear enhancement technology of metallurgical flow field”

No.	Institution	Core papers	Percentage of core papers/%	Citations	Citations per paper	Mean year
1	Islamic Azad University	10	8.33	893	89.30	2018.8
2	Xi'an Jiaotong University	8	6.67	499	62.38	2018.5
3	Ton Duc Thang University	7	5.83	491	70.14	2019.7
4	Nanyang Technological University	6	5.00	410	68.33	2019.0
5	Shanghai Jiao Tong University	4	3.33	453	113.25	2019.8
6	Chinese Academy of Sciences	4	3.33	433	108.25	2017.8
7	King Fahd University of Petroleum and Minerals	4	3.33	410	102.50	2020.2
8	Iran University of Science and Technology	4	3.33	309	77.25	2019.0
9	Indian Institute of Technology	4	3.33	284	71.00	2019.0
10	COMSATS University Islamabad	4	3.33	229	57.25	2020.2

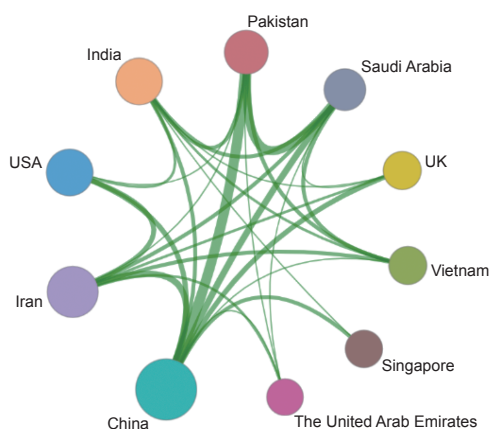


Figure 1.2.4 Collaboration network among major countries in the engineering research front of “chaotic nonlinear enhancement technology of metallurgical flow field”

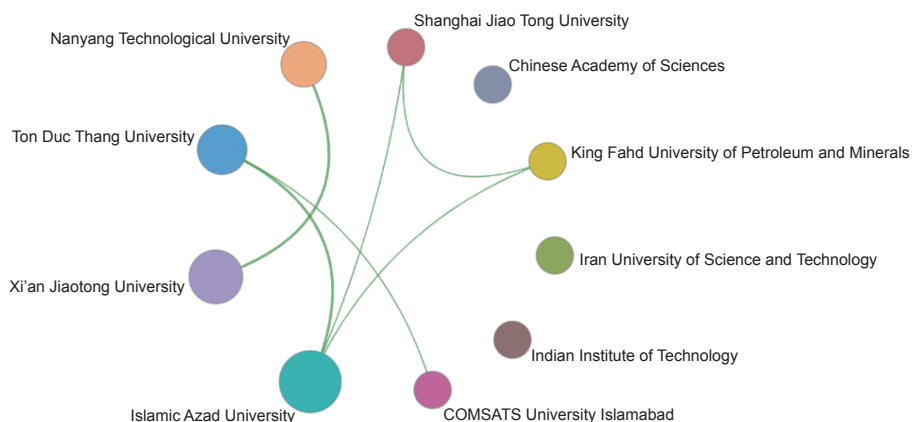


Figure 1.2.5 Collaboration network among major institutions in the engineering research front of “chaotic nonlinear enhancement technology of metallurgical flow field”

Table 1.2.7 Countries with the greatest output of citing papers on “chaotic nonlinear enhancement technology of metallurgical flow field”

No.	Country	Citing papers	Percentage of citing papers/%	Mean year
1	China	2 490	26.51	2021.0
2	Saudi Arabia	1 327	14.13	2021.3
3	Pakistan	1 157	12.32	2021.1
4	India	1 050	11.18	2021.2
5	Iran	1 003	10.68	2020.5
6	USA	560	5.96	2020.8
7	Egypt	458	4.88	2021.5
8	UK	366	3.90	2021.1
9	Vietnam	351	3.74	2020.2
10	Malaysia	315	3.35	2021.0

Table 1.2.8 Institutions with the greatest output of citing papers on “chaotic nonlinear enhancement technology of metallurgical flow field”

No.	Institution	Citing papers	Percentage of citing papers/%	Mean year
1	King Khalid University	360	14.84	2021.5
2	Islamic Azad University	306	12.61	2020.5
3	King Abdulaziz University	301	12.41	2021.2
4	Ton Duc Thang University	279	11.50	2020.0
5	Prince Sattam Bin Abdulaziz University	230	9.48	2021.6
6	Xi'an Jiaotong University	195	8.04	2020.9
7	China Medical University	191	7.87	2021.5
8	COMSATS University Islamabad	169	6.97	2021.4
9	Babol Noshirvani University of Technology	159	6.55	2019.4
10	Duy Tan University	129	5.32	2020.5

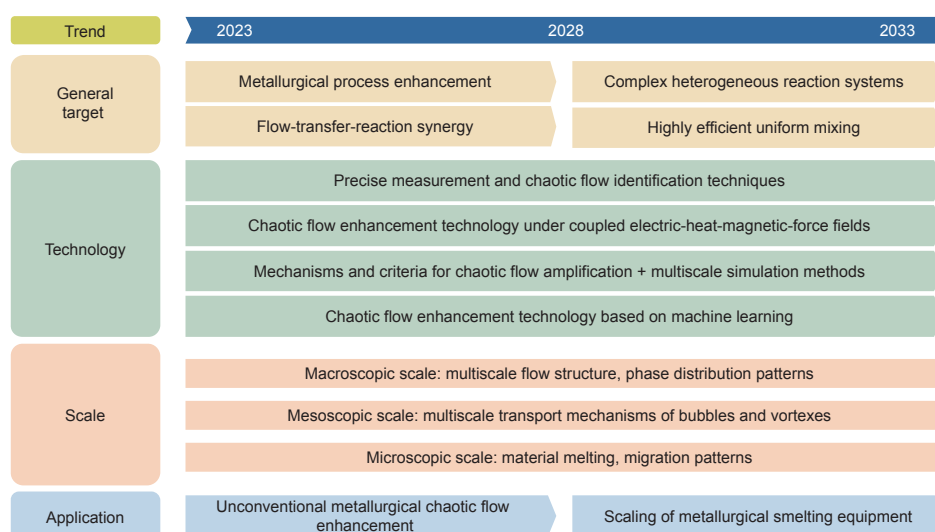


Figure 1.2.6 Roadmap of the engineering research front of “chaotic nonlinear enhancement technology of metallurgical flow field”

### 1.2.3 High-performance electrocatalysts and electrolysis systems for CO<sub>2</sub> conversion and utilization

The use of renewable energy to drive electrochemical reduction of CO<sub>2</sub> to produce high value-added chemicals provides an effective way to solve the energy crisis and environmental problems. In recent years, research on the development of electrocatalyst materials for CO<sub>2</sub> reduction has made great progress in terms of selectivity, efficiency, and reaction rate, and is moving towards practical applications. Electrochemical reduction of CO<sub>2</sub> can be used to produce various chemicals, such as alcohols, oxygenates, syngas, and olefins, on a large scale. The shift to renewable energy could greatly reduce CO<sub>2</sub> emissions.

Because of its high thermodynamic stability, CO<sub>2</sub> is difficult to activate. Additionally, it is difficult to generate high value-added C<sub>2+</sub> products through C–C coupling. Recently, significant progress has been made in the design of highly active or highly selective electrocatalysts and the mechanism of CO<sub>2</sub>RR. There are three main areas of focus in current research.



First, design and controllable preparation of highly efficient electrocatalysts through control of the crystal surface, morphology, and surface electronic structure to improve the CO<sub>2</sub>RR activity, selectivity, and stability. Second, various *in situ* characterization methods, such as *in situ* infrared spectroscopy, *in situ* Raman spectroscopy, and *in situ* electron microscopy, are used to monitor the evolution of the reaction intermediates and catalyst surface structures during the CO<sub>2</sub>RR process. The results are used to reveal the regulatory effects of the catalyst surface and electronic structure on the catalytic reaction and its kinetic mechanism. Third, design of the electrode structure through the modification of hydrophobic materials (such as polytetrafluoroethylene) and improvement of the hydrophobic performance of the electrode surface to avoid issues with flooding during long-term operation and improve the electrode stability. The structure of electrolytic reactor is optimized to enhance mass transfer and energy efficiency.

