*J Water Environ Nanotechnol* 2026, 11(SI): 1-4
10.22090/jwent.2026.2087985.2105

EDITORIAL

# Guest Editorial: Frontiers of AI-Driven Nanotechnology for Sustainable Water and Environmental Systems

***Mohsen Jahanshahi***[1,2]*
Guest Editor, Special Issue (SI)
Editor-in-Chief, JWENT

[1]Nanotechnology Research Institute, School of Chemical Engineering, Babol Noshirvani University of Technology, Shariati Ave, Babol, Iran
[2]Excellence Center of Nanotechnology in Water (ECNW), Babol Noshirvani University of Technology, Shariati Ave, Babol, Iran

* Corresponding Author.
Email: mjahan@nit.ac.ir, m.jahanshahi50@gmail.com

**Article History:**
Received: 2026-02-01
Revised: 2026-3-01
Accepted: 2026-04-16

How to cite this article
Jahanshahi M, Guest Editorial: Frontiers of AI-Driven Nanotechnology for Sustainable Water and Environmental Systems. J Water Environ Nanotechnol. 2026, 11(SI): 1-4, DOI: 10.22090/jwent.2026.2087985.2105

The increasing pressures of climate change, freshwater scarcity, emerging pollutants, ecosystem degradation, urbanization, and industrialization have fundamentally reshaped research in water and environmental sciences. Conventional approaches to monitoring, treating, and managing water and environmental resources are increasingly faced with the complexity, scalability, dynamics, and inter-relationships of environmental systems. In many cases, these methods are no longer able to respond to current challenges alone. In this context, the convergence of artificial intelligence (AI) and nanotechnology in achieving the Sustainable Development Goals (SDGs) is emerging not just as a technological trend, but as an emerging scientific paradigm; a paradigm that has the potential to fundamentally redefine the way we understand, predict, and challenge environmental concerns [1, 2]. The field of environmental sciences has drastically transformed from primarily a reactive, laboratory-based approach to a more predictive, data-rich, material-enabled, and systems-based discipline [3] over the last decade.

AI appears as one of the major driving forces in this paradigm, in which machine learning (ML), deep learning (DL), optimization, and hybrid modeling techniques are successfully utilized for predicting pollutant behavior, designing treatment strategies, understanding complicated sensor signals, and facilitating material discovery and real-time decision-making in water and environmental systems [4-7]. Nanotechnology, on the other hand, has established itself as a mature and multidisciplinary system design paradigm for producing sensitive, selective, and tunable advanced adsorbents, catalysts, photocatalysts, membranes, antibacterial materials, delivery systems, nanosensors [8-10], and nano-agrochemicals such as nanofertilizers, nanopesticides, nanonutrients, etc. [11-15].

©2026 The Author(s). Published by the Iranian Environmental Mutagen Society. This work is licensed under the Creative Commons Attribution 4.0 International License (CC BY 4.0). To view a copy of this license, visit http://creativecommons.org/licenses/by/4.0/.

Through the convergence of AI and nanotechnology, we are entering a new era where these technologies not only complement but are actually advancing each other in intelligent environmental systems. This integration is particularly critical for the water environment and ecosystems that inherently involve complicated, nonlinear, multiscale and uncertain behaviors. Pollutant transport and adsorption mechanisms, membrane scaling, catalytic deactivation, microbial interactions, drought stress dynamics, and ecological responses all involve highly coupled processes that are difficult to characterize by conventional single-factor or purely deterministic approaches [16-18]. AI provides potent capacities in pattern recognition, nonlinear approximation, surrogate modeling, multi-objective decision-making, and uncertainty analysis and prediction [19, 20]. Meanwhile, nanotechnology provides the material basis and functional capabilities for precision intervention, targeted remediation, and high-resolution environmental detection. This integration creates a pathway to intelligent environment diagnosis, prediction, treatment technology, an automated monitoring system, and adaptive sustainable strategies. This convergence is critically important as current research focuses on Contaminants of Emerging Concern (CECs), such as pharmaceuticals, agrochemicals, dyes, personal care products, endocrine disruptors, pesticides, pathogens, and recalcitrant industrial pollutants. CECs are often found in low concentrations in heterogeneous and dynamic matrices, and this makes detection, risk assessment, and treatment challenging. AI-assisted nanosensors provide a promising strategy to tackle these issues by highly sensitive detection using nanostructured materials and the interpretation and real-time analysis of the data obtained using AI. Moreover, AI could help to identify more specific adsorption materials, robust membrane separation techniques, or highly active photocatalysis systems without lengthy experimental procedures. While this convergence has led to significant advances in sustainable water and environmental systems, the development of reliable, scalable, and truly sustainable technologies remains a major challenge.

