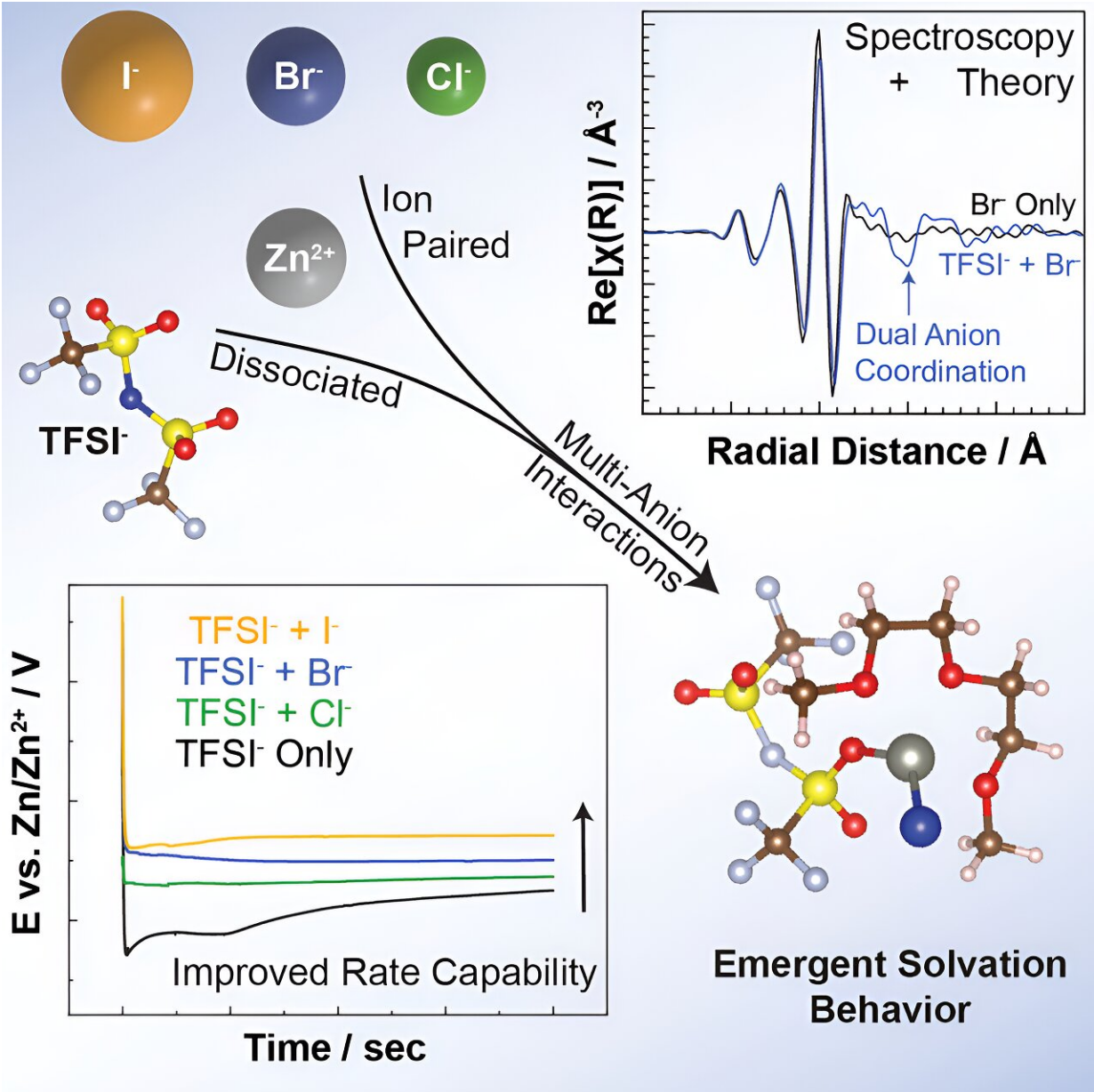


# A new blueprint for designing high-performance batteries

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Graphical abstract. Credit: *Chem* (2023). DOI: 10.1016/j.chempr.2023.03.021

A team of scientists at the U.S. Department of Energy's (DOE) Argonne National Laboratory discovered an intriguing cooperative behavior that occurs among complex mixtures of components in electrolytes in batteries. Electrolytes are materials that move charge-carrying particles known as ions between a battery's two electrodes, converting stored chemical energy into electricity.

