Journal of Zhejiang University-SCIENCE A 2026 27(8):779-782
www.jzus.zju.edu.cn; www.springer.com/journal/11582
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Editorial

https://doi.org/10.1631/jzus.A26ED001

Artificial intelligence for carbon neutrality: pioneering a new paradigm for future energy systems research

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1 Introduction

The transition toward carbon neutrality is reshaping the architecture and operation of modern energy systems. Rapid growth in wind and photovoltaic generation, deeper electrification of transport and industry, expansion of low-temperature heating, and the emergence of hydrogen as a flexible energy carrier are creating systems that are increasingly distributed, coupled, and uncertain. The central challenge is not only to install low-carbon technologies but also to coordinate generation, conversion, storage, networks, and demand across multiple spatial and temporal scales while maintaining reliability, affordability, safety, and resilience (Zhang et al., 2022; Lund et al., 2025).

Artificial intelligence (AI) is becoming a key enabler of this transformation. AI methods can learn nonlinear relationships, accelerate computationally expensive simulations, forecast renewable generation and demand, and adapt control policies in complex operating environments. Nevertheless, energy systems are safety-critical cyber-physical infrastructures governed by conservation laws, equipment limits, market rules, and human institutions. Trustworthy AI must therefore combine learning with physical knowledge, calibrated uncertainty, interpretability, data efficiency, and operational safeguards. Research on uncertainty quantification and long-sequence forecasting further shows that confidence, temporal structure, and distribution shifts can be as important as nominal prediction accuracy (Abdar et al., 2021; Zhou et al., 2021). Thus, AI for carbon neutrality should be understood not as a replacement for engineering knowledge but as a means of integrating data, physics, optimization, and decision-making into more capable and verifiable energy-system tools. Unfortunately, there has been no dedicated special issue or workshop devoted to it.

This special issue contains original and hitherto unpublished works on the applications of AI for carbon neutrality. Focal points of the issue include but are not limited to innovative applications of: (1) AI-based forecasting and uncertainty analysis for variable renewable energy sources; (2) intelligent scheduling and real-time control of integrated, multi-energy systems; (3) machine learning approaches for optimal dispatch of energy storage, hydrogen, and hybrid systems; (4) deep learning and digital-twin frameworks for carbon-neutral energy systems; (5) reinforcement learning and metaheuristic algorithms for energy system design and operation; (6) AI-driven techno-economic and life-cycle analyses of low-carbon energy pathways; (7) data-centric strategies for carbon accounting, emissions monitoring, and footprint reduction; (8) cyber-security, privacy, and resilience in AI-enabled energy networks; (9) case studies and pilot projects demonstrating AI for renewable integration and system decarbonization; (10) generative AI, large language models, and their applications in energy systems.

Bai et al. (2026) addressed the real-time scheduling of an electric-heat-hydrogen integrated energy system with high wind and photovoltaic penetration. Their

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Received Aug. 1, 2026; Revision accepted Aug. 5, 2026; Crosschecked Aug. 11, 2026; Online first Aug. 19, 2026

framework combines a coupled power state of charge soft penalty, a differentiable bidirectional incentive-based demand response mechanism, and a long short-term memory (LSTM)-augmented maximum entropy soft actor-critic scheduler. By explicitly representing temporal correlations among renewable output, loads, prices, and storage states, the method improves the stability of continuous high-dimensional control while reducing both operating cost and carbon emissions. This contribution illustrates how memory-enhanced deep reinforcement learning can coordinate electricity, heat, hydrogen conversion, and multiple storage assets without discarding the engineering constraints that determine feasible operation (Shi et al., 2023; Sadeghian et al., 2025).

Yan et al. (2026) extended AI-assisted decarbonization to engine-relevant combustion chemistry by constructing neural surrogates for reactive force field molecular dynamics simulations. Using trajectories of C_2H_4/NH_3 pyrolysis and the temporal evolution of C_6 intermediates associated with polycyclic aromatic hydrocarbon formation, the authors compare feed-forward neural networks with an LSTM-based recurrent model. The sequence-aware architecture achieves better predictive performance because its gated memory captures history-dependent chemical dynamics that static feed forward models cannot represent effectively. The study offers an efficient route for reducing the computational burden of ReaxFF simulations and supports the development of ammonia/hydrocarbon combustion strategies in which soot-relevant carbon-nitrogen chemistry must be resolved (Badra et al., 2021; Aliramezani et al., 2022).

Sun et al. (2026) proposed a hierarchical physics-informed learning method for 3D spatiotemporal wake-field prediction in large wind farms. The framework combines a data neural network with a partial differential equation neural network embedding the 3D Navier–Stokes equations, while hierarchical sampling retains dense information in highly dynamic wake regions and uses only a fraction of the data in smoother regions. This design substantially lowers the data requirement of large domain physics-informed neural networks while preserving accurate local and global ultrashort-term wake forecasts. This work is especially relevant because wind-farm wake interactions can cause major power losses and fatigue loading, whereas conventional high-fidelity simulations remain computationally demanding (Amiri et al., 2024; Liu et al., 2025).