The major countries and institutions in recent years for output of core papers on the engineering research front of “high-performance electrocatalysts and electrolysis systems for CO<sub>2</sub> conversion and utilization” are shown in Tables 1.2.9 and 1.2.10, respectively. Among the major countries producing core papers, China is ranked first, with 71 core papers (66.36% of the total), which is much higher than the numbers produced in the USA, Australia, Canada, and other countries. Among the major institutions producing core papers, Chinese Academy of Sciences is ranked first, followed by University of Science and Technology of China, and Stanford University. The major collaborations among countries and institutions are plotted in Figures 1.2.7 and 1.2.8, respectively. Most of China’s collaborations are with the USA, and it also closely cooperates with Australia, Canada, and Singapore. The top three countries in terms of the number of citing core papers are China, the USA, and Australia (Table 1.2.11). The proportion of citing papers from China is 57.95%, which indicates that Chinese scientists have paid close attention to the research trends in this area. Most of the major institutions producing citing core papers are in China, including Chinese Academy of Sciences, University of Science and Technology of China, and Tianjin University (Table 1.2.12)

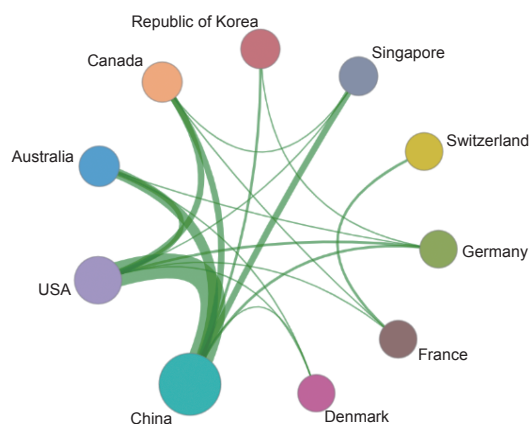
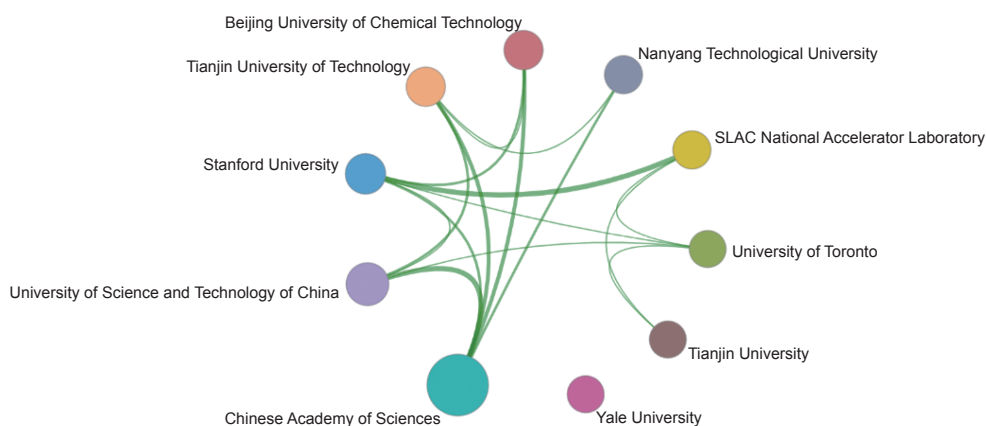
It is an important to develop green and low-carbon energy technology to activate and transform CO<sub>2</sub> through electrocatalytic mild conditions to synthesize the chemicals needed for social and economic development. The electrocatalytic conversion of CO<sub>2</sub> is a complex multi-scale process, involving CO<sub>2</sub> molecular adsorption and conversion, nano-scale catalysts, micron-scale membrane electrodes, and macro-scale electrolyzers. Current research is mainly focused on finding and improving high-performance electrocatalysts. Future research should look at combining various *in situ* characterization methods for electrode morphology

**Table 1.2.9 Countries with the greatest output of core papers on “high-performance electrocatalysts and electrolysis systems for CO<sub>2</sub> conversion and utilization”**

No.	Country	Core papers	Percentage of core papers/%	Citations	Citations per paper	Mean year
1	China	71	66.36	17 849	251.39	2019.0
2	USA	31	28.97	8 069	260.29	2018.8
3	Australia	12	11.21	2 946	245.50	2018.9
4	Canada	11	10.28	4 406	400.55	2019.1
5	Republic of Korea	9	8.41	1 429	158.78	2018.8
6	Singapore	7	6.54	2 569	367.00	2018.9
7	Switzerland	4	3.74	764	191.00	2018.5
8	Germany	4	3.74	686	171.50	2018.8
9	France	4	3.74	681	170.25	2019.2
10	Denmark	3	2.80	749	249.67	2018.3

Table 1.2.10 Institutions with the greatest output of core papers on “high-performance electrocatalysts and electrolysis systems for CO<sub>2</sub> conversion and utilization”

No.	Institution	Core papers	Percentage of core papers/%	Citations	Citations per paper	Mean year
1	Chinese Academy of Sciences	25	23.36	6 474	258.96	2019.1
2	University of Science and Technology of China	9	8.41	2 517	279.67	2019.4
3	Stanford University	7	6.54	1 813	259.00	2019.3
4	Tianjin University of Technology	6	5.61	1 616	269.33	2018.7
5	Beijing University of Chemical Technology	6	5.61	1 260	210.00	2019.0
6	Nanyang Technological University	5	4.67	1 846	369.20	2019.0
7	SLAC National Accelerator Laboratory	5	4.67	1 032	206.40	2019.4
8	University of Toronto	4	3.74	2 155	538.75	2020.0
9	Tianjin University	4	3.74	2 082	520.50	2018.0
10	Yale University	4	3.74	1 860	465.00	2017.5

Figure 1.2.7 Collaboration network among major countries for the engineering research front of “high-performance electrocatalysts and electrolysis systems for CO<sub>2</sub> conversion and utilization”Figure 1.2.8 Collaboration network among major institutions for the engineering research front of “high-performance electrocatalysts and electrolysis systems for CO<sub>2</sub> conversion and utilization”





evolution, reaction process condition optimization, electrode/electrolyte interface evolution, mass transfer transportation optimization, catalyst stability improvement, and electrolyte/solvent effect. Additionally, for the future industrial application of electrocatalytic reduction of CO<sub>2</sub>, the following points need to be considered: determining the practical application objectives, evaluating the economics of chemical products and market supply and demand, expanding the scale of CO<sub>2</sub> electrolyzers, improving the long-term continuous operation stability of electrocatalysts, and calculating the cost of product separation and raw material recovery. The roadmap of the engineering research front of “high-performance electrocatalysts and electrolysis systems for CO<sub>2</sub> conversion and utilization” is shown in Figure 1.2.9.

Table 1.2.11 Countries with the greatest output of citing papers on “high-performance electrocatalysts and electrolysis systems for CO<sub>2</sub> conversion and utilization”

No.	Country/Region	Citing papers	Percentage of citing papers/%	Mean year
1	China	8 508	57.95	2021.0
2	USA	1 928	13.13	2020.6
3	Australia	746	5.08	2020.8
4	Republic of Korea	612	4.17	2020.9
5	Germany	524	3.57	2020.8
6	Canada	521	3.55	2020.7
7	India	424	2.89	2021.1
8	UK	407	2.77	2020.8
9	Singapore	405	2.76	2020.8
10	Japan	386	2.63	2020.8

Table 1.2.12 Institutions with the greatest output of citing papers on “high-performance electrocatalysts and electrolysis systems for CO<sub>2</sub> conversion and utilization”

No.	Institution	Citing papers	Percentage of citing papers/%	Mean year
1	Chinese Academy of Sciences	1 705	36.28	2020.9
2	University of Science and Technology of China	525	11.17	2021.0
3	Tianjin University	405	8.62	2021.0
4	Tsinghua University	374	7.96	2021.0
5	Beijing University of Chemical Technology	303	6.45	2020.8
6	Zhengzhou University	300	6.38	2021.2
7	Soochow University	260	5.53	2020.9
8	Nanyang Technological University	230	4.89	2020.7
9	Zhejiang University	209	4.45	2021.0
10	Shenzhen University	196	4.17	2021.1

