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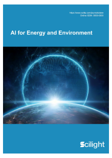

Commentary

AI-Driven Screening of Electrolyte Additives for Aqueous Zinc-Ion Batteries

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How To Cite: Wang, L.; Suna, P. AI-Driven Screening of Electrolyte Additives for Aqueous Zinc-Ion Batteries. *AI for Energy and Environment* **2025**, *1*(1), 2.

Received: 1 September 2025
Accepted: 22 September 2025
Published: 17 October 2025

Abstract: Aqueous zinc-ion batteries face significant challenges including dendrite growth and hydrogen evolution, which limit their practical application. Electrolyte additives offer a promising solution, yet traditional discovery methods remain inefficient. In this highlight, we found an exciting study that an AI-driven high-throughput screening strategy is employed to identify potential electrolyte additives from over 75,000 organic molecules. By evaluating adsorption energy on Zn(002) surfaces, electrochemical stability, and solubility, 48 candidate molecules were identified. Experimental validation confirmed that selected additives significantly enhance the performance of aqueous zinc-ion batteries.

Keywords: aqueous zinc-ion batteries; Electrolyte additives; AI-driven high-throughput screening strategy

Aqueous zinc-ion batteries (AZIBs) have garnered considerable attention owing to their low cost and intrinsic safety [1]. However, the practical deployment of AZIBs remains hindered by persistent interfacial challenges associated with the zinc metal anode and aqueous electrolytes [2]. In particular, the zinc anode suffers from uncontrolled dendrite growth, which risks internal short circuits, as well as the accumulation of “dead zinc” that severely reduces Coulombic efficiency [3,4]. Concurrently, the aqueous electrolyte triggers hydrogen evolution reactions at the zinc surface, leading to the generation of corrosive byproducts and passivation layers, both of which further degrade battery performance [5]. To address these limitations, electrolyte engineering has emerged as a promising strategy. For instance, tuning the salt concentration can significantly suppress free water activity and enhance the electrochemical stability of AZIBs [6]. Nevertheless, the high cost of such “water-in-salt” systems has limited their widespread application [7]. As a more practical and cost-effective alternative, the incorporation of trace-level electrolyte additives has proven to be a scalable approach. According to the Web of Science (as of 6 August 2025), more than 2300 papers have been published on additive-enabled optimization of AZIB electrolytes. Historically, the selection of electrolyte additives has relied heavily on trial-and-error experimentation, often guided by empirical insights or analogies from adjacent fields. Although this approach has yielded several effective organic and inorganic additives, the search for high-performance, generalizable, and scalable additives remains a major bottleneck in advancing AZIB technologies. Although some scientists have conducted screening and design of AZIB’s electrolytes based on multimodal optimization through molecular simulations, the scope of screening remains relatively limited [8].

With the advent of the artificial intelligence (AI) era, a critical question arises: can AI accelerate the discovery of next-generation AZIB additives? In a pioneering effort, Xu et al. leveraged AI-driven high-throughput screening to identify promising electrolyte additives for AZIBs, which publish in Angewandte Chemie International Edition [9]. Their workflow is illustrated in Figure 1. Starting with 75,024 electrically neutral organic molecules composed of C, H, O, N, and S atoms, extracted from the Materials Project database, the authors established a molecular library, using water as a key reference molecule due to its role in hydrogen evolution reactions and interfacial instability.

To evaluate additive performance, the authors generated adsorption structures of these molecules on the Zn(002) surface and predicted their redox potentials. Given that one of the crucial mechanisms by which additives improve performance is by modulating zinc nucleation, molecules with strong affinity toward the Zn(002) surface (i.e., lower adsorption energies) are desirable for guiding uniform Zn deposition. For each molecule, 100 adsorption configurations were automatically generated, and a graph neural network (GNN) model was employed to predict their adsorption energies. The lowest predicted energy was taken as the most stable configuration for subsequent density functional theory validation. This approach enabled rapid screening of vast chemical spaces, out of 75,024 molecules, 67,383 were successfully mapped to 6,738,300 unique Zn(002) surface configurations. The GNN predicted adsorption energies for all configurations, and the minimum value for each molecule was taken as its representative adsorption energy. For reference, the adsorption energy of H_2O on Zn(002) was predicted to be −0.155 eV. Notably, the majority of screened molecules exhibited lower adsorption energies than water, suggesting their preferential adsorption on the zinc surface and potential to mitigate parasitic hydrogen evolution reactions and improve zinc reversibility.

