Engineering 29 (2023) 22–26

Contents lists available at ScienceDirect

Engineering

journal homepage: www.elsevier.com/locate/eng

Views & Comments

Green Electrification of the Chemical Industry Toward Carbon Neutrality

Cheng Tang, Qiang Zhang

Beijing Key Laboratory of Green Chemical Reaction Engineering and Technology, Department of Chemical Engineering, Tsinghua University, Beijing 100084, China

1. Introduction

Achieving carbon neutrality and sustainable development demands an extensive and profound systemic reform of China's energy, industry, and economy structures. According to statistics [1,2], almost 90% of CO_2 emissions in China come from the energy sector, with the leading emission sources being power (48%), industry (36%), transport (8%), and buildings (5%) [1]. Therefore, a clean energy transition from fossil fuels to renewables is the inevitable choice, and it is estimated that renewables-based electricity (i.e., green electricity) generation, mainly using wind and solar photovoltaic (PV) power, will account for 80% of China's energy use by 2060 (Fig. 1(a)) [1]. Given its increasing penetration and plummeting price, renewable electrification via green electricity (whether direct or indirect) is emerging as an attractive and powerful approach to decarbonize the emission-intensive industry and transport sectors (Fig. 1(b)) [1,3,4] and to help buffer the high intermittency and fluctuation of renewables in the electricity grid [5–7].

As an example, the chemical industry generally accounts for 6%–10% of total CO_2 emissions across reports [8,9]. These emissions comprise direct emissions during raw material production, extraction, and refining (42%) and indirect emissions from electricity use (35%) and process heat (23%) [8]. The share of indirect emissions will be higher in China due to its heavy reliance on coal. Green electrification of the chemical industry (hereinafter denoted as "ge-CI") will promisingly contribute to deep emission cuts by phasing out fossil fuels in electricity use, heat supply, and high-emission chemical processes (e.g., the production of hydrogen, ammonia, methanol, olefins, and aromatics). The ge-CI route has been previously discussed using terms such as "Power-to-X" [5,10], "e-refinery" [11,12], and "e-chemistry" [13]; however, its exploration and implementation are greatly limited due to unclear targets and roadmaps, low technological readiness, limited scale, and high cost. In this article, we attempt to identify the key challenges and opportunities of ge-CI and to set out a roadmap toward long-term green, high-quality, and carbon-neutral development in China's chemical industry and energy sector.

2. A roadmap to green electrification with key challenges and priorities

Through a comprehensive assessment of their industry status, technological readiness, and potential contributions, we distinguish between the following ge-CI strategies to be gradually deployed at scale (Fig. 2): ge-electricity, ge-heat, ge-hydrogen, ge-

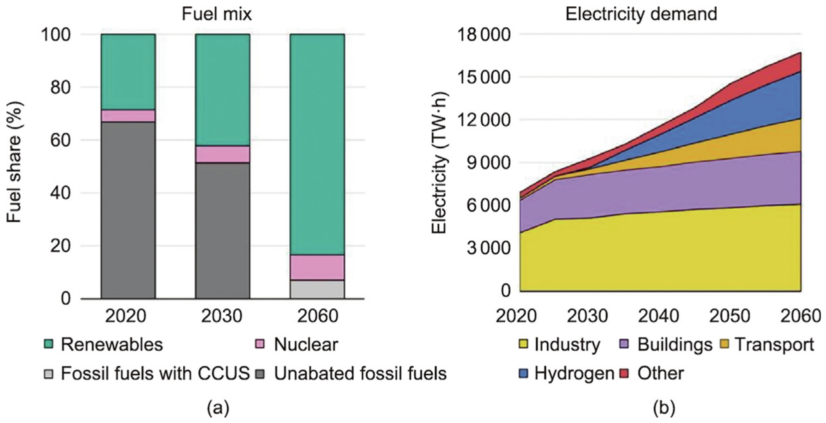

Fig. 1. The clean energy transition from fossil fuels to renewables. (a) Electricity generation in China using different fuel sources; CCUS denotes carbon capture, utilization, and storage. (b) Electricity demand of different sectors in China. Reproduced from Ref. [1] with permission.

https://doi.org/10.1016/j.eng.2023.04.018

fuels, and ge-chemicals, where "ge" denotes "green electrification" with an emphasis on the critical role and unique technical requirements of green electricity.