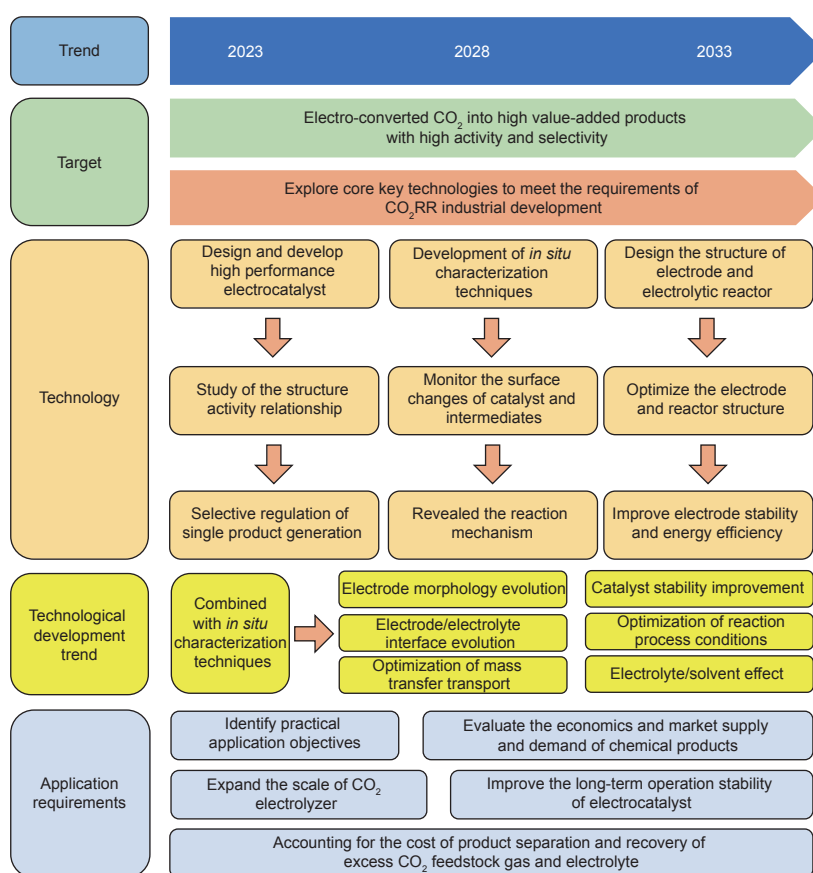


Figure 1.2.9 Roadmap of the engineering research front of “high-performance electrocatalysts and electrolysis systems for CO<sub>2</sub> conversion and utilization”

## 2 Engineering development fronts

### 2.1 Trends in Top 11 engineering development fronts

The Top 11 engineering development fronts as assessed by the Field Group of Chemical, Metallurgical, and Materials Engineering are shown in Table 2.1.1. “Design and preparation of metal matrix composites for high-temperature environments”, “construction and large-scale manufacturing technology of high-efficiency photovoltaic devices”, “low-temperature and low-pressure thermal catalytic ammonia synthesis over a wide loading range”, and “development of ironmaking technology for hydrogen-rich carbon cycle blast furnaces” were recommended by experts directly. The other fronts were chosen by a panel of experts according to core-paper statistics provided by Clarivate. The annual numbers of core patents for all fronts show overall growth, especially for “integration of large language models for the design and synthesis of advanced chemical engineering materials”, “efficient and energy-saving separation technologies for energy intensive chemical processes”, and “development of ironmaking technology for hydrogen-rich carbon cycle blast furnaces” (Table 2.1.2).

#### (1) Metallurgical low-carbon utilization of renewable energy

The smelting process of complex metal materials requires a large amount of electricity and relies on the reduction characteristics of fossil fuels and combustion heating. This is the key to restrict the low-carbon sustainable development of the metallurgical



Table 2.1.1 Top 11 engineering development fronts in chemical, metallurgical, and materials engineering

No.	Engineering development front	Published patents	Citations	Citations per patent	Mean year
1	Metallurgical low-carbon utilization of renewable energy	520	223	0.43	2020.4
2	Integration of large language models for the design and synthesis of advanced chemical engineering materials	482	1 354	2.81	2020.9
3	Design and preparation of metal matrix composites for high-temperature environments	596	1 033	1.73	2019.7
4	Efficient and energy-saving separation technologies for energy intensive chemical processes	697	774	1.11	2020.0
5	Chaotic enhancement technology for heating process in metallurgical furnaces	775	501	0.65	2019.8
6	Construction and large-scale manufacturing technology of high-efficiency photovoltaic devices	705	1 066	1.51	2019.4
7	Low-temperature and low-pressure thermal catalytic ammonia synthesis over a wide loading range	540	890	1.65	2019.5
8	Development of ironmaking technology for hydrogen-rich carbon cycle blast furnaces	353	582	1.65	2020.2
9	Development and application of ultra-high energy density aluminum-air batteries	400	656	1.64	2019.7
10	Key preparation technologies and applications of high-purity metals, alloys, and materials	358	335	0.94	2019.8
11	Molecular design and large-scale preparation of new bio-aviation fuels	208	464	2.23	2019.6

Table 2.1.2 Annual number of core patents published for the Top 11 engineering development fronts in chemical, metallurgical, and materials engineering

No.	Engineering development front	2017	2018	2019	2020	2021	2022
1	Metallurgical low-carbon utilization of renewable energy	40	48	48	90	140	154
2	Integration of large language models for the design and synthesis of advanced chemical engineering materials	12	22	46	66	123	213
3	Design and preparation of metal matrix composites for high-temperature environments	84	101	87	93	106	125
4	Efficient and energy-saving separation technologies for energy intensive chemical processes	83	90	92	105	131	196
5	Chaotic enhancement technology for heating process in metallurgical furnaces	97	113	109	132	157	167
6	Construction and large-scale manufacturing technology of high-efficiency photovoltaic devices	126	142	108	95	100	134
7	Low-temperature and low-pressure thermal catalytic ammonia synthesis over a wide loading range	101	76	93	81	86	103
8	Development of ironmaking technology for hydrogen-rich carbon cycle blast furnaces	32	48	39	55	59	120
9	Development and application of ultra-high energy density aluminum-air batteries	52	53	77	77	68	73
10	Key preparation technologies and applications of high-purity metals, alloys, and materials	46	50	55	53	72	82
11	Molecular design and large-scale preparation of new bio-aviation fuels	32	37	32	28	36	43

industry. Renewable energy can provide clean electricity, biomass energy, and green hydrogen with reducibility and combustion heating properties. It is expected that low-carbon green transformation of the industry will be achieved with the efficient application of renewable energy in metallurgy. China has developed a relatively complete iron and steel hydrogen metallurgy system and conducted metallurgy demonstration projects for more than one million tons of hydrogen. Hydropower silicon and hydropower aluminum have been achieved in Yunnan, China with an output value of more than 100 billion RMB. However, in the field of renewable energy combustion and reduction technology, there are still many problems to be further studied. The future development direction is mainly concentrated in three areas. First, metallurgical energy systems should be combined with multi-energy complementation and energy storage to develop clean energy supply systems using wind, light, water, hydrogen, and metallurgical waste heat and energy. Second, new technology for deep reduction of metallurgical slag by swirl injection of biomass fuel oil should be developed to replace fossil energy reducing agents with renewable energy. Third, swirl atomization enhanced combustion technology of biomass fuel should be developed to improve combustion and heating efficiency of macromolecular, low calorific value biomass fuel, and replace fossil fuel with renewable energy. These changes will provide clean energy, improve the efficiency of energy consumption, and reduce carbon emissions over the full lifecycle.

