Enhancing Magnesium Anode Performance via a Novel Active Learning Framework and Density Functional Theory

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Abstract The magnesium-air (Mg-air) battery, renowned for its remarkable energy density and cost-effectiveness, has the potential to revolutionize applications beyond the reach of conventional rechargeable batteries [1]. This includes serving as range extenders for electric vehicles and powering long-range drones. However, the persistent challenge of balancing efficiency and voltage has impeded its widespread adoption, hindering further progress in energy density. In this study, we addressed this obstacle by developing a novel active learning framework tailored to screen high-performance magnesium anodes. Our innovative framework integrates physically interpretable variables, machine learning, Pareto front exploration, experimental feedback, and feedback from generated data. Within an extensive compositional space (~350,000 possibilities), we identified a novel anode, Mg-1Ga-1Ca-0.5In, exhibiting exceptional energy density (2548±220 W h kg^{-1}). We attribute the excellent performance of Mg-1Ga-1Ca-0.5In to the concepts of "grain boundary activation" and "intra-grain inhibition". This concept diverges from the conventional design approach commonly reported in existing studies, which primarily emphasize the influence of second phases on discharge behavior, while overlooking the impact of solute atoms. We believe that our findings hold immense promise for the future of energy storage.

Keywords Magnesium anode; Corrosion; Machine learning; Theoretical calculation

Reference

[1] H. Liang, L. Wu, C. Zhao, C. Zhai, W. Du, Evading efficiency-voltage trade-off in magnesium-air batteries through solute atoms and second phases synergy, Journal of Magnesium and Alloys, in press (2024).