New hydrodynamic theory helps to understand the correlation of ions

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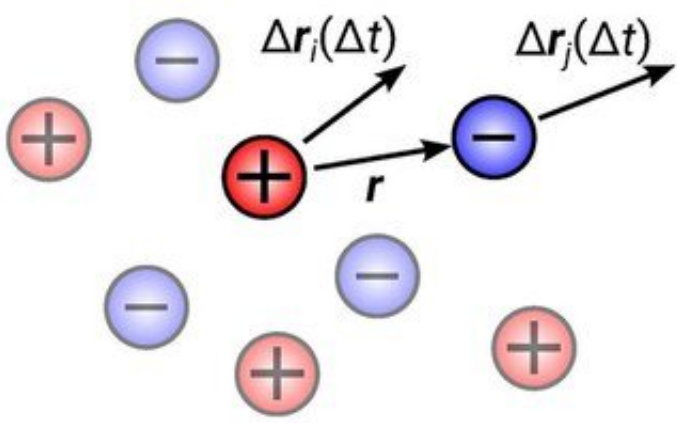

Credit: HI MS/Diddo Diddens

In their theoretical work, Dr. Diddo Diddens from Helmholtz Institute Münster of Forschungszentrum Jülich and Prof. Andreas Heuer from the Helmholtz Institute Münster and the Institute of Physical Chemistry of the University of Münster investigated the central question of the extent to which ions in liquid electrolytes move statistically correlated, i.e. together, in one direction.

With this knowledge, the influence of individual factors, such as ion pairs on conductivity, can be better determined. The detailed results of their study have been published in the *Journal of Chemical Physics* and

on the pre-print server *arXiv*.

It is often assumed that two ions with the same charge avoid each other due to mutual repulsion and thus move in opposite directions. Now, the researchers are able to show that two neighboring ions with the same charge move in the same direction.

"This counter-intuitive behavior can be explained by the fact that the electrolyte, as a liquid, is incompressible, unlike gases. Therefore, a single ion can only move as its molecular environment allows," Diddens explains.

In contrast, the electrostatic interactions—repulsion of equally charged ions, attraction of unequally charged ions—primarily influence the local arrangement of the ions, but less so the statistically correlated movement of neighboring ions.

Molecular dynamics simulations are often used in battery research to determine how strongly correlated individual ions move in certain electrolytes. However, the movements are often difficult to interpret. Diddens and Heuer have now developed a new theory that predicts how much two ions move statistically correlated (together) depending on their distance.

With the help of the theory, the influence of individual factors, such as ion pairing on conductivity, can be better determined. The hydrodynamic effects are universal in liquids. Thus, they occur in many electrolytes, including certain polymers.

Determining the collective ion dynamics helps to understand how efficiently an electrolyte can transport a certain type of ion, for example lithium ions in lithium-ion batteries, and thus improve the fast-charging behavior of a battery cell, among other things. The knowledge can be

used for the design of new types of electrolytes.

More information: Diddo Diddens et al, Hydrodynamic Interactions in Ion Transport—Theory and Simulation, *arXiv* (2023). DOI: 10.48550/arxiv.2302.10330

Diddo Diddens et al, Hydrodynamic interactions in ion transport—Theory and simulation, *The Journal of Chemical Physics* (2023). DOI: 10.1063/5.0147339