### (2) Integration of large language models for the design and synthesis of advanced chemical engineering materials

The development cycle for new chemical materials spans 15–25 years, requires significant investment, and is heavily reliant on expert experience. As the field has matured, the size of the total dataset has increased but data for some specific sub-systems are limited. Access to experts with experience to discern patterns in new materials is becoming increasingly challenging, and there is an urgent need for a paradigm shift in research methodologies. At the beginning of 2023, ChatGPT emerged, closely followed by Llama, Claude, Wenxin Yiyan, and Wu Dao, marking the dawn of the era of large language models (hereafter referred to as large models). Characterized by their large scale, emergent properties, and universality, these models are promising for application in the chemical engineering sector and show potential for accelerating the design and fabrication of new materials. Large models can comprehensively hasten the development of new materials across various stages, including literature information extraction, material structure generation, material property prediction, synthesis condition optimization, and intelligent characterization. Literature information extraction serves as the primary means to integrate chemical material data. Large language models can refine the output of natural language models to make them structured information, and improve the quality of data. Material structure generation is a key technology for the reverse design of new materials, and could benefit from the emergent properties of large models in breaking human cognitive biases. Material property prediction is a prerequisite for high-throughput screening and could be enhanced by large models, which consolidate various smaller models within the field to enable precise prediction of various material properties. Synthesis condition optimization and intelligent characterization are core steps in exploring material fabrication techniques. Large models possess superior pattern-recognition capabilities, allowing for faster identification of optimal points.

### (3) Design and preparation of metal matrix composites for high-temperature applications

Metal matrix composites (MMCs) are multiphase materials composed of a metal or alloy matrix and one or more types of reinforcement. These composites possess the combined characteristics of the metal or alloy matrix and the reinforcement, including high specific strength, specific modulus, low density, and good electrical and thermal conductivity. Consequently, they are used in many applications in the aerospace, automotive, electronic information, and national defense industries. However, most research on MMCs has focused on enhancing their mechanical properties at room temperature, particularly their strength and toughness, while high-temperature properties have received relatively little attention. Under high-temperature and stress conditions, solute atoms exhibit faster diffusion rates and are more vulnerable to adverse effects such as oxidation and corrosion from the service environment. Additionally, MMCs subjected to long-term use frequently experience failure in the form of thermal fatigue or creep damage. Consequently, their service lives tend to be shorter than those used at room temperature. This underscores the urgency for design of MMCs to meet the requirements of high-temperature use. Currently, material development efforts at both domestic and international levels are primarily focused on four aspects. First, high-throughput preparation and characterization of composites using material genetic engineering. Second, fine control of the configuration and interface in the



material forming process. Third, short process manufacturing technology for producing large-size components of heat-resistant aluminum matrix composites. Forth, understanding the evolution, property degradation mechanisms, and control technology of composites used in high-temperature environments.

### (4) Efficient and energy-saving separation technologies for energy intensive chemical processes

The chemical industry had large energy consumption and carbon emissions. Chemical separation processes account for approximately 70% of the total energy consumption in chemical product processing. Currently, although some industries have made significant improvements in technology and equipment, the overall technical level is still relatively low. The proportion of technology and equipment at an advanced international level in the entire industry is very small, and the energy utilization rate is approximately 15% lower than the average of developed countries. Some chemical products have an energy consumption more than 20% higher than those in developed countries. Improvements in production efficiency, energy conservation, emission reductions, and industrial upgrades can only be achieved by increasing technological innovation; vigorously developing and promoting new energy-saving processes, technologies, and equipment for chemical separation processes; reducing fossil energy consumption and improving energy utilization efficiency; and fully utilizing high-tech to enhance and transform traditional chemical industries. The future development of separation technology for energy intensive chemical processes should mainly focus on two aspects. First, development of alternative and efficient separation methods, such as molecular recognition separation technology, separation process integration, and intensification technology. Appropriate separation methods should be selected according to the characteristics of different separation systems to improve the energy utilization efficiency of the separation process. Second, development of new forms of renewable energy, such as solar energy, biomass energy, green hydrogen, and green electricity, to reduce the proportion of fossil energy used in the separation process. Development of new separation technologies using renewable energy could be used to promote the transition to a green, sustainable, and efficient chemical industry.

### (5) Chaotic enhancement technology for heating process in metallurgical furnaces

The main method to achieve energy savings and efficiency improvements in metallurgical furnace is to strengthen the heating process. Traditional intensified heating mainly relies on increasing the amount of heating, which leads to high energy consumption and carbon emissions, and shortens the equipment lifecycle. Additionally, the product quality does not meet the requirements for high-end uses. Chaotic enhanced heating technology in metallurgical furnace uses chaotic mathematical theory to establish a series of mathematical models of chaotic flow intensification, and then regulates the chaotic flow pattern to strengthen heat and mass transfer. Currently, industrial applications have been realized in molten pool melting furnaces and heating furnaces. Two key scientific problems, the enhancement mechanism of heat and mass transfer in furnaces and the multi-field collaborative enhancement mechanism, have not been solved. Consistency between the mathematical model and practical application is not sufficient. There are three main future directions. First, extensive research is required on the basic theory and nonlinear chaos technology in furnace heating, further improvements are needed in the minimum burn-up heating law and model, and the issue of inaccurate heating needs to be solved. Second, to address this problems of serious sputtering and short equipment life of molten pool melting furnace, the oxygen-enriched swirl chaotic stirring heating technology is developed to solve the problems of insufficient utilization of oxygen-enriched and insufficient self-heating and high energy consumption. Third, swirling chaotic combustion and heating system control technology should be developed to overcome issues with inaccurate heating and incomplete fuel combustion in the heating furnace. This will solve difficulties with uniformly heating metal workpieces, ensure heating quality, reduce energy consumption and achieve uniform and accurate heating.

### (6) Construction and large-scale manufacturing technology of high-efficiency photovoltaic devices

Developing photovoltaic technology is as a vital and transformative initiative for harnessing renewable energy. To overcome the limitations of traditional silicon-based photovoltaic cells, various emerging thin-film photovoltaic technologies, such as cadmium telluride solar cells, copper indium gallium selenide-based solar cells, perovskite solar cells, and polymer solar cells, have come to the forefront of renewable energy. Recently, remarkable progress has been made for these photovoltaic technologies in both power conversion efficiency and large-scale manufacturing techniques. These advancements are important for enhancing their

competitiveness and facilitating their commercialization. The unique advantages of these thin film photovoltaic technologies have significantly expanded the application horizons of photovoltaics, allowing for integration into urban infrastructure, consumer electronics, and beyond. These new applications include building integrated photovoltaics and portable devices. The future development of photovoltaic technology requires focused attention on the following four aspects. First, enhanced integration into new energy power systems to support the advancement of smart city construction. Second, integration with energy storage technology to achieve a steady supply and efficient utilization of green energy. Third, the recycling and reutilization of photovoltaic components to propel the industry towards green and sustainable growth. Fourth, pivotal technological breakthroughs for emerging photovoltaic technologies to reduce costs, extend the lifespan, and allow for successful mass production.

#### (7) Low-temperature and low-pressure thermal catalytic ammonia synthesis over a wide loading range

Ammonia, with an annual output of 180 million tons, plays an important role in modern agriculture and industry. Because of its easy liquefaction, high energy density, and zero carbon emissions, ammonia is called hydrogen 2.0 and is expected to become a next-generation energy carrier. Synthesis of  $\text{NH}_3$  by the reaction of  $\text{N}_2$  and  $\text{H}_2$  is an exothermic process accompanied by a decrease in volume. A low temperature and high pressure are conducive for this reaction. However, because of the high bond energy and weak coordination ability of  $\text{N}_2$  molecules,  $\text{N}_2$  is difficult to activate at low temperatures. Currently, synthesis of ammonia is carried out continuously under the high temperature and high pressure, which has a high energy consumption and high carbon emissions. Additionally, clean energy, such as photovoltaics and wind, are volatile, retarding the green upgrades of traditional ammonia synthesis. Future development of low temperature and low-pressure green ammonia preparation technology with a wide loading range should focus on the following aspects: development of catalysts with high intrinsic activity, reduction of the adsorption energy barrier of  $\text{N}_2$  on the catalyst surface, and improvement of the activation capacity of nitrogen at low temperature. In a traditional thermal catalytic reactor, electric, magnetic, and other external fields with variable frequency can be introduced to adjust the electronic structure of the active center of the catalyst to break the restrictions of adsorption and desorption. Devices and systems with rapid response abilities need to be developed to broaden the loading range of synthetic ammonia under low-temperature and low-pressure conditions.