In the short term (2022–2030), ge-CI will rely on energy-efficiency improvements and the direct use of green electrification to substitute for fossil-fired power and heat in existing emission-intensive processes; that is, ge-electricity and ge-heat will be implemented. In the medium term (2030–2045), green hydrogen generated from water splitting will serve as a versatile agent for long-term renewable energy storage and the decarbonization of hard-to-abate sectors; that is, ge-hydrogen and ge-fuels will be implemented. In the long term (2045–2060), innovative technologies are expected to produce a handful of high-value chemicals directly powered by green electricity using sustainable feedstocks; that is, ge-chemicals will become established.

2.1. ge-Electricity

Nowadays, there are already many direct electrification processes in industry (26% in 2019) [6,14], including electricity-intensive industries (e.g., the chlor-alkali industry, aluminum/zinc smelters, calcium carbide production, adiponitrile manufacturing, and electrowinning) and electricity-powered unit operations (e.g., electrodialysis, motor pumps, agitators, centrifuges, and compressors). These are straightforward and feasible examples of the implementation of ge-CI by directly integrating with a low-carbon power grid or distributed renewable energies, which is estimated to reduce the emissions from the chemical industry by over 35% [8]. However, the ge-electricity route is hindered by the great contradiction between intermittent and variable renewable supply and the demand for consistent, stable operation, resulting in many technical bottlenecks and extra cost for energy conversion and storage. The following research and development (R&D) priorities for ge-electricity have been identified:

(1) It is essential to explore the influence of dynamic power supply conditions on operation results and degradation phenomena. Acquired knowledge is crucial for the further optimization of materials, reactors, and processes, in order to maximize operational limits and minimize degradation issues.

(2) Intrinsic operation flexibility should be further increased by modifying facilities and operation protocols, adding back-up components, or deploying new technologies. An extended operating window will reduce the requirement and cost of compensating for the variability of green electricity.

(3) From the supply side, a "virtual power plant" with preconditioned renewable energies or a "source–network–load–storage" integrated operation model in a micro-grid are efficient approaches to upgrade large-scale existing assets with ge-electricity. System efficiency and cost-effectiveness can be enhanced by means of a smart central control system, process and capacity optimization, peak-valley electricity pricing, and the development of low-cost, high-power energy storage technologies such as batteries, supercapacitors, and flywheels.

2.2. ge-Heat

Heat with different working temperatures plays an important role across the whole chemical industry, in areas such as steam heating for drying, distillation, and curing (below 200 °C); oil refining, steam cracking, chemical separation, and reactions (400–1000 °C); and calcination and melting processes (900–2000 °C) [6,15]. Although fossil-fired heating is convenient and cheap, it is emission-intensive and inefficient, with much energy being wasted. Alternatively, electricity can power heating processes at almost any temperature using heat pumps, electrical resistance, electromagnetic heating, and electric arc heating. These ge-heat technologies are more efficient, modular, precise, and faster than their fossil-based alternatives [5,15]. However, several key barriers remain to be overcome, including reactor scalability, materials compatibility, and economic feasibility, in addition to the flexibility challenge presented by ge-electricity.