The team found that combining two different types of anions (negatively charged ions) with cations (positively charged ions) can significantly improve the overall battery's performance. This suggests that careful selection of ion mixtures can enable battery developers to precisely tailor their devices to produce desired performance characteristics.

The study focused on a type of next-generation battery called the multivalent battery. Today's lithium-ion batteries have a limited ability to provide performance attributes needed in critical applications like passenger electric vehicles and storing renewable energy on the grid. Many researchers see multivalent batteries as a potential alternative.

These potentially game-changing technologies use cations such as zinc, magnesium and calcium that have a charge of +2 as opposed to +1 for lithium ions. By moving more charge, multivalent batteries can store and release more energy. This makes them attractive candidates to replace existing lithium-ion battery technologies in electric vehicles. They are also envisioned for grid storage.

Another advantage of multivalent batteries is that they use abundant elements supplied through stable, domestic supply chains. In contrast, lithium is less abundant and has an expensive, volatile international

supply chain.

## **The quest to advance multivalent batteries**

Optimizing how an [electrolyte](#) moves ions between battery electrodes is crucial for good performance and long lifetimes. This back-and-forth process results in the deposition and stripping of metal atoms on the surface of a battery's anode (negative electrode). A high-performance, long-lasting battery should be able to reversibly deposit and strip a uniform layer of metal for thousands of cycles.

Today, most multivalent batteries under investigation by researchers do not perform well, limiting their commercial viability. The ions and electrodes tend to be unstable and degrade. As a result, the electrolytes are unable to efficiently transport cations, diminishing the battery's ability to generate and store electricity.

Researchers need to know what causes the degradation and inefficiency. This requires a much deeper understanding of how cations interact with other ions, atoms and molecules in the electrolyte. Gaining this knowledge is particularly important as researchers explore electrolytes with more complex mixtures of cations and anions.

"We can design better electrolytes by better understanding the mechanisms that drive instability and inefficiency," said Justin Connell, a materials scientist on the research team and one of the study's authors.

## **Unexpected ion interactions**

One of the main candidates for a multivalent battery is based on zinc metal. The Argonne team sought to characterize the interactions that occur—and the structures that form—when zinc cations are combined

with two different types of anions in the electrolyte. They also wanted to know how these interactions can impact key aspects of battery performance, such as metal deposition and stripping at the anode.

The team designed a laboratory-scale battery system comprised of an electrolyte and zinc anode. The electrolyte initially contained zinc cations and an anion, called TFSI, with a very weak attraction to the cations. Chloride anions were then added to the electrolyte. Relative to TFSI, chloride has a much stronger attraction to zinc cations.

The researchers probed the interactions and structures among these ions with the use of three complementary techniques:

- X-ray absorption spectroscopy: Conducted at Argonne's Advanced Photon Source, a DOE Office of Science user facility, this technique involved probing the electrolyte with synchrotron X-ray beams and measuring the absorption of the X-rays.
- Raman spectroscopy: Conducted at Argonne's Electrochemical Discovery Laboratory, this technique illuminates the electrolyte with laser light and evaluates the scattered light.
- Density functional theory: Conducted at Argonne's Laboratory Computing Resource Center, this is a type of modeling that simulates and calculates the structures formed by the interactions among the ions in the electrolyte.

The team selected these techniques because they inform one another and together can provide a stronger validation of the conclusions.

"These techniques characterize different aspects of the ion interactions and structures," said Mali Balasubramanian, a physicist on the research team and one of the study's authors.

