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The Art of Precision Measurement

WHITEPAPER

THE IMPORTANCE OF WATER ACTIVITY IN EMERGING BATTERY TECHNOLOGIES

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1. Executive Summary

By 2050, the world's energy consumption is expected to increase by nearly 50%, posing a significant challenge for current battery technologies to grow sustainably and cost-effectively.[1] Although lithium-ion systems still dominate the market, emerging chemistries such as redox flow, aluminum-air, and aqueous (water-based) batteries aim to address cost, safety, and environmental concerns.[2-4] However, moisture-induced instabilities remain a major issue. Even trace amounts of water can drastically alter electrolyte behavior, reducing conductivity or causing corrosion.[5-7]

Recent research indicates that water activity, a measure of the energy status of water, is a more accurate predictor of performance variation than total water content. This is because viscosity, ionic transport, and redox characteristics can change dramatically when small amounts of high energy water are introduced to deep eutectic solvents (DESs), such as ethaline (a 1:2 choline chloride:ethylene glycol mixture).[11-13] By controlling water activity using specialized meters and refined measurement techniques, manufacturers can maintain stable electrolyte performance.[14-16] These strategies help prevent moisture-related failures, extend battery lifespans, and capitalize on the distinctive advantages offered by emerging battery chemistries.

2. Introduction and Background

2.1. The Drive for Alternative Batteries

As the U.S. Energy Information Administration predicts that the world's energy demand may nearly double by 2050, the need for large-scale, reliable storage systems has become more pressing.[2,3] Although lithium-ion batteries remain essential, they face material and scalability challenges,[2,3] driving interest in alternative approaches such as water-based (aqueous) systems. Redox flow batteries utilize electrolyte solutions that when oxidized or reduced and passed through an electrochemical cell, create an electrical current [3]. Aluminum-air designs leverage high-density aluminum anodes combined with oxygen as the cathode to create electrical current, thereby decoupling power and energy.[4-6] Unfortunately, all of these options encounter difficulties in controlling water content; if moisture is not managed effectively, performance can deteriorate under humid conditions.[7]

2.2. Deep Eutectic Solvents and Moisture Sensitivity

As an example, deep eutectic solvents (DESs) have attracted attention for their low toxicity, straightforward synthesis, and tunable chemical structures.[8-10] Typically composed of hydrogen bond donors (e.g., glycols) and acceptors (e.g., choline chloride), many DES are highly hygroscopic, readily absorbing water from ambient air.[11-13] This extra water can alter hydrogen-bonded networks and compromise electrochemical stability. Conventional drying methods such as vacuum or molecular sieves may reduce overall moisture, but they do not distinguish between lower energy water that is chemically bound within the solvent and high energy water that remains free to interface with electrochemical processes.[14]

2.3. Water Activity as a Guiding Metric

Water activity, or the thermodynamic activity of water, has proven to correlate more reliably with changes in viscosity conductivity, or redox potential than does total water content.[15-18] Water that is chemically bound in stable complexes tends to be relatively inert, whereas even minor fluctuations in high energy water can accelerate corrosion, lower capacity, or lead to phase separation.[19-22] Consequently, industrial and academic research has shifted from merely drying solvents to precisely regulating water energy levels, aiming for more accurate and reproducible results in both laboratory and practical applications.

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3. Description of the Problem

Conventional drying methods (e.g., vacuum suction or sieving) lower bulk moisture but do not indicate how much water remains chemically bound. Redox flow and aluminum-air batteries are considered safer and more scalable than Li-ion batteries; however, if water activity is not properly controlled, their electrolytes can become unstable.[3] Even a small increase in water uptake can shift ethaline-type DESs from nearly ideal to noticeably less ideal conditions.[7,11] This occurs because newly absorbed water molecules rearrange local hydrogen-bond networks, a change not detectable by conventional total-water measurements.[14]

Furthermore, standard drying techniques do not distinguish between energy levels of water; they merely remove the bulk portion.[16,23] At low water concentrations where non-ideal behavior is more pronounced, any residual high energy water can corrode metal components, skew electrochemical data, and obscure true solvent stability thresholds if it is allowed to react.[12-14] Such oversight threatens the economic viability of emerging battery technologies that aim to surpass Li-ion cells in cost, safety, or scalability. Moreover, without precise monitoring of water activity, researchers risk misinterpreting critical electrochemical results, introducing manufacturing inconsistencies, and shortening device lifespans.[24,25]

In **Figure 1**, the behavior of ethylene glycol (EG) and its deep eutectic solvents (DES) variant, ethaline, is compared under increasing water content ranging from 0% to 100%. **Figures 1a** and **1b** plot the water activity (a_w) against the mole fraction of water (x_w). Both EG and ethaline deviate from the ideal (dashed) reference line at low water concentrations, indicating that solvent-water interactions are suboptimal. As water content increases, these curves gradually converge with the idea line, suggesting that the mixtures behave more like conventional solutions beyond a certain concentration.

