Machine Learning for Dendrite Suppression: Designing Stable Anodes for Aqueous Zinc-Ion Batteries

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PROJECT PROFILE

Topic: Zinc & Lead Batteries| Vertical: Materials and Systems Innovation

Strategic Pathway: Optimize

Project start and finish: FY25-FY26

PROBLEM

Advancing AZIBs technology is essential for the development of grid-scale energy storage systems. This project aims to accelerate the development of advanced aqueous zinc-ion batteries (AZIBs) by addressing the dendrite formation problem on anodes.

- Suppressing dendrite growth through improved anode design is necessary to enable the practical deployment of AZIBs.
- Traditional approaches to anode design, based on trial-and-error experimentation, are often time-consuming and limited in scope.

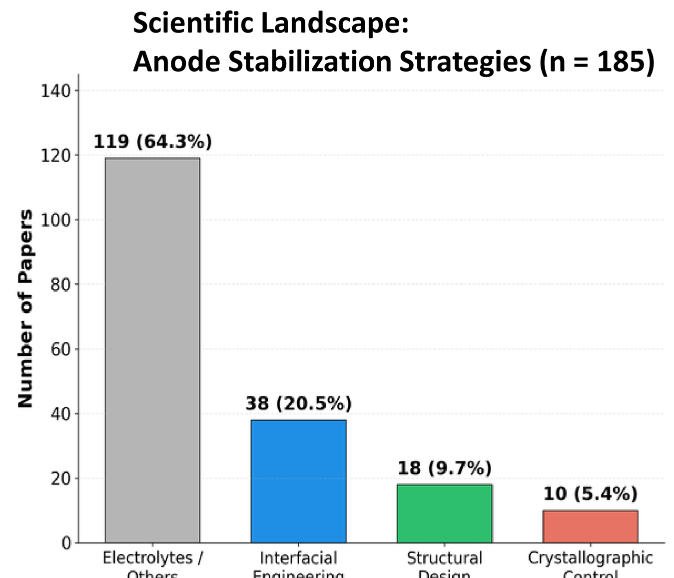
APPROACH

This project incorporates machine learning to guide the design of stable zinc anodes with suppressed dendrite formation for aqueous zinc-ion batteries.

- Data engineering with auto search and semi-auto paper collection.
- Data mining to create a comprehensive database.
- ML/AI techniques are applied to this high-dimensional dataset for feature extraction, enabling the identification of hidden correlations and design principles that suppress dendrite growth and improve battery stability.

Fig. 1. Data-to-Insight pipeline.

RESULTS



Category	Estimated Count	Description
Electrolyte Additives	~70 papers	Using liquid "salts" or molecules to change the bulk electrolyte. Easy to do, but often causes side reactions.
Purely Fundamental	~30 papers	Theoretical modeling or microscopy studies that don't propose a new anode design.
Alternative Metals	~10 papers	Research into Zn-Mn or Zn-V alloys, rather than focusing on the anode structure itself.
Optimization /Standard	~9 papers	Minor tweaks to current collectors or commercial foil treatments.

Fig. 2. Dataset composition.

- Data engineering pipeline was generated which enable the bulk acquisition with automatic search, which cast a wide net across ~239 papers.
- The Python-driven DOI-to-Local-Library bridge was developed to synthesis the library with the papers in the list. Extra filtration was conducted to reduce the noise, which left us with 185 literatures.