#### (8) Development of ironmaking technology for hydrogen-rich carbon cycle blast furnaces

Blast furnace ironmaking is the main method for iron production currently. The global production of pig iron from blast furnaces exceeded 1.3 billion tons in 2022. The blast furnace–basic oxygen furnace (BF-BOF) process will still be an important method for iron and steel production in the future. Because approximately 2/3 of carbon emissions from iron and steel manufacturing comes from the blast furnace process, reducing carbon emissions from blast furnace ironmaking process is a focus of research in the global steel industry. The ironmaking technology for hydrogen-rich carbon cycle can minimize carbon emissions, by injecting hydrogen-rich gas (such as coke oven gas) into the blast furnace, which can replace the coke and coal, using the top gas recycling (TGR) technology and carbon capture, utilization and storage (CCUS) technology to reuse the  $\text{CO}$  and  $\text{H}_2$ , and capture  $\text{CO}_2$  from blast furnace gas. The ironmaking technology for hydrogen-rich carbon cycle blast furnaces is the first choice for reducing carbon emission from traditional blast furnace because it does not need to change the process structures and charge structures. Companies such as Nippon Steel, ThyssenKrupp, and China Baowu are actively developing and experimenting the ironmaking technology for hydrogen-rich carbon cycle blast furnaces, and have achieved phased carbon reduction goals. The key points of ironmaking technology for hydrogen-rich carbon cycle blast furnaces include full-oxygen blast furnace iron-making technology, reheating and recycling of top gas after  $\text{CO}_2$  capture, injection of hydrogen-enriched compound gases into the blast furnace, and self-circulation of the blast furnace gas under full-oxygen blast furnace conditions.

#### (9) Development and application of ultra-high energy density aluminum-air batteries

With the development of the global economy, energy demands have increased rapidly, which is of great concern. Currently, common traditional energy sources, such as lead-acid batteries, nickel-metal hydride batteries, and lithium-ion batteries, have limitations in their energy densities, safety, and production costs. Aluminum-air batteries (AABs) show potential as an energy storage system because of their high voltage (2.7 V), high capacity density (2 980 mAh/g), high energy density (8 100 Wh/kg), high



safety, abundance of source materials, and environmentally friendly features. Research on the inhibition of hydrogen evolution on the anode surface has progressed in the key areas, such as alloying of anode materials, introduction of electrolyte additives, and use of organic electrolytes. The international community has established new goals for energy demand and technical indicators, and it is particularly important to design and develop AABs with ultra-high energy density, high safety, and high power that can be mass produced. Specifically, three key technological breakthroughs need to be achieved in the basic research and industrial applications of aluminum-air batteries in the future: ① development of battery modification technology (including anode alloying techniques and electrolyte additives) and understanding of the corresponding surface/interface reaction mechanism; ② development of a coupling model for battery components and subsequent optimization to simplify the battery structure and facilitate large-scale application; and ③ continuous development of AABs with low carbon emissions, high safety, and low cost, and utilization of the battery by-products to enhance the economic benefits of the AABs.

### (10) Key preparation technologies and applications of high-purity metals, alloys, and materials

High-purity metals, alloys, and materials are mainly used in semiconductor, wireless electronics, aerospace, and military fields, and in other cutting-edge science and technology. The methods for preparation of high purity materials include chemical purification and physical purification. Chemical methods mainly rely on the reactivity-selectivity principle of the chemical reaction, and impurities are removed through selective chemical reactions by modifying the reaction system, controlling the reaction conditions, and optimizing the reaction environment. In physical methods, similarities and differences in the physical characteristics of different elements are used to remove impurities through vacuum distillation, zone melting, and electromigration methods. Chemical and physical purification methods are usually combined to obtain highly purified materials. The core problems to be solved in the preparation of high purity metals, alloys and their materials include: ① the dispersion and distribution mechanism of impurity elements in materials; ② the similarity of elements and their selective separation kinetics, which are needed to calculate the interaction force, heat of absorption and desorption, and kinetic equilibrium parameters between the matrix and impurities; and ③ the mechanisms behind impurity phase morphology transformation, migration behavior, and the regulation of purification process parameters.

### (11) Molecular design and large-scale preparation of new bio-aviation fuels

New bio-aviation fuels could be synthesized from biomass raw materials by precise chain breaking and re-synthesis through chemical bonding. Current research on new bio-aviation fuels focuses on four aspects. First, biofuel molecular design should be conducted by investigating the structure-activity relationship between the fuel molecular structure and physicochemical properties. Additionally, rational design and screening methods for high-throughput fuel molecules should be established, which could help to produce target molecule structure libraries from the molecular structure characteristics of the biomass raw materials. Second, an efficient and mild synthesis method is required to achieve high atom utilization for high output conversion of biomass feedstock to aviation fuel. Third, the mechanism of the catalytic reaction and the relationship between the catalyst structure and its performance in biomass conversion should be studied. This will guide the development of hyperdispersed low-load noble metal catalysts or non-noble metal catalysts with high activity and selectivity. Fourth, continuous improvement of catalysts and processes, development of integrated processes and optimization of reactor structures, improvement of the reaction efficiency, and reduction of the energy consumption are required for large-scale fuel preparation. There is an urgent demand for carbon emission reductions in the aviation field, and it is necessary to accelerate the pace of design, efficient synthesis, and large-scale preparation of bio-aviation fuel. New bio-aviation fuels that can replace petroleum-based aviation fuels will assist with this.

## 2.2 Interpretations for three key engineering development fronts

### 2.2.1 Metallurgical low-carbon utilization of renewable energy

The process of mining, smelting, and heat treatment in the steel and non-ferrous metallurgical industries directly consumes large quantities of fossil fuels. Implementation of clean energy substitutes is an effective measure to solve carbon emission problems. The



green metallurgical industry need reconstruct the layout and overall arrangement, facilitate the transition of metallurgical production capacity to metal resources areas or renewable energy-rich areas of wind energy, solar energy, hydropower. For example, aluminum electrolysis companies can be constructed near nuclear power plants. Biomass energy, which has a mature manufacturing process but has always been limited in its application scale, is the only carbon-containing renewable energy source and is the best green and low-carbon alternative for metallurgical fuels and reducing agents. Exploring the efficient application of renewable energy in the metallurgical field is a new way to achieve green and low-carbon transformation of the metallurgical industry.

For steel metallurgy, the utilization of renewable energy has developed rapidly in recent years. Clean energy sources such as hydrogen energy, solar energy, wind energy, hydropower, and coal-to-gas conversion have been introduced. The use of multi-energy systems and complementary technologies has increased the use of clean energy in the metallurgical industry. New methods of energy recovery, such as waste heat utilization, have been developed, and cross-process and cross-industry energy recycling have been promoted by optimizing key processes and improving equipment. However, renewable energy has issues with intermittent instability, and it is difficult to achieve a continuous and stable energy supply. China has developed a relatively complete metallurgy system for steel hydrogen. As an example, the 1.2-million-ton hydrogen metallurgy demonstration project of the Hebei Province HBIS Group is the first in the world to use the coke oven gas self-reforming method to produce hydrogen. The obtained hydrogen has been used to directly reduce iron-containing raw materials and produce high-quality iron.

Development of green electricity in the non-ferrous metallurgical industry has been very rapid. For example, in Yunnan Province, China, which is rich in renewable energy, interest in electrolytic aluminum enterprises has increased. The scale of green aluminum and silicon production capacity in this region ranks among the top in the country, with an output value exceeding 100 billion RMB. Combination of silicon-aluminum industry with clean energy can realize the green development of integrated hydropower, silicon, and aluminum industries. However, the research and development and application of alternative technologies for biomass combustion and emissions reductions in the metallurgical industry are still in their infancy, and the future emission reduction potential is huge.

The relevant patents are mostly from China (Tables 2.2.1 and 2.2.2), which is consistent with its position as “the largest metallurgical country”. Kunming University of Science and Technology is ranked first in the number of patents because of its advantages of regional new energy resources and metallurgical technology research.

A roadmap for the next 20 years for the research front of “metallurgical low-carbon utilization of renewable energy” is shown in Figure 2.2.1. The main focuses are construction of a metallurgical energy system that combines multi-energy sources and energy storage systems to form a complementary clean energy supply system of wind, solar, water–hydrogen, and metallurgical waste heat and energy; development of a new technology for reduction of metallurgical slag by swirl injection of biomass fuel oil, and replacing fossil fuel energy reducing agents with renewable energy; and development of enhanced combustion technology for swirl atomization of biomass fuel oil and replacement of fossil fuels with renewable energy to achieve clean and low carbonization of metallurgical energy structure. The overall goal is transformation from carbon metallurgy to disruptive green low-carbon metallurgy in the next 10 years, and in the following 10 years reduction in the energy consumption of smelting and carbon emissions intensity. This will provide a metallurgical process with zero emissions.

