Accelerating Electrolyte Discovery via a Closed-Loop Physical AI Platform

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1. Introduction

The electrification of transportation and grid infrastructure is driving demand for safer, longer-lasting, and more affordable batteries [1]. Liquid electrolytes are the linchpin of this transition, but their formulation is a high-dimensional optimization problem: a handful of salts and solvents combine into more than 10^{60} practical mixtures, and conductivity, electrochemical stability, and interfacial behavior emerge from coupled chemistries that intuition cannot resolve [2]. Discovery has therefore been bottlenecked by slow, manual trial-and-error. Closed-loop physical AI platforms, integrating automated experimentation, structured data management, and machine learning, have recently emerged as a powerful paradigm for navigating such spaces [3,4]. Here we report a closed-loop platform that operationalizes this paradigm for electrolyte discovery and demonstrate its capabilities on liquid sodium electrolytes.

2. Closed-loop physical AI platform

Our platform closes the loop between formulation, characterization, and prediction (Figure 1). Sobol sampling coupled to a pre-trained high-dimensional machine-learning model proposes candidate formulations from a high-dimensional combinatorial space; an automated robot dispenses, mixes, and assembles the cells; temperature-controlled electrochemical impedance spectroscopy (EIS) measures ionic conductivity; resulting in structured datasets that are fed into the loop.

2.1 High-dimensional design space

We construct a high-dimensional combinatorial design space spanning 5 salts, 15 solvents, multiple ratios, and salt concentrations, enabling systematic exploration far beyond conventional electrolyte design heuristics. Sobol low-discrepancy sampling combined with controlled normalization strategies generates thousands of distinct formulations under varied conditions, capturing the complex interactions that govern multi-component liquid electrolyte transport [4, 5].

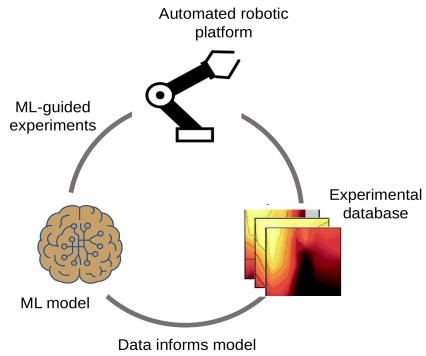

Figure 1. The closed-loop physical AI platform integrates an automated robotic platform, an in-house experimental database, and machine-learning models that guides and informs the next round of experiments.

2.2 Automated experimental workflow

Our robotic workflow can handle both liquid and polymer electrolyte materials[5, 6]. For liquids, the platform can formulate and assemble ~144 cells per week, perform several temperature-resolved EIS and auto-fit Nyquist responses to a Randles equivalent circuit to extract bulk and interfacial resistances. For polymers, the same backbone casts and dries films, measures film thickness, and assembles symmetric cells. The end-to-end throughput is ~8× that of manual experimentation while sharply reducing operator-driven variability, yielding consistent, model-ready data.

3. Demonstration: liquid sodium electrolytes

We demonstrate the platform on liquid sodium electrolytes, a chemically rich and underexplored space relative to lithium [7]. From 5 sodium salts (NaTFSI, NaFSI, $NaPF_6$, $NaClO_4$, NaOTf) and 15 organic solvents spanning ethers, carbonates, sulfonamides, nitriles, phosphates, and esters, the platform generated 3,400 unique data points — the first structured experimental databases for sodium electrolytes to date.

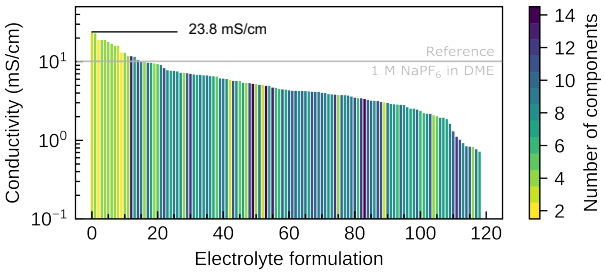

Figure 2. Measured ionic conductivity of 119 unique liquid sodium electrolytes, sorted in descending order and colored by number of components. The horizontal line marks the 1 M $NaPF_6$ in DME reference. The platform identified mixtures exceeding 20 mS cm^{-1}, with a record of 23.8 mS cm^{-1}.

Figure 2 shows that the platform discovers electrolyte formulations with record-level ionic conductivity within the explored design space (>20 mS cm^{-1}), substantially above the 1 M $NaPF_6$ in DME reference. The highest measured value, 23.8 mS cm^{-1} is — to our knowledge — the highest reported room-temperature value for any liquid sodium electrolyte. Color-coded by number of components, the figure further reveals that the highest conductivities cluster at moderate compositional complexity (5–7 components), pointing to a tractable optimization regime.

4. Cross-chemistry machine learning

Our models is trained jointly on Li and Na conductivity datasets — spanning multiple salt and solvent families, ratios, salt concentration, and broad mixture compositions — and accurately predicts conductivity across chemistries. Initial validation on sodium and lithium systems demonstrate cross-chemistry generalization [6,7]. The model actively guide the next experiments, replacing exhaustive sampling with targeted exploration and closing the discovery loop. Together, these results show that a unified physical AI platform can transform electrolyte discovery from artisanal trial-and-error into a structured, data-generating engine for AI-guided closed-loop design.

Acknowledgments

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