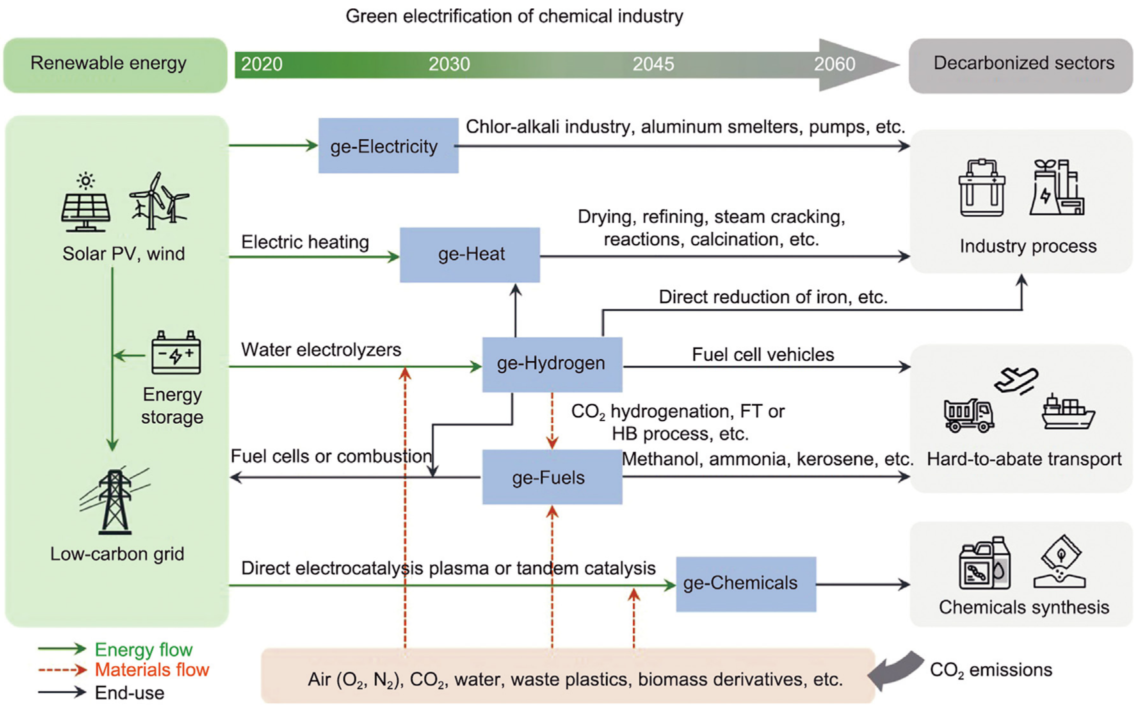

Fig. 2. A roadmap and key strategies for the green electrification of the chemical industry. FT denotes Fischer–Tropsch, and HB denotes Haber–Bosch.

The following R&D priorities for ge-heat have been identified:

(1) Some ge-heat technologies that are applicable at the industrial scale with little change to existing processes or infrastructure, such as heat pumps and electrically heated steam cracker furnaces, should be developed and demonstrated first. These technologies hold high potential to halve their energy use [5] and lower carbon emissions by as much as 90% [16].

(2) More research efforts are required to explore the new catalytic mechanisms induced by the unique features of ge-heat, which include fast temperature modulation, temperature gradients, and dynamic operation [17]. Such research can lead to novel opportunities to intensify the reaction rate, selectivity, and stability.

(3) To take full advantage of ge-heat, it is necessary to redesign established processes and develop next-generation catalysts and reactors with new geometries and characteristics [6,17], which will lead to maximized benefits in energy efficiency, emission reduction, and economic feasibility.

2.3. ge-Hydrogen

Green hydrogen produced from water splitting powered by renewables or a low-carbon grid—namely, ge-hydrogen—is expected to play a crucial role in the green transition and decarbonization. As a green energy carrier with high energy density, ge-hydrogen can help store renewable energy for long durations and power heavy-duty or long-distance transport; moreover, as a carbon-free feedstock, ge-hydrogen is versatile for decarbonizing emission-intensive industries, such as iron and steel, cement, and chemical synthesis [1,18]. The International Energy Agency (IEA) has predicted that China's electrolyzer capacity will increase to 750 GW (nearly 40% of the global capacity) with an electricity consumption of 3300 TW·h by 2060 [1]. However, the wide deployment of ge-hydrogen presents multiple challenges, such as a much higher cost compared with coal or natural gas routes, technical limitations in hydrogen storage and transport, and immature integration with targeted industrial processes.

The following R&D priorities for ge-hydrogen have been identified:

(1) Materials innovation is required to further reduce the overpotential with higher energy efficiency for both alkaline and acidic water splitting. Efforts should focus on exploring electrocatalysts with large current densities, low overpotential, long-term durability, and low cost. It is also important to develop scalable and controllable technologies for manufacturing large-scale hierarchically nanostructured electrodes.

(2) The degradation mechanisms of catalysts, membranes, and electrolyzers under industrially relevant operating conditions and fluctuating power input should be systematically explored. The derived mitigation strategies are crucial for achieving stack and system technical targets, such as a lifetime of 80 000 h, an average degradation rate of 2.1 mV per 1000 h, and a variable output of 20%–110% for alkaline electrolyzers [19].

(3) The exploration and demonstration of ge-hydrogen in hard-to-abate sectors should be prioritized in order to maximize the impact; such sectors include oil refining, hydrogen-rich smelting, coal to olefin, ammonia synthesis, and heavy-duty transport. This calls for innovative hydrogen-based technologies and facilities, as well as breakthroughs in process integration and regulation.

