WREN2026 - World Renewable Energy Network Conference

November 2026 - Pará, Brazil

Artificial Intelligence Applications in Renewable Energy Device Development: Recent Advances and Emerging Trends

David L. Azevedo

Institute of Physics, University of Brasília - UnB, Brasília, Brazil

ABSTRACT

The global energy transition has driven the search for more efficient technologies in the conversion and storage of energy from renewable sources. In this context, computational methods based on machine learning have emerged as essential tools for accelerating the development of new materials and devices. This review presents recent advances in the application of artificial intelligence algorithms for the design and optimization of solar cells, solid-state batteries, wind turbines, and electrolyzers for green hydrogen production.

In the domain of photovoltaic cells, the development of high-efficiency perovskites stands out. Researchers at EPFL developed a methodology combining hybrid functional calculations with predictive models, identifying 14 promising new materials from a database of approximately 15,000 candidates. In a study published in *Science* in 2024, an international team used machine learning algorithms to discover new charge transport materials, achieving a conversion efficiency of 26.2%, close to the world record of 26.7%. The Karlsruhe Institute of Technology demonstrated that only 150 computationally guided experiments were sufficient to obtain results that would normally require hundreds of thousands of conventional tests.

For solid-state batteries, interatomic potentials derived from neural networks are replacing density functional theory calculations in high-throughput screening. Guo and collaborators identified 130 promising new solid electrolytes using this approach. Recent studies demonstrate reductions of 70-80% in experimental iterations during fabrication process optimization. Autonomous laboratories integrating robotics, automated characterization, and adaptive planners operate continuously, producing previously unknown electrolytes in days rather than the months required by traditional methods.

In wind energy, genetic algorithms combined with surrogate models have optimized Savonius turbines, increasing the power coefficient by 33%. Vertical-axis turbines designed with Gaussian process regression exhibited power output three times greater than conventional models. For polymer membrane electrolyzers, artificial neural networks achieved a coefficient of determination of 0.999 in predicting operational parameters, while computationally optimized high-entropy alloy catalysts demonstrated activity eight times higher than commercial platinum.

The main trends identified include: integration of atomistic simulations with surrogate models for accelerated materials screening; closed-loop cycles combining computational prediction, automated synthesis, and characterization; application of generative models for inverse design of molecular structures; and increasing emphasis on interpretable methods that allow extraction of physical knowledge from predictions. These approaches are significantly reducing development times and costs, accelerating the commercialization of technologies essential for decarbonizing the global energy matrix.

Keywords: machine learning, perovskite solar cells, solid-state batteries, wind turbines, electrolyzers, green hydrogen, materials discovery

REFERENCES

[1] Wu, J., et al. (2024). Inverse design workflow discovers hole-transport materials tailored for perovskite solar cells. *Science*, 386(6727), 1256. https://doi.org/10.1126/science.ads0901

[2] Wang, H., & Pasquarello, A. (2024). Machine learning accelerates discovery of solar-cell perovskites. *Journal of the American Chemical Society*. https://doi.org/10.1021/jacs.4c02847

[3] Mao, L., & Xiang, C. (2025). A comprehensive review of machine learning applications in perovskite solar cells: Materials discovery, device performance, process optimization and systems integration. *Materials Today Energy*, 47, 101742. https://doi.org/10.1016/j.mtener.2024.101742

[4] Guo, X., Wang, Z., Yang, J., & Gong, X. (2024). Machine-learning assisted high-throughput discovery of solid-state electrolytes for Li-ion batteries. *Journal of Materials Chemistry A*, 12, 10124-10136. https://doi.org/10.1039/D4TA00721B

[5] ACS Applied Energy Materials (2025). Path to Machine Learning-Driven Autonomous Systems for Solid-State Electrolyte Batteries: Design, Fabrication, and Lifetime Prediction. *ACS Appl. Energy Mater.*, 8(20), 14971-14986. https://doi.org/10.1021/acsaem.5c02002

[6] Wang, S., et al. (2025). Artificial Intelligence Empowers Solid-State Batteries for Material Screening and Performance Evaluation. *Nano-Micro Letters*, 17, 287. https://doi.org/10.1007/s40820-025-01797-y

[7] ASME (2025). A Machine Learning Optimized Vertical-Axis Wind Turbine. *Journal of Applied Mechanics*, 92(8), 081006. https://doi.org/10.1115/1.4067890

[8] Energies (2025). Review of Artificial Intelligence-Based Design Optimization of Wind Power Systems. *Energies*, 5(3), 18. https://doi.org/10.3390/energtic5030018

[9] Yang, Q., et al. (2025). Machine learning-assisted prediction and optimization of solid oxide electrolysis cell for green hydrogen production. *Green Chemical Engineering*, 6(2), 154-168. https://doi.org/10.1016/j.gce.2024.04.004

[10] Gu, Y., et al. (2025). Design and Application of Electrocatalyst Based on Machine Learning. *Interdisciplinary Materials*. https://doi.org/10.1002/idm2.12249

[11] ACS Nano (2024). Generative Artificial Intelligence for Designing Multi-Scale Hydrogen Fuel Cell Catalyst Layer Nanostructures. *ACS Nano*, 18(31), 20504-20517. https://doi.org/10.1021/acsnano.4c04943

[12] Nature Reviews Materials (2025). Understanding solid-state battery electrolytes using atomistic modelling and machine learning. *Nature Reviews Materials*. https://doi.org/10.1038/s41578-025-00817-y