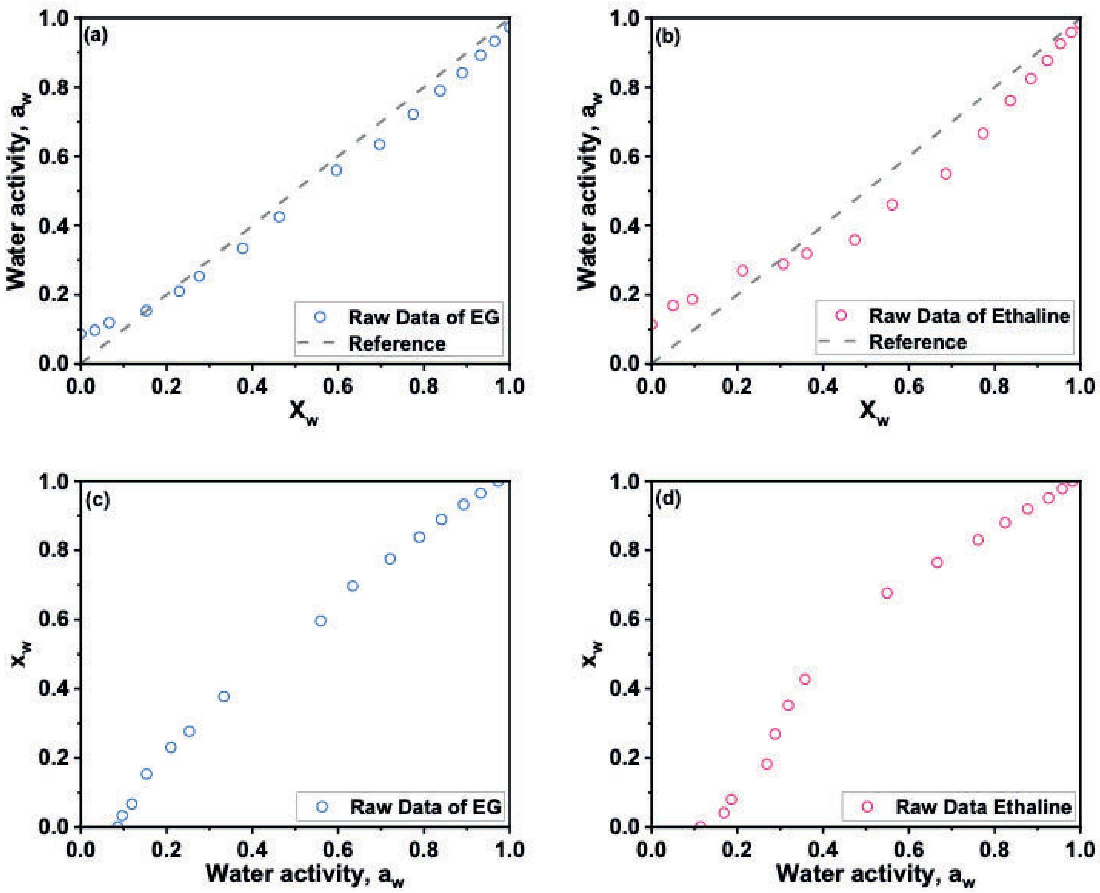

Figure 1. Water activities (a_w) of (a) ethylene glycol (EG) and (b) ethaline with varying mole fractions of water at 25 ^{0}C. Moisture sorption isotherm of (c) ethylene glycol (EG), and (d) ethaline. Each point on the graph represents the data collected at different water additions, from 0 wt.% to 100 wt.%.

The moisture sorption isotherms depicting the system's water content by weight are shown in **Figures 1c** and **1d**. According to **Figure 1c**, EG readily absorbs water, demonstrating a high affinity. In contrast, ethaline exhibits a low initial absorption rate, followed by a noticeable increase once more water is introduced. These observations help identify the point at which the energy of water begins to more rapidly with increase in moisture content, impacting processes such as hydrogen evolution or degradation and indicate how readily each solvent can take up and retain water and the corresponding changes in water energy in industrial applications. This information is invaluable for process development, where controlling water content and understanding solvent stability are both critical.

4. Possible Solutions

Accurate measurements of water activity directly address moisture-related issues because they are more sensitive to changes in the energy water than conventional dryness analyses at various water contents.[14,15] They can effectively monitor the solvent's water activity during cell fabrication, storage, and blend preparation, providing more precise humidity regulation. For example, carrying out critical procedures in a glove box can prevent moisture reabsorption that would otherwise negate earlier drying efforts. Furthermore, by detecting variations in water activity at an early stage, real-time adjustments can be made to vacuum drying or molecular sieve treatment to minimize residual moisture. Maintaining the energy of water below a certain threshold preserves the intended ionic pathways and redox window of the solvent, promoting stable device performance across a range of operating conditions.

In addition to strict humidity control, the performance of DESs can be improved through "electrolyte tailoring." Introducing co-additives with ionic interactions that compete for water can mitigate the adverse effect on the energy of water by trace moisture.[28,29] Alternatively, modifying functional groups in choline chloride or ethylene glycol can reduce changes in hydrogen bonding or viscosity upon water introduction.[30,31] Another strategy is to create hybrid mixtures by combining DESs with suitable co-solvents, thereby extending the electrolyte's stable operating range.[32] These modifications, coupled with precise water activity control, retain the advantage of DES-based electrolytes for large-scale battery systems.

5. Conclusion

Water activity measurements are ideal for investigating battery solvents, such as DESs or ionic liquids, which are regarded as viable options for battery electrolytes. By examining the water activity in such solvent systems, one can gain a deeper understanding of their performance as electrochemical systems in the presence/absence of water. This is extremely important since changes in the energy of water changes every physical parameter of these solutions. In particular, the electrochemical performance and stability can be affected directly by changes in water activity.

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