A critical bottleneck in this field is data-related limitations. The performance of AI systems depends heavily on training data. However, environmental datasets are often sparse, heterogeneous, noisy, spatially and temporally variable, and in many cases, acquired from controlled laboratory settings rather than real-world field settings. These problems become even more pronounced in studies with smaller sample sizes, the absence of standardized protocols, and the lack of external validation, which could limit the generalizability and reliability of models in practical applications. Another major challenge relates to the interpretability and mechanistic transparency of AI models. Many ML and DL models can provide highly accurate predictions, but in environmental, regulatory, and policy contexts, models need to be not only good at prediction but also explainable, traceable, and consistent with the physical and chemical principles governing the systems under study. Therefore, the development of explainable AI frameworks, physics-informed models, and hybrid modelling strategies can be one of the most important directions for future research.

Comprehensive assessment of the environmental impacts of nanomaterials is increasingly important from a sustainability perspective. Although nanomaterials have shown outstanding performances in adsorption, catalysis, separation, sensing, and intelligent delivery systems, questions remain regarding their life cycle, environmental fate, ecotoxicity, and recoverability. Thus, approaches such as Safe-by-Design, green synthesis, life cycle assessment, and the design of circular systems for nanomaterial reuse are increasingly recognized as essential for the sustainable development of these technologies. Moreover, scalability and successful transfer of technology from laboratory to real-world applications are still major barriers. Some of the reported advances are still limited to proof-of-concept studies and have not undergone pilot-scale validation, and require an analysis to understand their costs, benefits, and potential problems. They need to be examined for their technical feasibility, long-term performance, and how they fit with existing rules and regulations. Bridging this gap needs an interdisciplinary collaboration between materials scientists, data scientists, environmental engineers, toxicologists, regulatory agencies, and industrial stakeholders. Governance issues are also getting more important, as the use of AI-enabled systems brings up questions about data governance, algorithmic bias, cybersecurity, accountability in decision-making, and fair access to technology [21, 22].

Nevertheless, the opportunities ahead are significant and potentially transformative. A major revolution in managing water and resources could happen with the help of intelligent nanosensors, real-time monitoring systems, self-optimizing treatment processes, and data-guided materials design by generative models. The application of AI and nanotechnology convergence in biological systems leads to the development of nano-bio-digital systems, which can help science move from traditional approaches to predictive, adaptive approaches, and systems-oriented frameworks. Water and environmental resource management will benefit from these advancements. This vision can be achieved by standardized environmental and materials datasets, explainable models, field-scale validation, and broad interdisciplinary collaboration. Some of the key research priorities that need our attention right now include: (1) establishment of high quality, standardized, and interoperable environmental datasets, (2) development of explainable, physics-informed and hybrid AI models, (3) integration of life cycle assessment, techno-economic analysis and risk assessment in nanotech-based research, (4) increased focus on



*J Water Environ Nanotechnol,* 2026, 11(SI): 1-4
10.22090/jwent.2026.2087985.2105

pilot-scale validation and field developing, (5) combine real-time monitoring, adaptive control, and predictive analytics in operational systems, (6) create transdisciplinary frameworks capable of linking laboratory innovation with policymaking, regulation, and implementation.

As Guest Editor, I am pleased to introduce this special issue (SI) entitled "Frontiers of AI-Driven Nanotechnology for Sustainable Water and Environmental Systems." This SI includes a collection of original research and comprehensive review articles that reflect the convergence of intelligent computational systems with nanoscale materials, devices, and processes, as one of the most promising interdisciplinary transitions in contemporary environmental sciences, to develop more efficient and adaptive solutions for the sustainable management of water resources and environmental systems. The papers in this SI offer a multi-dimensional view of the increasing convergence of AI with nanotechnology and water and environmental sciences. The issue initiates with a conceptual overview presenting emerging frameworks linking ML with nanomaterial design and environmental systems management, thus providing a theoretical basis for evolving interdisciplinary fields.