2.4. ge-Fuels

Despite the rapid penetration of battery electric vehicles and the expected application of hydrogen energy, direct electrification and decarbonization of the transport sector are still difficult. More specifically, long-distance aviation, shipping, and long-haul heavy-duty road transport will continue to greatly rely on energy-dense liquid fuels [20,21]. Converting green hydrogen into liquid fuels—namely, ge-fuels—via a reaction with captured CO_2 (e.g., for green methanol, formic acid, dimethyl ether, and kerosene) or by coupling with the Haber–Bosch process (i.e., for green ammonia) offers a low carbon footprint, high energy density, and high compatibility with existing infrastructure. This is considered to be a pragmatic and reliable alternative to petroleum-derived fuels, and one that can contribute not only to transport but also to the chemical industry and long-term energy storage [18,20–23]. However, the ge-fuels route is widely debated, as it presents significant barriers in terms of high cost, low life-cycle efficiency, and immature process integration [20,23].

The following R&D priorities for ge-fuels have been identified:

(1) With a comprehensive evaluation of technological readiness, technoeconomic characteristics, and life-cycle CO_2 emissions and energy efficiency, specific no-regret ge-fuels and end-uses should be identified, prioritizing sectors that are not only hard to abate but also inaccessible to direct electrification [20].

(2) A fundamental mechanistic understanding and innovative catalysts design are crucial to improving hydrogen conversion, reducing reaction temperature, and regulating product distribution for drop-in use [21]. More investigation is strongly required to explore the effects of actual CO_2 sources and impurities on catalytic performance and durability.

(3) To smoothly integrate electrocatalytic water splitting and thermocatalytic steps with different dynamics and conditions, research on collaborative control technologies and system simulation is urgently needed, along with pilot-scale demonstrations. Green methanol and green ammonia are among the earliest ge-fuels for implementation.

2.5. ge-Chemicals

Given the substantial advances that have been achieved in electrocatalytic water splitting, there has recently been increasing interest in extending the direct electrocatalytic approach to produce more complex and valuable chemical products, such as oxygen reduction to hydrogen peroxide, CO_2 reduction to oxygenates and hydrocarbons, nitrogen reduction to ammonia, C–N coupling for N-containing compounds, the upgrading of biomass derivatives, and more [11,13,24]. In addition to direct electrification, the ge-chemicals route is highly attractive due to its use of renewable feedstock (e.g., CO_2, water, air, and biomass), modularized and decentralized reactor for onsite/on-demand operation, and faster industrialization via parallel stacking configurations. Despite intense effort, the direct electrocatalytic synthesis of green chemicals is at an early stage, and its role in the future chemical industry is uncertain with respect to technological maturity, economic feasibility, and market volume. Challenges in fundamental understanding, efficient catalysts, and well-designed reactors call for revolutionary research.

The following R&D priorities for ge-chemicals have been identified:

(1) For materials, the development of highly active, selective, and durable electrocatalysts is essential yet challenging. This should be conducted with new mechanistic approaches different from thermal catalysis and by combining theoretical computations, atomic-level material design, *in situ* spectroscopy tests, and interfacial engineering [11,24].

(2) For reactors, typified by flow electrolyzers, comprehensive innovation and engineering are required to enable practical implementation. Key issues include reactor design and scale-up, electrolyte optimization, mass (gas/water) transport management, membrane identification, and stability retainment [24].

(3) For processes, it is necessary to customize decentralized application scenarios in order to maximize the uniqueness, competitiveness, and impact of ge-chemicals. Novel electrification approaches, such as plasma catalysis and tandem reactions integrating multiple catalytic steps that may be more efficient in activating molecules, are also worth further exploration [6,11,23].

3. Conclusions and outlook

The electrification of the chemical industry powered by green electricity is an important and feasible green transition option, via the direct routes of ge-electricity and ge-heat and the indirect routes of ge-hydrogen, ge-fuels, and ge-chemicals, which are highly interactive (Fig. 2). The change in the energy input and operation modes is likely to reduce the CO_2 emissions from processes, improve energy efficiency, help decarbonize hard-to-abate sectors, create new industrial opportunities, reduce environmental pollution, and benefit the renewable energy transition by means of flexible load balance or long-term storage.

