Advanced Electrolyte Model (AEM)

The Advanced Electrolyte Model (AEM) developed at the INL is a proven capability designed to explore molecular-to-macroscale level aspects of electrolyte behavior, and can be used to drastically reduce the time required to characterize and optimize electrolytes. Although it is applied most frequently to Li-ion and Na-ion battery systems, it is general in its theory and can be used toward numerous other targets.

Selected key features:

- The chemical physics or statistical-mechanical basis of the AEM is found in the non-primitive non-restricted associative form of the Mean Spherical Approximation (NPNRAMSA), a powerful computational approach to accurate interpretation of chemical physics behind real electrolyte systems. The NPNRAMSA enables robust predictions over solvent composition, salt concentration, temperature, and permittivity domains.
- Added to this is an ion-solvation equation of state (IS-EOS) that renders accurate values of various quantities tied to ion solvation in such systems, such as effective solvated ion sizes, solvent-ion binding energies, solvation numbers, etc. The effects of ion solvation are central to accurate prediction of all properties of electrolytes and lithium solvation/desolvation parameters.
- To address relevant contemporary electrolytes, the AEM accurately predicts properties of multiple-solvent systems (up to 5 solvents or more), and also handles two-salt systems.
- Key interfacial issues are targeted, including double-layer behavior, field effects on solvent in the presence of the SEI, and lithium desolvation.
- The double-layer regions can and should exhibit local regions of non-electroneutrality, and hence, the AEM was developed to predict properties for such conditions.
- Contributing theories and mathematics are seamlessly integrated and self-consistent.
- AEM Component Database covers many battery-relevant solvents and salts, and is growing.
- Predictions for many systems have average percent deviations with lab data that fall within 5-10%, with many conditions below 5% deviation. The model has been validated with scores of electrolyte systems over hundreds of unique conditions.
- The AEM has been used to help a growing list of private sector companies and DOE partners with electrolyte characterization and optimization, with more collaborations under development.

The AEM generates numerous separate reports, covering issues and quantities such as

1. Transport Properties (viscosity, conductivity, diffusivity, transference numbers, ionic hopping),
2. Thermodynamic Properties (activity coefficients, osmotic coefficient, osmotic pressure, etc.)
3. Ion Association Speciation (ion pairs, triple ions, solid solvates),
4. Solvent-to-ion Binding Energies and solvation numbers for both cations and anions,
5. Ligand-wise and net Lithium Desolvation energy and kinetics,
6. Relative molal enthalpy,
7. Solvent and Solution Permittivity, and related Dielectric Depression,
8. Transport Analysis of Double-Layer Regions and related electrolyte properties therein,
9. Attenuation of properties under Faradaic transport conditions,
10. Field Effects on solvent dipole orientation, considering both ionic and surface charge fields,
11. Arrhenius Analysis (activation energies) of ten foremost electrolyte properties,
12. Large-Scale Optimization of solvent composition, given a multi-solvent system (there are about ten distinct optimization parameters that are considered),
13. Summary of non-convergent cases,
14. and other quantities.

This disruptive capability is unique, powerful, relevant to present and future electrolyte development, and without peer. It redefines electrolyte modeling for highly-complex contemporary systems, *wherein significant steps have been taken to capture the reality of electrolyte behavior in the electrochemical cell environment.* This capability can have a very positive impact on accelerating domestic battery development to support aggressive vehicle and energy goals in the 21st century.

Dr. Kevin Gering is the sole developer of the AEM, and he can arrange to apply this state-of-the-art tool to systems of interest per your request.

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