Table 2.2.1 Countries with the greatest output of core patents on “metallurgical low-carbon utilization of renewable energy”

No.	Country	Published patents	Percentage of published patents/%	Citations	Percentage of citations/%	Citations per patent
1	China	513	98.65	218	97.76	0.42
2	India	2	0.38	0	0.00	0.00
3	Republic of Korea	2	0.38	0	0.00	0.00
4	Netherlands	1	0.19	5	2.24	5.00
5	Russia	1	0.19	0	0.00	0.00



Table 2.2.2 Institutions with the greatest output of core patents on “metallurgical low-carbon utilization of renewable energy”

No.	Institution	Published patents	Percentage of published patents/%	Citations	Percentage of citations/%	Citations per patent
1	Kunming University of Science and Technology	14	2.69	16	7.17	1.14
2	CISDI Engineering Company Limited	13	2.50	4	1.79	0.31
3	Jiangsu Binxin Iron and Steel Group Company Limited	7	1.35	1	0.45	0.14
4	Baoshan Iron & Steel Company Limited	6	1.15	2	0.90	0.33
5	Cangzhou China Railway Equipment Manufacturing Technology Company Limited	5	0.96	2	0.90	0.40
6	Yunnan Desheng Steel Company Limited	4	0.77	1	0.45	0.25
7	Wuhai Desheng Coal Coking Company Limited	4	0.77	0	0.00	0.00
8	Qingdao University of Technology	3	0.58	6	2.69	2.00
9	Xinhua Qunhua Ceramics Technology Company Limited	3	0.58	4	1.79	1.33
10	Angang Steel Company Limited	3	0.58	3	1.35	1.00

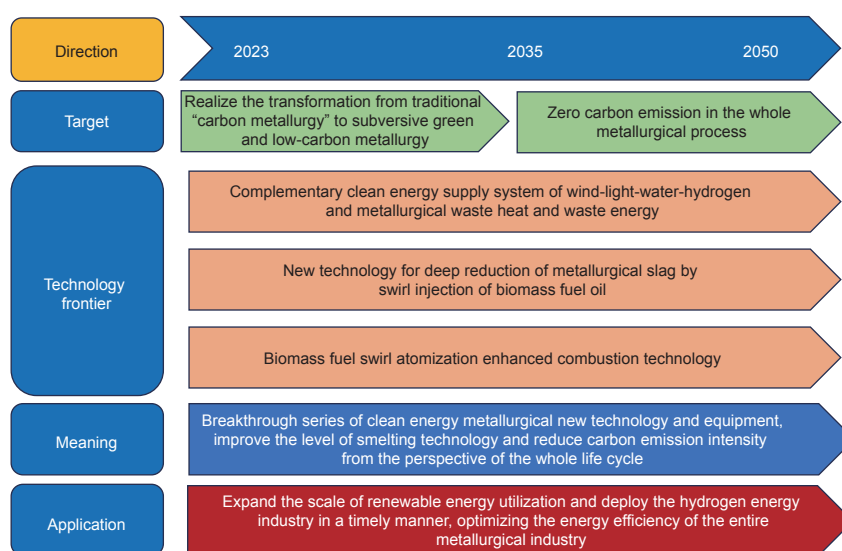


Figure 2.2.1 Roadmap of the engineering development front of “metallurgical low-carbon utilization of renewable energy”

### 2.2.2 Integration of large language models for the design and synthesis of advanced chemical engineering materials

The chemical and materials industry is a pillar of industrial society and forms the cornerstone of humanity's endeavor to explore and transform the material world. Each discovery and mass production of a new material signifies a leap forward. However, the traditional R&D paradigm of trial and error through experimentation and human summarization of patterns has reached its limits, which slows the design and preparation of new chemical materials. A paradigm shift is required in research methodologies. In the realm of new chemical materials, the data are characterized by large volumes yet sparse distributions. Relying on manual efforts or traditional models is inadequate to effectively unearth the patterns underlying the massive datasets. Large models offer the promise of integrating domain knowledge and tuning for specific material systems. This allows for a broad-to-specific technical

trajectory to help scientists break from conventional thinking and accelerate material development.

As early as 2011, the USA took the lead by initiating the Materials Genome Initiative. China also launched a key project on the fundamental techniques and platforms for material genome engineering. With the continuous development of artificial intelligence, the number of patents geared towards the development of new chemical materials has been growing annually. China and the USA together account for over 70% of global patents in this field (Table 2.2.3), with the rest primarily originating from developed nations. Although the patent numbers are similar for China and the USA, the citation gap is significant, which suggests that the USA is the leader in this domain. Whereas patents from the USA are produced by both universities and enterprises, those from China are primarily produced by universities (Table 2.2.4). This highlights the need for China to catch up in terms of industry–academia–research integration. Moreover, China lags the USA in international collaboration and communication within this domain (Figure 2.2.2), and there is a need to further expand its global influence. Currently, this domain is a focus for international research, and the number of related patents published is increasing annually. According to the average citation count, this domain is at the forefront of developmental innovations. However, patents directly applying large models for material development remain scarce, which suggests that the field is still in its nascent stages and has vast potential for growth.

**Table 2.2.3** Countries with the greatest output of core patents on “integration of large language models for the design and synthesis of advanced chemical engineering materials”

No.	Country	Published patents	Percentage of published patents/%	Citations	Percentage of citations/%	Citations per patent
1	USA	180	37.34	877	64.77	4.87
2	China	177	36.72	337	24.89	1.90
3	India	33	6.85	0	0.00	0.00
4	Republic of Korea	24	4.98	33	2.44	1.38
5	Japan	21	4.36	24	1.77	1.14
6	UK	11	2.28	28	2.07	2.55
7	Germany	10	2.07	8	0.59	0.80
8	Canada	8	1.66	13	0.96	1.62
9	Australia	5	1.04	3	0.22	0.60
10	Switzerland	3	0.62	13	0.96	4.33

**Table 2.2.4** Institutions with the greatest output of core patents on “integration of large language models for the design and synthesis of advanced chemical engineering materials”

No.	Institution	Published patents	Percentage of published patents/%	Citations	Percentage of citations/%	Citations per patent
1	International Business Machines Corporation	14	2.90	34	2.51	2.43
2	Intel Corporation	8	1.66	35	2.58	4.38
3	Guangzhou University	8	1.66	2	0.15	0.25
4	Micron Technology Incorporated	7	1.45	0	0.00	0.00
5	Peptilogics Incorporated	6	1.24	14	1.03	2.33
6	Freenome Holdings Incorporated	6	1.24	13	0.96	2.17
7	University of California	6	1.24	7	0.52	1.17
8	Zhejiang University	5	1.04	10	0.74	2.00
9	Ro5 Incorporated	5	1.04	6	0.44	1.20
10	Stanford University	4	0.83	26	1.92	6.50

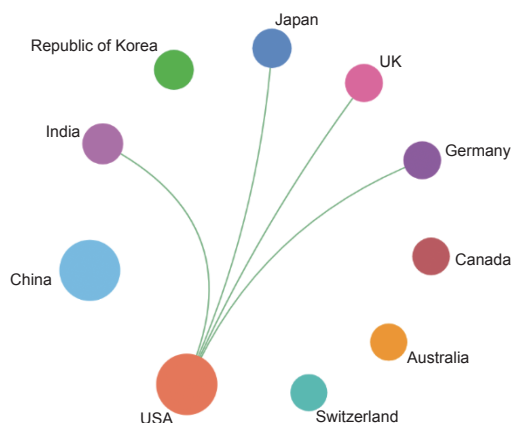


Figure 2.2.2 Collaboration network among major countries for the engineering development front of “integration of large language models for the design and synthesis of advanced chemical engineering materials”

