

滾軋製程設計搭配計算相圖與機器學習法開發鋅離子電池陽極鋅箔

CALPHAD- and Machine Learning-Assisted Alloy Design with Rolling Optimization for Zn Foil Anodes in Aqueous Zn-Ion Batteries

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Abstract

Alloying modification and microstructural regulation enhance Zn anodes in aqueous zinc-ion batteries (AZIBs). However, integrated strategies remain scarce. In this work, we combine CALPHAD-assisted Zn-X alloy design with rolling process optimization to regulate alloy composition and microstructure. CALPHAD provides thermodynamic predictions of phase fractions, whereas rolling refines grains and reinforces preferential crystallographic orientation. Electrochemical evaluation of the fabricated electrodes is further combined with machine learning (ML) analysis to facilitate the optimization of alloy composition and processing parameters. This holistic strategy enables uniform Zn deposition, enhances corrosion resistance, and provides a scalable route toward durable Zn anodes.

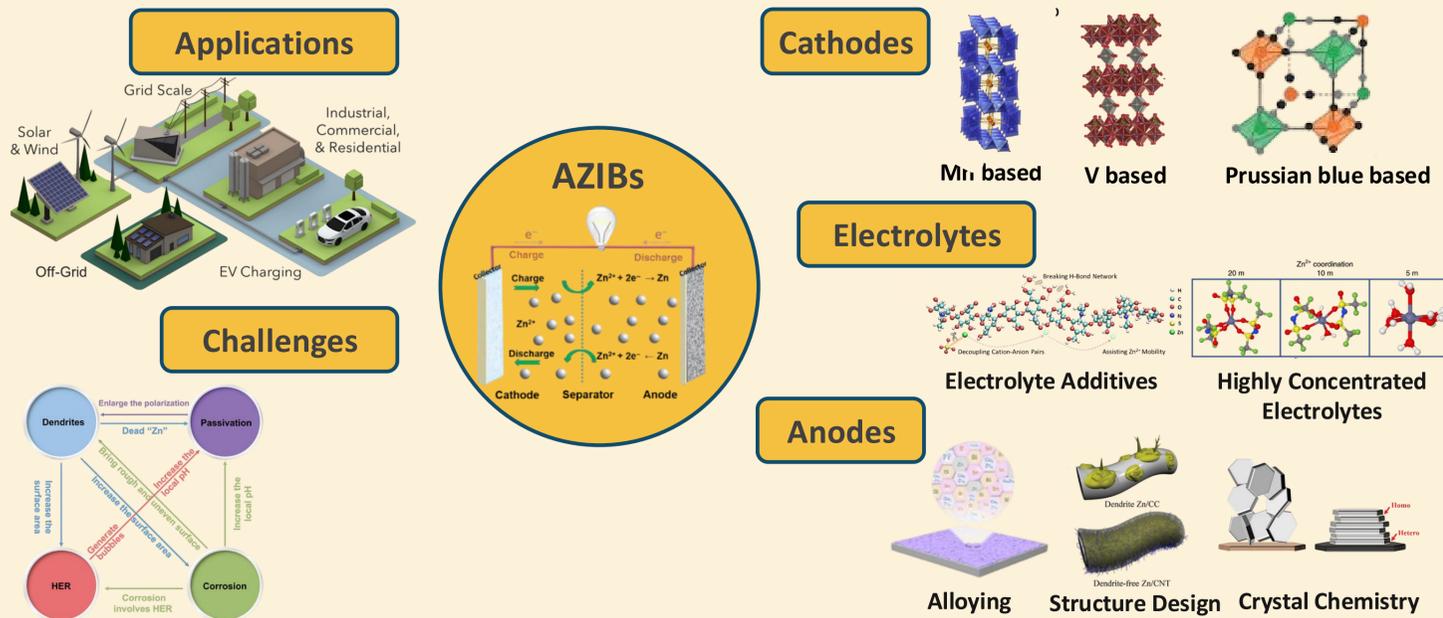
Outlook

- Applying physical metallurgy to Zn anodes shows great potential.
- Controlling alloy phases and microstructures from a materials science perspective enhances Zn anode stability.
- CALPHAD- and ML-Assisted process design offers a reliable framework for developing Zn alloy anodes.

Acknowledgement

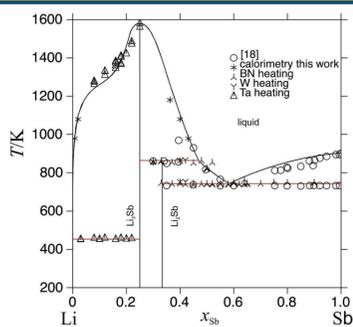
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Introduction

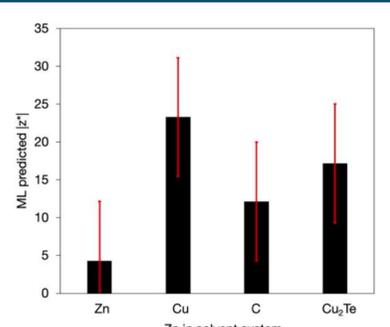
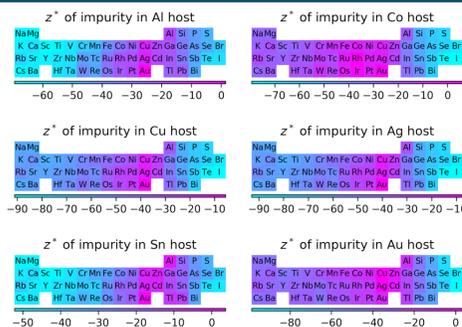


CALPHAD- and ML-Assisted Alloying in Anode Design

CALPHAD

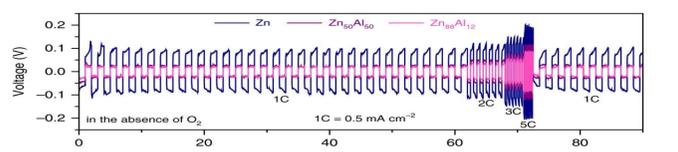
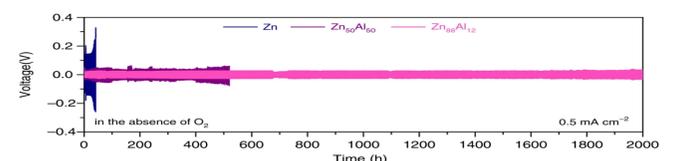
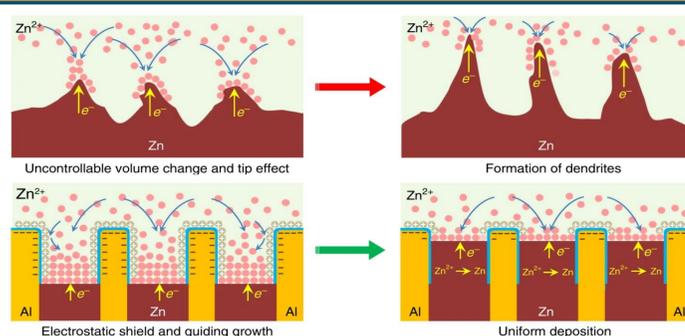


Machine Learning-Assisted



Ingot Composition and Anode Performance

Electrostatic Shielding and Structural Hosting Enabled by Hetero-Metal Alloying



Rolling Process for Manipulating Textured Electrodes