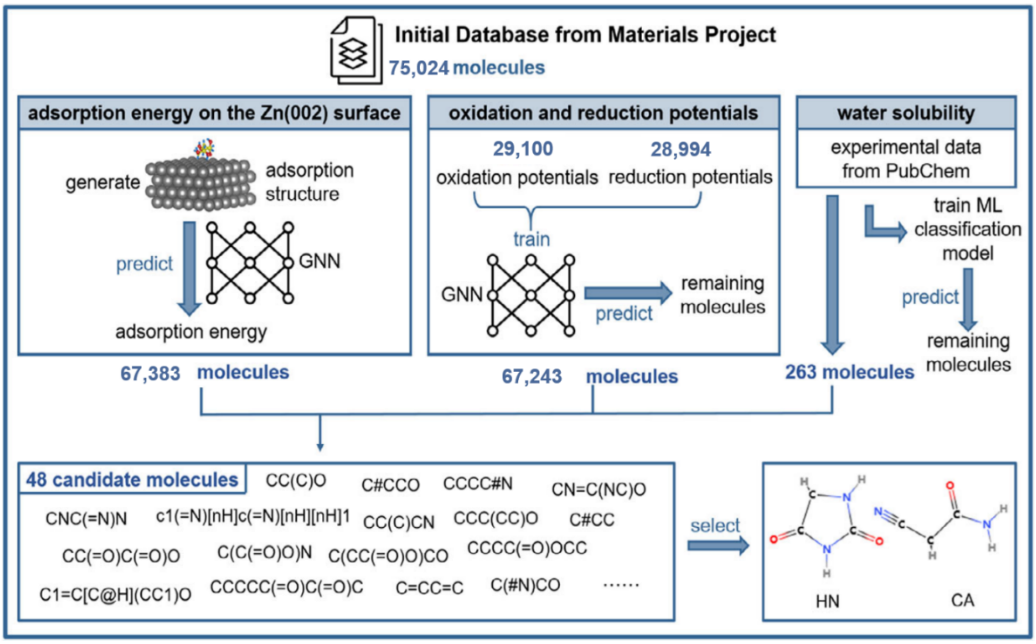

Figure 1. The workflow of electrolyte additive high-throughput screening for AZIBs [9]. Copyright 2025, Wiley-VCH.

Beyond strong surface affinity, candidate molecules must also exhibit sufficient electrochemical stability to function effectively as electrolyte additives in AZIBs. In practical systems, the operational voltage window should be carefully controlled to suppress water decomposition. Therefore, an ideal additive should not further narrow the already limited electrochemical stability window of AZIBs. Given that additives are typically used at low concentrations, their redox activity should not occur prior to that of water within the same voltage range. Specifically, to avoid unwanted side reactions, an ideal additive should possess a lower reduction potential and a higher oxidation potential than H_2O.

To assess the electrochemical stability of the molecular candidates, the authors extracted oxidation potentials for 29,910 molecules and reduction potentials for 28,994 molecules from the Materials Project API, based on the initial dataset of 75,024 molecules. These values were then used to train a graph neural network (GNN) model capable of predicting the redox potentials of the remaining molecules. Ultimately, among the 67,383 molecules for which adsorption energies were predicted, redox potential values were successfully obtained for 67,243 molecules. By referencing the oxidation and reduction potentials of H_2O as the coordinate origin, molecules residing in the second quadrant (i.e., those with oxidation potentials higher than and reduction potentials lower than H_2O) were considered electrochemically stable. From the original dataset of 75,024 molecules, 14,907 molecules satisfied both the adsorption energy and electrochemical stability criteria. To further evaluate their experimental feasibility in AZIBs, the authors retrieved solubility data from the PubChem API. Experimental aqueous solubility values were successfully obtained for 263 of these molecules. Among them, 48 water-soluble molecules met all selection criteria and were ultimately identified as promising electrolyte additive candidates.

To examine the structural similarity between the screened candidates and previously reported additives, molecular fingerprints were computed and subjected to two-dimensional dimensionality reduction. The resulting distribution revealed that many of the shortlisted candidates shared similar chemical backbones with known additives, reinforcing the validity and reliability of the AI-driven screening strategy. From this candidate pool, three molecules, propyl propionate, 1,4-butanediol, and butyric acid, were selected for experimental validation. Electrochemical tests confirmed their effectiveness as AZIB electrolyte additives, highlighting the potential of this AI-guided approach for accelerating rational additive discovery.

In summary, Xu et al. [9] developed a scalable, data-driven framework for the discovery of electrolyte additives in AZIBs. Specifically, they automatically generated large sets of molecular adsorption configurations and employed a GNN to efficiently predict their adsorption energies on the Zn(002) surface. Concurrently, oxidation and reduction potentials for tens of thousands of molecules were extracted from databases to train a GNN model capable of predicting the electrochemical stability windows of the remaining molecules. To assess solubility, experimental data for 263 molecules were obtained via the PubChem API and used to train a machine learning model for solubility prediction. Applying these criteria, 48 molecular candidates were identified as potential electrolyte additives. Among them, two were experimentally validated and demonstrated promising electrochemical performance. These molecules exhibited stronger Zn(002) surface affinity than H_2O, broader electrochemical stability windows. We believe that this work will offers a powerful blueprint for accelerating the rational design of next-generation electrolyte additives through artificial intelligence.

Author Contributions

L.W.: data curation, writing—original draft preparation; P.S.: supervision, writing—reviewing and editing. All authors have read and agreed to the published version of the manuscript.

Funding

This research was funded by the National Natural Science Foundation of China (Grant No. 22209058), the Guangdong Basic and Applied Basic Research Foundation (Grant Nos. 2023A1515011994 and 2023A1515110008), and the Science and Technology Planning Project of Guangzhou, China (Grant No. 2024A04J3799).

Institutional Review Board Statement

Not applicable.

Informed Consent Statement

Not applicable.

Data Availability Statement

The data that support the findings of this study are openly available in *AI for Energy and Environment*.

Conflicts of Interest

The authors declare no conflict of interest.

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