The papers that follow focus on the methodological improvements in modeling adsorption, treatment, and purification processes, and explain how AI algorithms can provide more accurate predictions and a deeper understanding of the dynamics of complex systems compared to conventional statistical methods. Another part of this issue is devoted to the use of nanosensors and smart monitoring systems for the construction of real-time water quality monitoring infrastructures. AI-driven nanotechnology enables the development of next-generation environmental monitoring networks. This SI also presents some research in materials and process engineering that uses ML to optimize the performance of advanced membranes, data-driven analysis of photocatalytic systems, and supporting intelligent characterization of nanomaterials, thereby facilitating the data-driven design of functional materials. In addition to water treatment technologies, two of the articles discuss the convergence of AI, nanotechnology, microbial biotechnology, and agriculture to address environmental challenges such as sustainable bioremediation strategies for contaminated soils and the exploration of nano-biosystems for enhancing resilience to stresses such as drought and water scarcity and for increasing the efficiency and specificity of agrochemicals (e.g., nanofertilizers, nanopesticides, nanonutrients, etc.) to reduce their environmental impacts. Collectively, the articles in this issue demonstrate that AI-based nanotechnology offers new horizons for sustainable water and environmental management, and also promotes sustainable food security. I would like to sincerely appreciate all the authors of this SI for their valuable contributions. I thank the reviewers for their rigorous and constructive evaluations. This effort helped ensure the scientific quality of this SI. I also appreciate the editorial team and the publishing staff for their support throughout the preparation and publication process. It is hoped that this SI will not only reflect the state-of-the-art advances in this field but also serve as a strategic platform for future research, interdisciplinary collaboration, and responsible development of emerging technologies in AI-driven nanotechnology for sustainable water and environmental systems.

## REFERENCES:


1. Mehmood, Hamid, Mukkavilli, S. Karthik, Weber, Ingmar, Koshio, Atsushi, Chinaporn, Meechaiya, Piman, Thanapon, Mubea, Kenneth, Tortajada, Cecilia, Mubea, Kenneth, and Liao, Danielle (2020). Strategic Foresight to Applications of Artificial Intelligence to Achieve Water-related Sustainable Development Goals. UNU-INWEH Report Series. United Nations University Institute for Water, Environment and Health (UNU-INWEH). https://www.unwater.org/news/strategic-foresight-applications-ai-achieve-water-related-sdgs.
2. Gabric, A. J. (2023). The Climate Change Crisis: A Review of Its Causes and Possible Responses. Atmosphere, 14(7), 1081. https://doi.org/10.3390/atmos14071081.
3. Artificial Intelligence-Driven Models for Environmental Management (2025) Editor(s): Shrikaant Kulkarni, Print ISBN:9781394282524, Online ISBN:9781394282555, https://doi.org/10.1002/9781394282555.
4. Safeer, S., Pandey, R. P., Rehman, B. Safdar, T. Ahmad, I. Hasan, S.W., Ullah, A. (2022) A review of artificial intelligence in water purification and wastewater treatment: Recent advancements. Journal of Water Process Engineering, 49, 102974. https://doi.org/10.1016/j.jwpe.2022.102974.
5. Ahmadi M., Davallo M., Jahanshahi M., Kiarostami V., Peyravi M. (2024). 'Investigating the Efficiency of Machine Learning Methods for Simulating the Effects of the Paper-Pulp Industry on Aqua Ecosystem Pollution', Journal of Water and Environmental Nanotechnology, 9(4), 458-468. https://doi.org/10.22090/jwent.2024.04.07.
6. Bohao He, Yanghe Zhao, Wei Mao, (2022) Explainable artificial intelligence reveals environmental constraints in seagrass distribution, Ecological Indicators, 144, 109523. https://doi.org/10.1016/j.ecolind.2022.109523.
7. Abdul Gaffar Sheik, Arvind Kumar, Chandra Sainadh Srungavarapu, Mohammad Azari, Seshagiri Rao Ambati, Faizal Bux, Ameer Khan Patan, (2025). Insights into the application of explainable artificial intelligence for biological wastewater treatment plants: Updates and perspectives. Engineering Applications of Artificial Intelligence, 144, 110132. https://doi.org/10.1016/j.engappai.2025.110132.
8. Torkamanzadeh, M.; Jahanshahi, M.; Peyravi, M.; Shokuhi Rad A. (2016) Comparative experimental study on fouling mechanisms in nano-porous membrane: cheese whey ultrafiltration as a case study Available to Purchase.
Water Sci Technol 74 (12): 2737–2750. https://doi.org/10.2166/wst.2016.352.
9. Sangchi, Z.G., Peyravi, M., Jahanshahi, M. (2026) A Comparative Study of Bio-Based Antimicrobial Membranes Induced by

Medicinal Plant-Derived Biocide for Dairy Wastewater Treatment. J Polym Environ 34, 51. https://doi.org/10.1007/s10924-025-03757-4.

