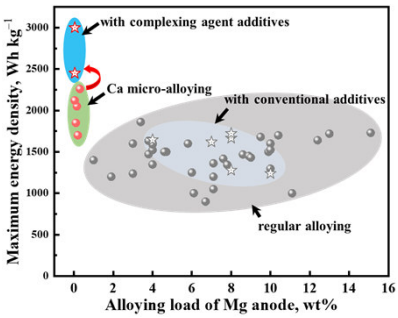
Selection of Electrolyte Additives for Enhanced Mg-air Battery Performance Supported by Data-driven Approach

Darya Snihirova[1], L. Wang[1], M. Deng[1], B. Vaghefinazari[1] , Y. Wu[1], T. Würger[1,2], R. Meißner[1,2], D.A. Winkler[3], C. Feiler[1], D. Höche[1], S. Lamaka[1], M. Zheludkevich[1, 4]

[1] Institute of Surface Science, Helmholtz-Zentrum Hereon, Germany;
[2] Institute of Polymers and Composites, Hamburg University of Technology, Germany;
[3]Department of Biochemistry and Chemistry, Latrobe University, Bundoora, Australia;
[4]Institute of Materials Science, Kiel University, Germany;

Motivation

- Mg possesses negative electrode potential (-2.37V vs. SHE), high volumetric capacity (3833 mA h cm^{-3} vs. 2061 mA h cm^{-3} for Li), long shelf life and environmentally benignity.
- Severe self-corrosion and blockage of Mg surface by discharge products lead to the loss of utilization efficiency and discharge potential.



Objectives

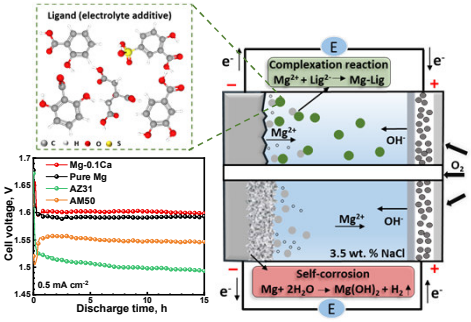
With the aim to boost Mg-air battery performance, Mg^{2+} complexing agents were adopted as electrolyte additives. The main objectives are:

- investigate the potential of Mg^{2+} complexing agents to regulate the interfacial condition of the Mg anode/electrolyte;
- establish data-driven quantitative structure–property relationship (QSPR) models to searches for promising battery booster candidates.

Such batteries can be used for power the automated equipment with sensors to operate in remote and sensitive locations; autonomous sea vehicles, emergency power sources.

Results

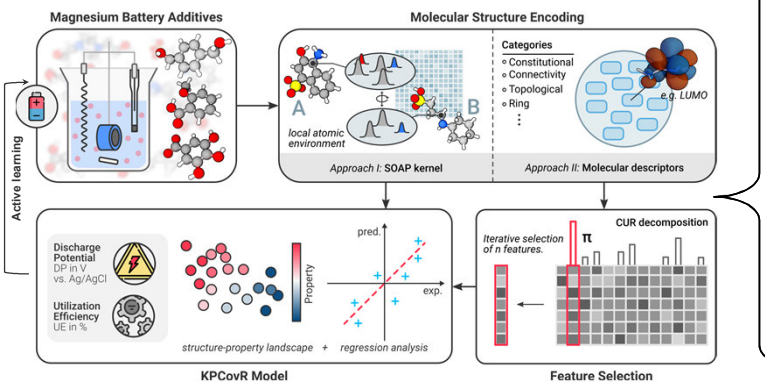
Mg^{2+} complexing agents as electrolyte additives for Mg-Ca based Mg-air battery[1-3]



Mg^{2+} complexing agents improve the cell voltage of Mg-air battery via hindering the precipitation of discharge products.

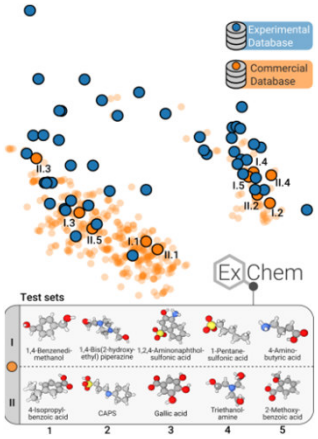
Different Mg^{2+} complexing agents should be used for various discharge loads to obtain optimal effect, according to their complexation abilities with Mg^{2+}.