Zhou et al. (2026) provided a comprehensive review of AI integration throughout the lifecycle evolution of district heating networks, covering planning and design, construction and renewal, operation and control, and maintenance and fault diagnosis. The review documents substantial gains reported in the literature, including order of magnitude improvements in design computation, major reductions in load forecasting errors, and fault localization accuracies above 95% in representative applications. More importantly, it identifies application fragmentation and persistent data silos as systemic barriers and proposes a digital-thread framework to maintain data continuity and decision feedback across lifecycle stages. This perspective moves AI-enabled district heating beyond isolated forecasting or control tasks toward coordinated, lifecycle-based infrastructure intelligence (Boussaid et al., 2024; Lu et al., 2024).

Zhao P et al. (2026) developed a mechanism-enhanced multitask knowledge distillation framework for the predictive and interpretable design of biomass-derived activated carbons. Their proposed architecture jointly predicts specific surface area, total pore volume, and mass yield using a shared residual neural network informed by teacher-model outputs. Repeated train-test evaluations show robust performance across one-step and two-step activation routes, with particularly strong improvements for mass-yield prediction. Permutation importance and Shapley additive explanations (SHAP) analyses identify activating agent, thermal severity, impregnation conditions, and precursor composition as dominant drivers, while Pareto screening translates predictions into practical operating windows. The study demonstrates how AI can replace trial-and-error material development with interpretable multi-objective decision support for carbon capture, separation, catalysis, and energy-storage materials (Yuan et al., 2021; Li et al., 2024).

Zhao K et al. (2026) investigated the performance degradation and geometry optimization of staggered-fin heat exchangers over altitudes from sea level to 5000 m. Their simulations show that at 5000 m, the pressure drop and heat-transfer coefficient decrease by approximately 23% and 18%, respectively. To avoid the prohibitive cost of evaluating thousands of computational fluid dynamics designs, the authors train surrogate models and identify a gradient boosting decision tree with near-unity determination coefficients for both target variables. Coupling this surrogate with an improved nondominated sorting genetic algorithm II (NSGA-II) yields designs that increase the heat-transfer coefficient by approximately 23% at comparable pressure drops or reduce the pressure drop by approximately 17% at comparable heat-transfer performances. The work exemplifies the productive combination of high-fidelity simulation, machine learning, and multi-objective optimization for climate- and environment-adaptive thermal equipment (He et al., 2024; Wen et al., 2024).

Huang et al. (2026) introduced a physics-informed deep-learning hybrid model for photovoltaic power forecasting under limited data and changing weather distributions. The physical front end generates plane-of-array irradiance and module-temperature features, which are then integrated with meteorological and historical power information in a convolutional neural network (CNN)–LSTM architecture. Validation across photovoltaic plants in China and Australia and across 15 min, 4 h, and 24 h horizons shows root-mean-square-error reductions of up to 8.93% relative to a purely data-driven baseline. The model retains high accuracy with only three months of training data and improves performance by 6.87% under strong cross-seasonal distribution shifts. These results show that physically grounded feature construction can improve both data efficiency and robustness, two requirements for dependable renewable-energy forecasting in rapidly changing operational settings (Niccolai et al., 2021; Mayer, 2022).

Zheng et al. (2026) proposed a hierarchical thermal-management strategy for hybrid electric drive tracked vehicles that combines a gated recurrent unit (GRU) and multi-head attention-enhanced twin delayed deep deterministic policy gradient (TD3) agent with model predictive control. The reinforcement-learning layer seeks energy-efficient global actions, whereas a dynamic threshold mechanism transfers authority toward the model-predictive controller as thermal states approach safety limits. Compared with deep deterministic policy gradient (DDPG) and standard TD3, the proposed learning architecture accelerates convergence by approximately 28% and 40%, respectively. Under off-road operation at 25 ℃, it reduces the fluctuation ranges of the high- and low-temperature circuits by 44.19% and 6.45%, lowers total energy consumption by 5.54%, and decreases peak power demand by 10.63% relative to standalone model predictive control (MPC); at 45 ℃, the energy reduction reaches 13.41%. This safety-prioritized hybrid control paradigm is a valuable model for deploying AI in energy-intensive equipment where exploration, uncertainty, and hard thermal limits must be reconciled (Atkinson et al., 2021; Ghate et al., 2024).

This special issue will be published in two parts. The first part appears in the present publication, and the second part will be published in due course. We believe this special issue will provide a special viewpoint for researchers and engineers to present and discuss recent developments in AI for carbon neutrality. The interdisciplinary integration of machine learning and energy engineering was well highlighted by the selected publications. We sincerely hope that the new algorithms and advanced methodologies shared in this special issue will improve the understanding of AI technologies and strategies, promote their application in carbon-neutral energy systems, and accelerate the intelligent development of future energy systems. We expect the selected articles to stimulate further discussion among researchers and bring new inspiration to the readers of this journal.

Author contributions

Xiaojie LIN and Jian LI provided the concept and wrote the draft of the manuscript. Rui JING and Zuming LIU conducted the literature review. Bowen WANG and Peng LI edited the first draft of the manuscript. Chang HUANG edited the draft of the manuscript.

Conflict of interest

Xiaojie LIN, Jian LI, Rui JING, Zuming LIU, Bowen WANG, Peng LI, and Chang HUANG declare that they have no conflicts of interest.

Declaration on the use of generative AI tools

No generative AI tools were used in the preparation of this manuscript.

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