Automated development of PFAS-free aqueous electrolytes for Na-ion batteries

Dr Wessel Van Ekeren[1], Andreas Tuxen[1], Dr Sergio Rodriguez[1], Prof Jin Hyun Chang
[1]Danmarks Tekniske Universitet, , Denmark

Developing safe and sustainable electrolytes is a critical hurdle for next-generation batteries. Commercial systems rely on flammable organic solvents and fluorinated salts (e.g., $LiPF_6$), which, while forming stable interphases, pose significant fire risks and release toxic hydrofluoric acid (HF). Furthermore, tightening PFAS regulations and high dry-room manufacturing costs necessitate moisture-tolerant, PFAS-free alternatives.

This work addresses these challenges by exploring High-Entropy Electrolytes (HEEs) within aqueous systems. While water-based electrolytes are intrinsically safe and cost-effective, they typically suffer from a narrow Electrochemical Stability Window (ESW). By leveraging the complex solvation structures of multiple salts, HEEs can widen the ESW while maintaining high ionic conductivity.

To navigate the vast, high-dimensional design space of HEEs, we developed an automated electrolyte development platform integrating high-fidelity characterization with Bayesian Optimization (BO). This system enables the autonomous profiling of 24 electrolytes per day across a 0–40°C range. Utilizing a three-electrode cell (Pt electrodes and Ag/AgCl reference), the platform performs Electrochemical Impedance Spectroscopy (EIS) and Linear Sweep Voltammetry (LSV) to measure ionic conductivity (mS cm^{-1}) and ESW (V).

Through high-throughput screening, we identified optimized combinations of NaAc, $NaNO_3$, and Na_2SO_4 that achieve the stability required for practical galvanostatic cycling. This automated approach accelerates the discovery of PFAS-free formulations, bridging the gap between environmental sustainability and the rigorous performance demands of next-generation energy storage.