Workflow for data-driven discovery of battery electrolyte additives[4]



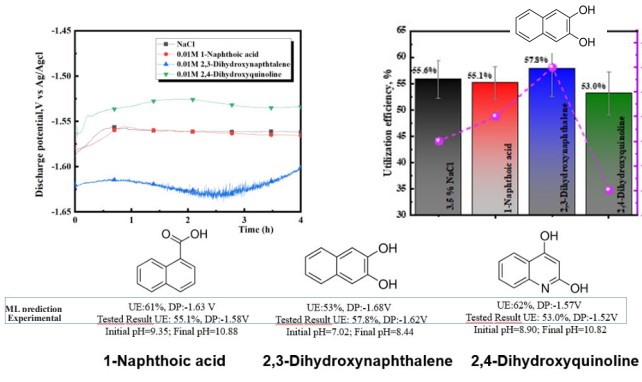
Experimental screening and data processing [4]

- Seed database comprising 50 electrolyte additives
- Measured **discharge potential (DP)** and **utilization efficiency (UE)**
- ExChem routine suggested two test sets of compounds of interest for the **active design of experiments**



Improvement of model prediction by active learning

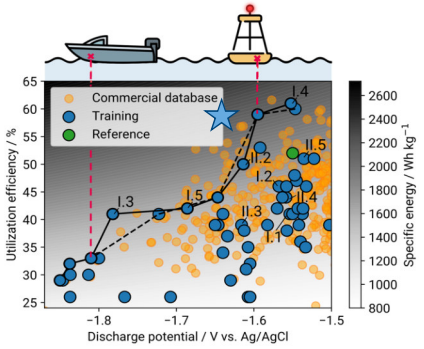
Every several additional experimental data-points do improve the ML predictions.



1-Naphthoic acid **2,3-Dihydroxynaphthalene** **2,4-Dihydroxyquinoline**

Summary and Outlook

- Mg^{2+} complexing agents improve the cell voltage of Mg-air battery via hindering the precipitation of discharge products.
- Different Mg^{2+} complexing agents should be used for various discharge loads to obtain optimal effect, according to their complexation abilities with Mg^{2+} and **application area (**power the automated equipment with sensors to operate in remote and sensitive locations; autonomous sea vehicles, emergency power sources).
- SOAP-based model generates intuitive structure– property landscapes that facilitate exploration of large areas of the chemical space.
- When provided with more training data, significant improvements of the prediction accuracy were observed.
- Large, more representative dataset is needed for correct ML prediction.



Multi-Objective Optimization, by establishing the Pareto front and looking for the compounds either with high UE or DP

References

[1] B. Vaghefinazari, D. Höche, S.V. Lamaka, D. Snihirova, M.L. Zheludkevich, Tailoring the Mg-air primary battery performance using strong complexing agents as electrolyte additives, J. Power Sources, 453 (2020) 227880.
[2] D. Snihirova, L. Wang, S.V. Lamaka, C. Wang, M. Deng, B. Vaghefinazari, D. Höche, M.L. Zheludkevich, Synergistic Mixture of Electrolyte Additives: A Route to a High-Efficiency Mg-Air Battery, Journal of Physical Chemistry Letters, (2020) 8790-8798.
[3] L. Wang, D. Snihirova, M. Deng, B. Vaghefinazari, D. Höche, S.V. Lamaka, M.L. Zheludkevich, Enhancement of discharge performance for aqueous Mg-air batteries in 2,6-dihydroxybenzoate-containing electrolyte, Chem. Eng. J., (2021) 132369.
[4] T. Würger, L. Wang, D. Snihirova, M. Deng, S.V. Lamaka, D.A. Winkler, D. Höche, M.L. Zheludkevich, R.H. Meißner, C. Feiler, Data-driven selection of electrolyte additives for aqueous magnesium batteries, Journal of Materials Chemistry A, 10 (2022) 21672-21682.

Acknowledgement

A sincere acknowledgement is given to the team of Dr. Jan Bohlen from Institute of Material and Process Design and Günter Meister from Institute of Metallic Biomaterials of Hereon for help with preparation of Mg alloy.

High-Performance Seawater Magnesium Batteries for Marine Application

SEAMAG MarTERA ERA-NET COFUND HELMHOLTZ GEMEINSCHAFT Bundesministerium für Bildung und Forschung

Helmholtz-Zentrum Hereon • Max-Planck-Straße 1 • 21502 Geesthacht I Germany • www.hereon.de
Contact: Dr. Darya Snihirova • T +49 4152 87-01936 • darya.snihirova@hereon.de