In the next 5 to 10 years, large models are expected to aid multiple facets of the new chemical materials industry, accelerating design and preparation through literature information extraction, material structure generation, material property prediction, synthesis condition optimization, and intelligent characterization (Figure 2.2.3). First, literature information extraction is the main way to collect data for the chemical materials data platform. Large model is able to refine the extraction results of traditional models and output highly structured information so as to build a high-quality domain database. The creation of a high-quality domain-specific dataset and fine-tuning with domain knowledge are critical steps to optimize large model performance in this area. Second, large models that mine connections behind the data and formulate logical hypotheses could provide breakthroughs for material structure generation, which is vital for the reverse design of new materials. Generative models, a challenge in the artificial intelligence domain, are essential to enable artificial intelligence-driven scientific hypotheses. Third, material property prediction, which is a foundation for high-throughput screening, can be streamlined using large models that integrate various smaller models within the domain for precise predictions for various material properties. Integration of these smaller models into large models allows for discerning patterns by learning the parameters of the smaller models. Synthesis condition optimization and intelligent characterization are at the heart of exploring material fabrication techniques. Large models, with their superior

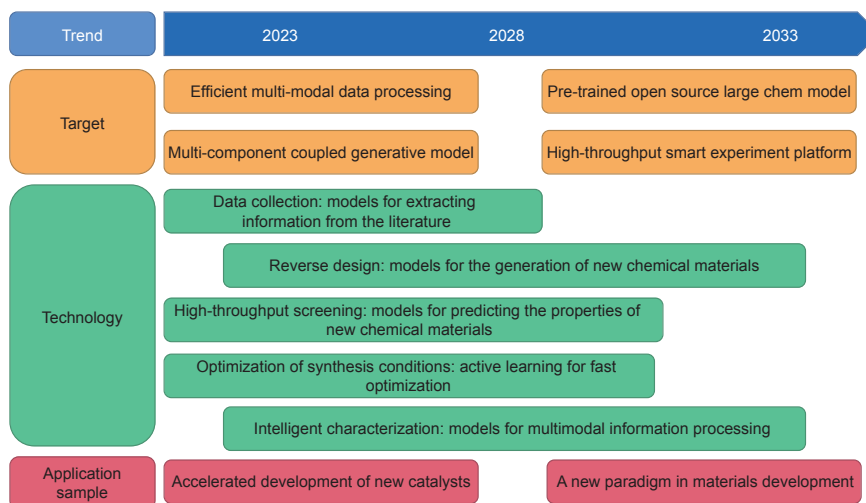


Figure 2.2.3 Roadmap of the engineering development front of “integration of large language models for the design and synthesis of advanced chemical engineering materials”

ability to discern patterns, can fully account for various influencing factors and swiftly optimize processes. Investigating multi-tiered active learning and establishing a universal framework in the chemical materials domain is crucial.

Taking polyolefin catalysts as an example, the chemical community currently relies on traditional methods for catalyst development. A single formula, from design and synthesis to characterization and final polymer evaluation, often takes several months, and most catalysts developed through this process do not meet final requirements. Leveraging the predictive abilities of large models can speed up the development of polyolefin catalysts. Further development of efficient high-end polyolefin catalysts could reduce the production costs of the key material, POE, used in photovoltaic industry encapsulation films. This will hasten the industrial production of domestic POE materials.

### 2.2.3 Design and preparation of metal matrix composites for high-temperature environments

Metal matrix composites (MMCs) are new materials made by adding inorganic non-metallic (or metallic) reinforcements of different sizes and morphologies (e.g., particles, fibers, whiskers, and nanosheets) to metals (e.g., aluminum, titanium, magnesium, and copper) using artificial methods. Compared with traditional homogeneous metals, MMCs have higher strength, corrosion resistance, electrical and thermal conductivity and other properties. They have broad application prospects in aerospace, national defense, rail transit, electronic information, and other fields. In the USA, particle-reinforced MMCs were first prepared by stir casting as early as the 1980s. In China, MMCs research began in 1981 and has already been applied in key components in many major projects. The field is currently in the stage of popularization and rapid development. Taking the aluminum matrix as an example, although it has high strength at room temperature, when used at 300–400 °C, this strength is eliminated. This mainly occurs because of the precipitation phase present in traditional high-strength aluminum alloys, which undergoes rapid destabilization and coarsening above 200 °C. Consequently, the material loses its strength, resulting in rapid softening and failure. The sharp decline in the mechanical properties of aluminum alloys in use is a key shortcoming that restricts structural design and affects the service safety, especially between 300 °C and 400 °C. This is of particular concern in the aerospace field. The 7075 aluminum alloy is widely used in aerospace and its tensile strength at 200 °C and 300 °C is only approximately 30% and 10% of that at room temperature, respectively. This hinders its effective use in heat-resistant structural components.

The principle behind thermal stability strengthening lies in the use of high thermal stability second-phase particles that pin grain boundaries, effectively hindering grain boundary slip and improving the stability of the matrix grain. At high temperatures, the load is transferred to the reinforcing particles through the interface, allowing for higher hardness of the reinforcing particles to bear a greater load and thereby enhancing the thermal stability of the material. For instance, Lavernia et al. successfully prepared a reinforced aluminum matrix composite containing TiC nanoparticles (35%) with tensile strength of up to 220 MPa and elongation of 10% at 300°C. However, it is worth noting that with further increases in the volume fraction of the reinforcement, the elongation greatly decreased. New materials with high strength-to-mass ratios at high temperatures, such as the high-strength 3D-printing aluminum alloy code-named Al250C developed by the WU Xinhua team in Australia, can have significant benefits in various applications. These materials, particularly MMCs, can be used to optimize thermal stability by adjusting and controlling the characteristics of the reinforcement particles and the interface between the reinforcement and the matrix. However, it is worth noting that the current tensile strength of aluminum matrix composites at 300 °C is generally below 250 MPa, and their plasticity and toughness are significantly lower than those of pure aluminum. Nevertheless, the improved performance, lightweight nature, and functionality of MMCs make them highly advantageous in many technological areas. Therefore, the design and preparation technology of MMCs in high-temperature environments are of great importance for enhancing scientific and technological strength, and particularly in achieving strategic goals.

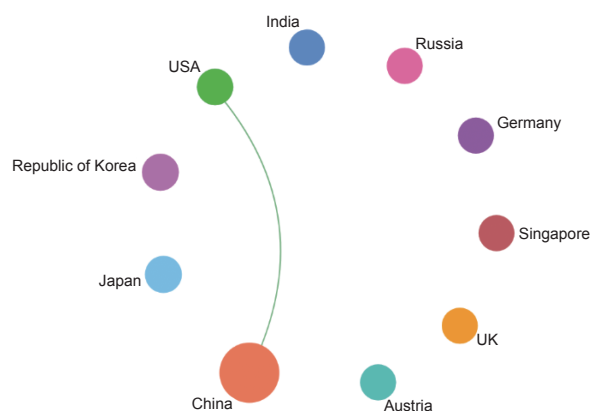
Table 2.2.5 reveals the main countries that produce core patents in the engineering development front of “design and preparation of metal matrix composites for high temperature environments”. Most of these patent outputs are from Asian countries, with China prominent in terms of patent disclosure and citation. There is some degree of international cooperation between China and the USA, while other countries and regions have not yet engaged in extensive collaboration (Figure 2.2.4). Notably, internationally

relevant technologies are currently embargoed, particularly in the USA, where research reports in this field are predominantly concentrated in national laboratories, and the core technologies have not been made public yet. Major metal materials research institutions in China, such as the University of Science and Technology Beijing, Harbin Institute of Technology, and the Institute of Metal Research of the Chinese Academy of Sciences, have prioritized research and development of MMCs for high temperature environments (Table 2.2.6). In terms of enterprises, Wuxi Hengteli Metal Products and Anhui Nicola Electronic Technology are leaders, but there is no collaboration between the main institutions. The widespread distribution of research institutions also illustrates the significant research status and value of heat-resistant MMCs.