10. Rawat, S., Tauseef, S.M., Sharma, M., Rautela, A., Gurav, R. G. (2026) A comprehensive review on emerging nanoparticle-based sustainable water treatments: Synthesis, characterization, and treatment efficiency, Desalination and Water Treatment, 326, 101724., https://doi.org/10.1016/j.dwt.2026.101724.
11. Debasmita Behera, Jesna Fathima, Noori M. Cata Saady, Sohrab Zendehboudi, Talib M. Albayati, Abbas Al-nayili, Pritha Chatterjee, V. Ponnusami, Brian Peach, Juan E. Ruiz Espinoza, (2026). 'Sustainable agriculture through environmental adaptation engineering for waste management' Green Technologies and Sustainability, 4 (1), 100242. https://doi.org/10.1016/j.grets.2025.100242.
12. Raiesi Ardali T., Soleimanpour L., Mamani L., Chorom M. (2024). 'Opportunities and Future Perspective of Nanofertilizers and Controlled Release Nanofertilizers in Agriculture', Journal of Water and Environmental Nanotechnology, 9(2), 223-247. https://doi.org/10.22090/jwent.2024.02.08.
13. Arbabi Bidgoli S. (2020). 'Endocrine Disrupting Effects of Carbon Nanotubes: A Systematic Review on Next Generation Nanotechnology based Agrochemicals', Journal of Water and Environmental Nanotechnology, 5(2), 102-113. https://doi.org/10.22090/jwent.2020.02.001.
14. Najafzadeh Nansa M., Jokarshoorijeh F., Tavakoli Hasanaklou N., Hosseni R., Ghorbanloo M., Mamani L. (2024). 'Nanoformulation: An efficient approach to natural insect repellent formulations', Journal of Water and Environmental Nanotechnology, 9(3), pp. 248-262. https://doi.org/10.22090/jwent.2024.03.01.
15. Niazian, M., Molaahmad Nalousi, A., Azadi, P. Ma'mani L., Chandler SF. 'Perspectives on new opportunities for nano-enabled strategies for gene delivery to plants using nanoporous materials. Planta 254, 83 (2021). https://doi.org/10.1007/s00425-021-03734-w.
16. Molaghan, P., Jahanshahi, M., Jahanshahi, M. (2024). A detailed molecular dynamics simulation and experimental investigation of CO2 adsorption on graphene oxide-polyaniline nanocomposite. Materials Chemistry and Physics, 314, 128835. https://doi.org/10.1016/j.matchemphys.2023.128835.
17. Belkhode PN, Awatade SM, Prakash C, Shelare SD, Marghade D, Gajghate SS, Noor MM, Dennison MS. (2025) An integrated AI-driven framework for maximizing the efficiency of heterostructured nanomaterials in photocatalytic hydrogen production. Sci Rep. 10;15(1):24936. https://doi.org/10.1038/s41598-025-10785-6.
18. Krishnan, A. Sundaram, T., Nagappan, B., Devarajan, Y., Bhumika, (2024) Integrating artificial intelligence in nanomembrane systems for advanced water desalination, Results in Engineering, 24, 103321. https://doi.org/10.1016/j.rineng.2024.103321.
19. Biglarijoo, N., Shams, A., Bagheri, M., Gill, L., Keypour, S. (2026) From data to sustainable clean water: AI/ML contributions to the UN Sustainable Development goals. Physics and Chemistry of the Earth, Parts A/B/C, 144, Part 1, 104427, https://doi.org/10.1016/j.pce.2026.104427.
20. De Temmerman, A., Verbeke, M. (2025) Improved multi-objective decision-making in manufacturing processes through uncertainty quantification and robust pareto front modelling. Sci Rep 15, 14411. https://doi.org/10.1038/s41598-025-97508-z.
21. Martin, K. D., & Murphy, P. E. (2016). The role of data privacy in marketing. Journal of the Academy of Marketing Science, 45(2), 135–155. https://doi.org/10.1007/s11747-016- 0495-4.
22. Mathew, D., Brintha, N. C., & Jappes, J. T. W. (2023). Artificial Intelligence Powered Automation for Industry 4.0. In A. Nayyar, M. Naved, & R. Rameshwar (Eds.), New Horizons for Industry 4.0 in Modern Business. Contributions to Environmental Sciences & Innovative Business Technology. Cham: Springer. https://doi.org/10.1007/978-3-031-20443-2_1.