Targeted at a substantial reduction of the industry's carbon footprint and technical/economic competitiveness, the critical features of ge-CI are identified as follows: ① low-carbon electricity input with a high proportion of renewables; ② dynamic or batch operation modes to integrate with fluctuating power; ③ high energy efficiency with direct heating, quick response, and a short process; ④ highly interactive energy and materials flows for process decarbonization; ⑤ decentralized and modular plant schemes for quicker scale-up and novel onsite/on-demand applications; and ⑥ smart grid–load interaction to maximize economic and operational benefits. However, these unique features also contribute to significant barriers and risks in materials, technologies, investments, and markets. We propose the following suggestions to accelerate the development and full-scale implementation of ge-CI, which will ultimately assist in achieving carbon neutrality.

At the national level, policymakers should identify priorities for ge-CI with a farsighted action plan and guidance. Although the promotion of renewable energy, industrial electrification, and green hydrogen has been highlighted, the current policy framework is not adequate to accelerate the innovation, demonstration, and implementation of ge-CI. Additional regulations, incentives, and enabling policies are important to stimulate and ensure the activity of researchers, industries, investors, and markets to develop next-generation technologies that are not yet economically attractive in the short term. Risk management and overall planning must be enhanced to foster a reliable and orderly transition in industrial implementation while ensuing process safety, supply security, people's well-being, and climate benefits.

At the industry level, it is crucial to formulate sectoral and thematic roadmaps and targets for key areas in order to promote large-scale demonstration in the short term (e.g., ge-electricity for the chlor-alkali industry and aluminum/zinc smelters; ge-heat for steam cracker furnaces) and technological innovation in the long term (e.g., ge-chemicals for hydrogen peroxide, fertilizers, and biomass upgrading). Reliable, comprehensive, transparent, and accurate statistics on energy consumption, carbon emissions, market size, and technological status are urgently needed for each sector. An Industry and Innovation Alliance for ge-CI is needed to bridge and unite the chemical industry, energy and grid sectors, manufacturers, end-users, policymakers, investors, and scientists, in order to regularly refine the roadmap with a focus on no-regret sectors and to devise strategies for large-scale deployment.

At the academic level, it is highly recommended to form a specialized academic committee for ge-CI in order to accelerate communication, collaboration, and innovation in this important and challenging direction. Some common issues and opportunities are identified in addition to the aforementioned R&D priorities for each strategy:

(1) Comprehensive assessment of life-cycle carbon emissions and technoeconomic characteristics is essential in order to rigorously evaluate the technical and economic feasibility of specific ge-CI strategies. The parallel development of alternative technologies should also be considered.

(2) Addressing the impact of fluctuating electricity via energy storage allocation for peak and frequency regulation is highly promising; however, energy storage technologies must be further developed for lower cost, longer life, lower dissipation, and an extended operating-temperature window.

(3) Smart regulation of ge-CI processes empowered by artificial intelligence (AI), the Internet of Things (IoT), and big data are crucial to maximize the efficiency and benefits of electrification, with forecasted or real-time weather, power supply, load demand, electricity pricing, carbon tax, and more.

(4) The innovation and development of materials and reactors should target certain emerging and unique features for ge-CI, such as dynamic/batch operation, onsite/on-demand applications, and faster and more precise manipulation. This will require a refined understanding of electrochemistry at the atomic scale and under *operando* conditions, as well as fresh mechanistic approaches (e.g., reactive catalysis [13,17,23]).

(5) The gap between laboratory research and industrial implementation can be filled not only by learning knowledge and know-how from existing electrified processes (e.g., the chlor-alkali industry, and water electrolyzers) but also by entirely redesigning electrode and reactor configurations, electrolytes, processes, and systems.

Acknowledgments

This work was supported by the National Natural Science Foundation of China (21825501) and the Ordos–Tsinghua Innovative and Collaborative Research Program in Carbon Neutrality.