"X-ray absorption spectroscopy probes how atoms are arranged in

materials at very small scales. Raman spectroscopy characterizes the vibrations of the ions, atoms and molecules. We can use the data on atom arrangements and vibrations to determine whether ions are separated or move together in pairs or clusters. Density functional theory can corroborate these characterizations through powerful computation."

The team found that the presence of chloride induced TFSI anions to pair with zinc cations. This outcome is significant because the pairing of anions with a cation can affect the rate at which the cation can be deposited as metal on the anode during charging or subsequently stripped back into the electrolyte during discharge. Faster electrode reactions requiring less energy enable a more efficient conversion of [chemical energy](#) into electricity.

The team repeated these experiments with two other ion mixtures. In one mixture, bromide ions were used instead of chloride, and in the other, iodide ions were used instead of chloride. Like chloride, bromide and iodide attract strongly to zinc cations, though less strongly than chloride. The outcome was similar to what happened with chloride: bromide and iodide induced TFSI anions to pair with zinc cations.

"What was particularly exciting about this result is that we didn't expect to see what we saw," said Connell. "The idea that we can use one anion to draw a second anion closer to a cation was very surprising."

With all three combinations of ions, the researchers measured the electrochemical activity at the interface between the electrolyte and the anode. Electrochemical activity involves the conversion of chemical energy into electricity. Bromide and iodide were more active than chloride because they held zinc cations less strongly. In other words, it took less energy to add electrons to the cations, pull zinc metal out of solution and deposit it on the anode. In practical terms, this can enable a zinc-ion battery to charge and discharge more quickly.

## Cooperation among ions

A fascinating aspect of the study's conclusions is the cooperation that occurred among different types of ions in an electrolyte. The Argonne researchers believe that the presence of the weakly attracting anions reduced the amount of energy needed to pull zinc metal out of solution. Meanwhile, the presence of the strongly attracting anions reduced the amount of energy needed to put the zinc back in solution. Overall, less energy was needed to drive this back-and-forth process and enable a constant flow of electrons (electrical current).

The discovery of this behavior points to an exciting new approach to designing electrolytes for advanced batteries.

"Our observations highlight the value of exploring the use of different anion mixtures in batteries to fine-tune and customize their interactions with cations," said Connell. "With more precise control of these interactions, battery developers can enhance cation transport, increase electrode stability and activity, and enable faster, more efficient electricity generation and storage.

"Ultimately, we want to learn how to select the optimal combinations of ions to maximize battery performance," Connell added.

As a research next step, Connell said it would be worthwhile to investigate how other multivalent cations like magnesium and calcium interact with various anion mixtures.

Another new line of research at Argonne involves the use of machine learning to rapidly calculate the interactions, structures and electrochemical activity that occur with many different ion combinations. The aim would be to accelerate the selection of the most promising combinations.

"Researchers can't study everything in laboratory experiments," said Darren Driscoll, a research team member and the study's lead author. "There are too many possible combinations of ions to consider and not enough manpower to synthesize them and measure the resulting interactions."

"If a machine learning study were to look at 1,000 different combinations of [ions](#) and find five promising combinations, an experimental scientist could then take a closer look at those five in the laboratory," said Lei Cheng, a chemist on the team and one of the study's authors.

The Advanced Photon Source is undergoing an extensive upgrade that will increase the brightness of its X-ray beams by up to 500 times. "The upgrade could enable more advanced analyses of electrolyte behaviors, such as how complex anion-[cation](#) structures and ion motion change over time," said Balasubramanian.

This research is published in [Chem](#). The study's other authors are Sydney Lavan, Milena Zorko, Paul Redfern, Stefan Ilic, Garvit Agarwal, Timothy Fister, Rajeev S. Assary and Dusan Strmcnik.

**More information:** Darren M. Driscoll et al, Emergent solvation phenomena in non-aqueous electrolytes with multiple anions, *Chem* (2023). [DOI: 10.1016/j.chempr.2023.03.021](https://doi.org/10.1016/j.chempr.2023.03.021)

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