

Chemistry

Special Topic: Artificial Intelligence and Energy Revolution

Artificial intelligence and energy revolutionShanshan Wang^{2,3} & Jin Zhang^{1,2,*}¹*School of Materials Science and Engineering, Beijing Science and Engineering Center for Nanocarbons, Beijing National Laboratory for Molecular Sciences, College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, China;*²*School of Advanced Materials, Shenzhen Graduate School, Peking University, Shenzhen 518055, China;*³*College of Aerospace Science and Engineering, National University of Defense Technology, Changsha 410073, China**Corresponding author (email: jinzhang@pku.edu.cn)

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Artificial intelligence (AI) is closely integrated with energy technology. On one hand, the rapid development of AI has led to a significant increase in electricity demand. It is estimated that the electricity consumption related to AI will grow at a rate of 50% per year from 2025 to 2030, in which the electricity consumption of data centers alone will exceed 3% of the global total electricity demand. Therefore, the sustainable development of AI urgently requires transformative breakthroughs in the fields of energy generation, storage, and conversion. On the other hand, AI technology is also strongly empowering the paradigm revolution in energy research. Through the deep intersection of machine learning, automation, and chemistry, researchers can achieve efficient screening, autonomous synthesis, and quantitative mechanism explanation of energy materials with superior properties in a shorter period and at a lower cost, promoting the evolution of energy chemistry research from trial-and-error to a rational exploration paradigm dual-driven by data and knowledge.

Here, we organize a special topic on “Artificial Intelligence and Energy Revolution”, which includes 4 high-quality papers covering the latest research, reviews, and perspectives of AI-empowered energy material investigations. Li and the Nobel Prize winner in the field of lithium-ion batteries (LIBs), Whittingham *et al.* [1], systematically reviewed the AI-assisted integration of the advanced digital simulations with comprehensive lifecycle management to rationally promote battery performance, safety, and durability. Multiscale models spanning from atomic to pack levels, cloud-based battery management systems, the “Battery Passport” concept, and a framework to converge standardization, modularization and digitization were discussed with an outlook of the future breakthroughs in advancing battery intelligence and sustainability. Ouyang *et al.* [2] presented an AI-driven Battery Design Automation (BDA) software, which integrates multiscale simulations and AI algorithms into a unified platform to tackle cross-scale, long-process, and multifactor challenges in the next-generation LIB research and development. It is anticipated that BDA in the battery field, which is seen as an analogue to electronic design automation (EDA) in the semiconductor industry, can facilitate a better understanding of the migration behavior of lithium ions in the chemical and electrochemical

reactions of LIB so that functions including materials screening, particle and electrode microstructure design, and the evaluation and prediction of cell and module lifespan and failure can be accomplished. Zhang *et al.* [3] reported a perspective on how to overcome the data scarcity challenges in AI-driven energy chemistry research, where the synergistic integration of four strategies, including high-throughput computation, self-driving experimentation, text mining from published papers and patents, as well as synthetic data generated by domain-appropriate transformations, was raised as a comprehensive solution. Finally, Wang *et al.* [4] conducted an experimental and data-driven study of hydrophilic and hydrophobic ionic liquids (ILs) for supercapacitors, where molecular fingerprints and machine learning approaches were combined to identify the structural determinants of conductivity in ILs, giving insight into the rational design of high-performance electrolytes for supercapacitors.

As the space of this special issue is limited, we cannot list all the recent progress made in the field of AI & energy revolution. However, we believe that this topic will inspire researchers to integrate AI with energy chemistry to drive a paradigm shift and promote discoveries and team building in cross-disciplinary areas. We would like to thank all the authors who have contributed high-quality peer-reviewed articles to this special topic. We are also grateful to the deputy editors in chemistry who invited these papers, as well as the editorial and production staff of the *National Science Open* for their high-quality assistance.

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