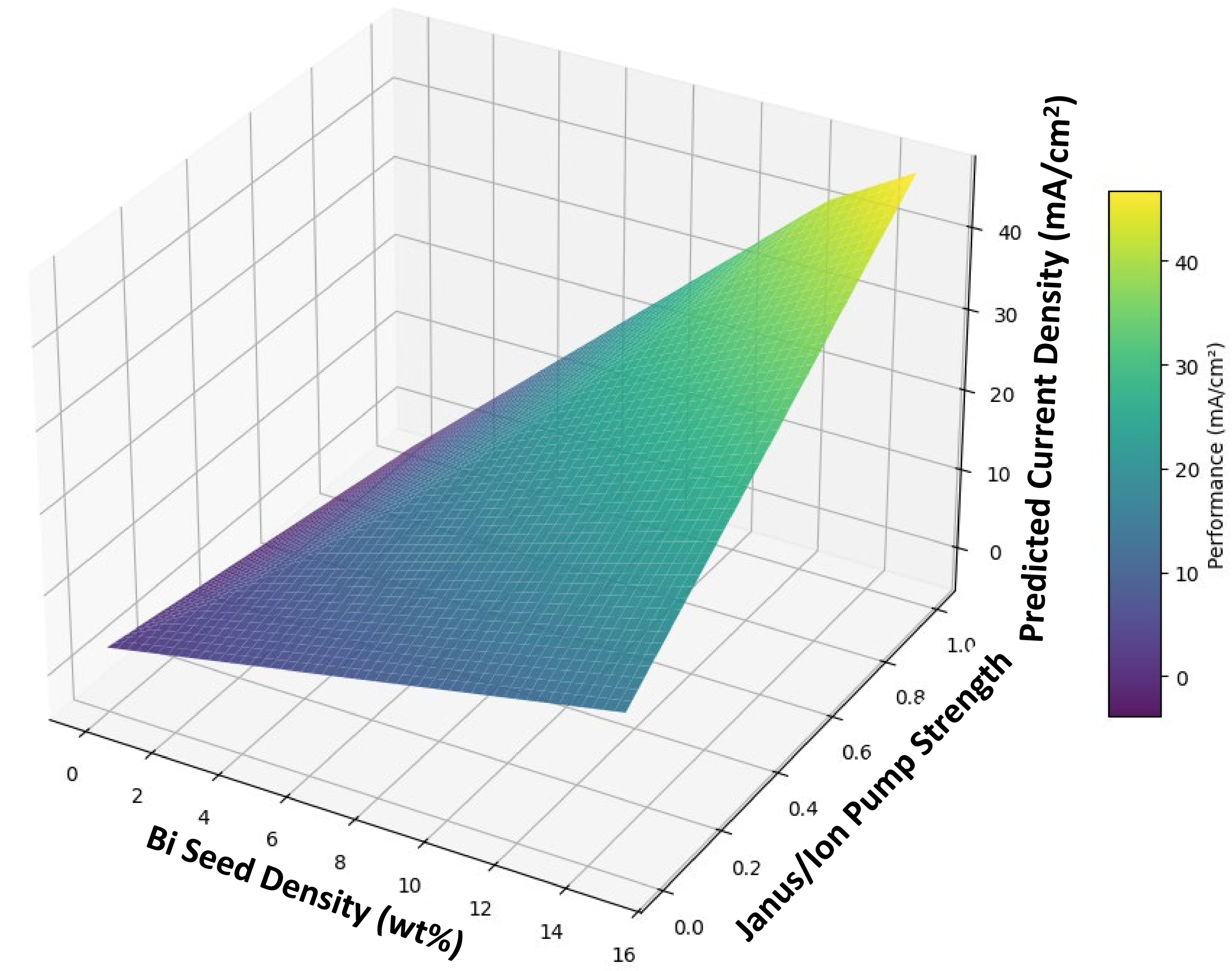


Fig. 3. The 3D sensitivity map.

- Data mining was conducted to convert 185 technical PDFs to a quantitative dataset.
- Random Forest (RF) model was implemented for data training and feature importance ranking. With the trained random forest model, 2nd order sensitivity analysis was conducted to examine how they interact.

CONCLUSIONS & IMPACT

The RF model identified the top three drivers that determine whether an anode successfully suppresses dendrite formation: nucleation & diffusion control (44%), Janus separator / ion pump (22%), and porosity (9%). Based on the sensitivity analysis, the finalized design is updated in Table 1.

Table 1. Finalized design specification.

Parameter	Target Specification	ML Rationale
Bi-Seed Density	10.0 – 12.0 wt%	Moves the design into the "High Stability" plateau on the X-axis, ensuring sufficient nucleation sites to support high-flux deposition.
Janus Charge Gradient	~18 mC/m^2	Identifies the "sweet spot" along the Y-axis, providing active Zn^{2+} pumping to sustain ~20 mA cm^{-2} without inducing local depletion.
Pore Confinement	< 5 nm (mesoporous)	Enables effective 2D diffusion suppression, directing ions into vertically controlled pathways governed by the Janus ion pump.

FUTURE DIRECTIONS

Different machine learning algorithm will be applied for comparison. Exploring the use of a multi-agent system in which different “agents” handle specific stages of the discovery cycle using limited experimental data.

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