MMCs for high-temperature environments are facing an important period of strategic opportunity and are expected to be widely used in livelihood equipment in the next 5 to 10 years. Many foundational studies have been conducted on technology for the design and preparation of heat-resistant MMCs, but there are still many unsolved technical and scientific problems. Because of equipment replacement and technology upgrade requirements, research and development of heat-resistant MMCs is facing new challenges and demands. Breakthroughs are required for enhancing the heat-resistant limit temperature of the material, improving the stability of the material preparation, reducing the cost, and developing precision processing equipment and an evaluation system suitable for heat-resistant MMCs. To further promote the improvement and application of design theory and technology, several key aspects should be considered (Figure 2.2.5). First, biomimetic design should be conducted at the microstructural and morphological levels. Taking inspiration from the structural analysis of plants and animals

**Table 2.2.5 Countries with the greatest output of core patents on “design and preparation of metal matrix composites for high-temperature environments”**

No.	Country	Published patents	Percentage of published patents/%	Citations	Percentage of citations/%	Citations per patent
1	China	529	88.76	892	86.35	1.69
2	Japan	24	4.03	23	2.23	0.96
3	Republic of Korea	23	3.86	53	5.13	2.30
4	USA	9	1.51	56	5.42	6.22
5	India	4	0.67	1	0.10	0.25
6	Russia	2	0.34	2	0.19	1.00
7	Germany	2	0.34	0	0.00	0.00
8	Singapore	1	0.17	5	0.48	5.00
9	UK	1	0.17	4	0.39	4.00
10	Austria	1	0.17	0	0.00	0.00



**Figure 2.2.4 Collaboration network among major countries for the engineering development front of “design and preparation of metal matrix composites for high-temperature environments”**

Table 2.2.6 Institutions with the greatest output of core patents on “design and preparation of metal matrix composites for high-temperature environments”

No.	Institution	Published patents	Percentage of published patents/%	Citations	Percentage of citations/%	Citations per patent
1	University of Science and Technology Beijing	7	1.17	39	3.78	5.57
2	Harbin Institute of Technology	7	1.17	16	1.55	2.29
3	Institute of Metal Research Chinese Academy of Sciences	6	1.01	23	2.23	3.83
4	Wuxi Hengteli Metal Products Company Limited	6	1.01	5	0.48	0.83
5	Jilin University	5	0.84	35	3.39	7.00
6	Taiyuan University of Technology	5	0.84	11	1.06	2.20
7	Anhui Nigula Electronics Technology Company Limited	5	0.84	0	0.00	0.00
8	AVIC Manufacturing Technology Institute	4	0.67	46	4.45	11.50
9	Xi'an University of Technology	4	0.67	23	2.23	5.75
10	Zhejiang University	4	0.67	19	1.84	4.75

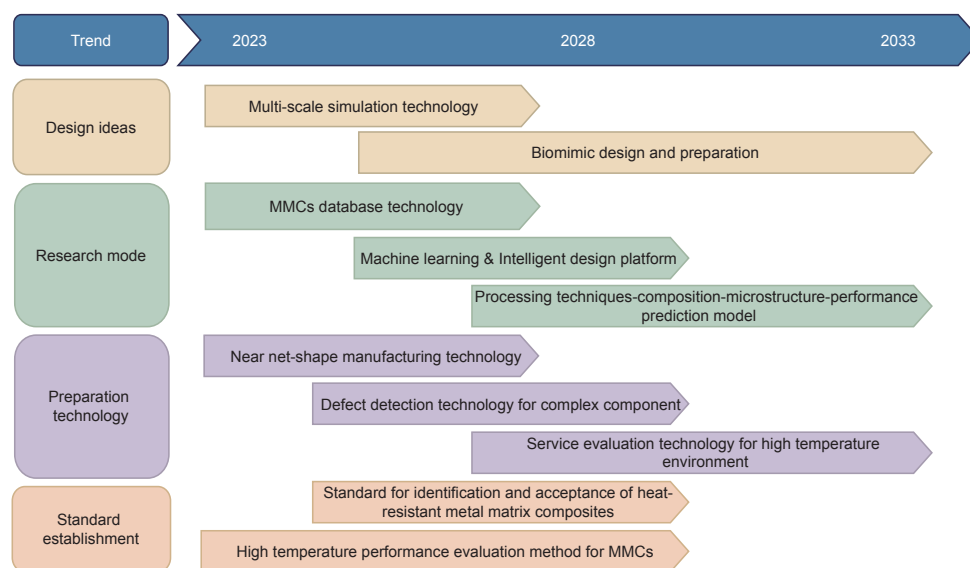


Figure 2.2.5 Roadmap of the engineering development front of “design and preparation of metal matrix composites for high-temperature environments”

residing in extreme environments, materials should be designed with a multi-scale approach from micro to macro. This design process could be further enhanced by developing a multi-scale computing platform that utilizes computational simulations to optimize the structural characteristics. Second, a new research paradigm should be established for genetic engineering of transitional materials. A multidimensional database could be constructed by exploring the physical and chemical properties of various materials such as metal oxides, carbides, nitride, borides, and nano-carbon,. This database, combined with simulation calculations of matrix composition, interface structure, and reinforcement distribution configuration, will facilitate the design and optimization of heat-resistant MMCs. Additionally, special near-net shape preparation and processing technology needs





to be developed. This technology will address the technical challenges associated with processing MMCs, leading to improved utilization rates and formation accuracy for the materials. To achieve this, the technical prototype should be designed and improved according to the interface and reinforcement configuration of the MMCs. Furthermore, efficient forming technology, defect detection technology, and service evaluation technology for MMCs components with complex shapes should be developed. Finally, a comprehensive system of national and industry standards should be studied and established. This should include the establishment of high-temperature performance evaluation methods, identification criteria, and acceptance criteria for different sub-materials of MMCs used in high-temperature environments. The implementation of such a system will ensure standardized and reliable performance of these materials.

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## Participants of the Field Group

### Directors

TAN Tianwei YUAN Yingjin

### Working group

**Liaisons:** MA Xinbin, HE Zhaohui, TU Xuan

**Secretaries:** CHNEG Luli, HUANG Yaodong, LI Yanni, LI Sha, ZHU Xiaowen

### Report writers

GAO Xin, HE Chunnian, HU Wenbin, JI Kemeng, LIU Yongchang, LUO Langli, LV Yongqin, PAN Lun, WANG Shibo, WANG Xiaonan, WEI Yonggang, WU Zhong, XU Haoyuan, YANG Chunpeng, YANG Shiliang, YAO Changguo, YU Yifu, ZHANG Sheng, ZHANG Xiang, ZHANG Zhiguo, ZHOU Kaige

## Exports for data mining and argumentation

### Beihang University

DENG Yuan, ZHU Wei, GUO Siming, HAN Guangyu, HU Shaoxiong, ZHANG Qingqing, ZHOU Jie

### Beijing University of Chemical Technology

LV Yongqin, ZHANG Zhiguo, GUO Yuman

### Central Research Institute of China Baowu Steel Group Corporation Limited

GU Haifang, WANG yuan, YAO Changguo

### Central South University

LI Yang

### East China University of Science and Technology

LU Jingyi, WANG Yiming

**Guangxi University**

NIE Shuangxi

**Harbin Institute of Technology**

KE Hua, LI Daxin

**Kunming University of Science and Technology**

HU Tu, QI Xianjin, TIAN Guocai, WANG Hua, WANG Shibo, WANG Xun, WEI Yonggang, XU Haoyuan, XU Jianxin, XU Lei, YANG Shiliang, YAO Qinwen, ZHENG Yongxin, ZENG Xiaoyuan

**National Science Library, Chinese Academy of Sciences**

WENG Yanqin, YANG Qiwen

**Sichuan University**

ZHU Huacheng

**Tianjin University**

CHEN Xing, CUI Chunyan, DING Ran, DU Xiwen, FEI Zhuping, GAO Xin, HAN You, HE Chunnian, HE Guangwei, HU Wenbin, JI Kemeng, LIU Jiachen, LIU Wenguang, LIU Yongchang, LUO Langli, LOU ShiNee, PAN Lun, PEI Chunlei, REN Xiangkui, SUN Zhe, WANG Can, WANG Yin, XU Lianyong, YANG Chunpeng, YANG Yongan, YANG Zhenwen, YU Tao, YU Yifu, ZHANG Bao, ZHANG Lei, ZHANG Peng, ZHANG Sheng, ZHANG Xiang, ZHANG Yumiao, ZHAO Lei, ZHAO Zhengyu, ZHOU Kaige, ZHU Guorui, CHEN Yuan, CHONG Boyang, DING Qiuyan, KUANG Siyu, LU Qi

**Tsinghua University**

WANG Xiaonan, YIN Haoyu

**University of Electronic Science and Technology of China**

YAN Yichao

**Zhejiang University**

YANG Haocheng