References

[1] International Energy Agency (IEA). An energy sector roadmap to carbon neutrality in China. Report. Paris: IEA; 2021.
[2] Dai H, Su Y, Kuang L, Liu J, Gu D, Zou C. Contemplation on China's energy-development strategies and initiatives in the context of its carbon neutrality goal. Engineering 2021;7(12):1684–7.
[3] Luderer G, Madeddu S, Merfort L, Ueckerdt F, Pehl M, Pietzcker R, et al. Impact of declining renewable energy costs on electrification in low-emission scenarios. Nat Energy 2022;7(1):32–42.
[4] Yu S, Fu S, Behrendt J, Chai Q, Chen L, Chen W, et al. Synthesis report 2022 on China's carbon neutrality: electrification in China's carbon neutrality pathways. Beijing: Energy Foundation of China; 2022. Chinese.
[5] Van Kranenburg K, Schols E, Gelevert H, de Kler R, Van Delft Y, Weeda M. Empowering the chemical industry: opportunities for electrification. Report. Petten: The Energy Research Centre of the Netherlands (ECN); 2016.
[6] Mallapragada DS, Dvorkin Y, Modestino MA, Esposito DV, Smith WA, Hodge BM, et al. Decarbonization of the chemical industry through electrification: barriers and opportunities. Joule 2023;7(1):23–41.
[7] Armaroli N, Balzani V. Towards an electricity-powered world. Energy Environ Sci 2011;4(9):3193–222.
[8] Eryazici I, Ramesh N, Villa C. Electrification of the chemical industry—materials innovations for a lower carbon future. MRS Bull 2021;46(12):1197–204.
[9] Chen JM, Yu B, Wei YM. CO_2 emissions accounting for the chemical industry: an empirical analysis for China. Nat Hazards 2019;99(3):1327–43.
[10] Buffo G, Marocco P, Ferrero D, Lanzini A, Santarelli M. Power-to-X and power-to-power routes. In: Calise F, D'Accadia MD, Santarelli M, Lanzini A, Ferrero D, editors. Solar hydrogen production: processes, systems and technologies. New York: Academic Press; 2019. p. 529–57.
[11] Tang C, Zheng Y, Jaroniec M, Qiao SZ. Electrocatalytic refinery for sustainable production of fuels and chemicals. Angew Chem Int Ed 2021;60(36):19572–90.
[12] e-Refinery Institute [Internet]. Delft: Delft University of Technology; [cited 2022 Nov 5]. Available from: https://www.tudelft.nl/e-refinery/.

[13] Papanikolaou G, Centi G, Perathoner S, Lanzafame P. Catalysis for e-chemistry: need and gaps for a future de-fossilized chemical production, with focus on the role of complex (direct) syntheses by electrocatalysis. ACS Catal 2022;12(5):2861–76.

[14] International Renewable Energy Agency (IRENA). World energy transitions outlook 2022: 1.5 °C pathway. Report. Abu Dhabi: IRENA; 2022.

[15] Beyond Zero Emissions Inc. Zero carbon industry plan: electrifying industry. Report. Melbourne: Beyond Zero Emissions Inc.; 2018.

[16] Nonnast T, Kateva E, Clarkmead L, Stamm M, editors. BASF, SABIC and Linde join forces to realize the world's first electrically heated steam cracker furnace [Internet]. Ludwigshafen: BASF SE; 2021 Mar 24 [cited 2022 Nov 5]. Available from: https://www.basf.com/cn/en/media/news-releases/global/2021/03/p-21-165.html

[17] Centi G, Perathoner S. Catalysis for an electrified chemical production. Catal Today 2022;423:113935.

[18] Oliveira AM, Beswick RR, Yan Y. A green hydrogen economy for a renewable energy society. Curr Opin Chem Eng 2021;33:100701.

[19] Satyapal S, Rustagi N, Green T, Melaina M, Penev M, Koleva M. U.S. national clean hydrogen strategy and roadmap. Report. Washington, DC: US Department of Energy; 2022.

[20] Ueckerdt F, Bauer C, Dirnaichner A, Everall J, Sacchi R, Luderer G. Potential and risks of hydrogen-based e-fuels in climate change mitigation. Nat Clim Chang 2021;11(5):384–93.

[21] Ramirez A, Sarathy SM, Gascon J. CO_2 derived e-fuels: research trends, misconceptions, and future directions. Trends Chem 2020;2(9):785–95.

[22] Yao D, Tang C, Wang P, Cheng H, Jin H, Ding LX, et al. Electrocatalytic green ammonia production beyond ambient aqueous nitrogen reduction. Chem Eng Sci 2022;257:117735.

[23] Papanikolaou G, Centi G, Perathoner S, Lanzafame P. Transforming catalysis to produce e-fuels: prospects and gaps. Chin J Catal 2022;43(5):1194–203.

[24] Xia R, Overa S, Jiao F. Emerging electrochemical processes to decarbonize the chemical industry. JACS Au 2022;2(5):1054–70.