Modelling reveals new insight into the electrical conductivity of ionic liquids

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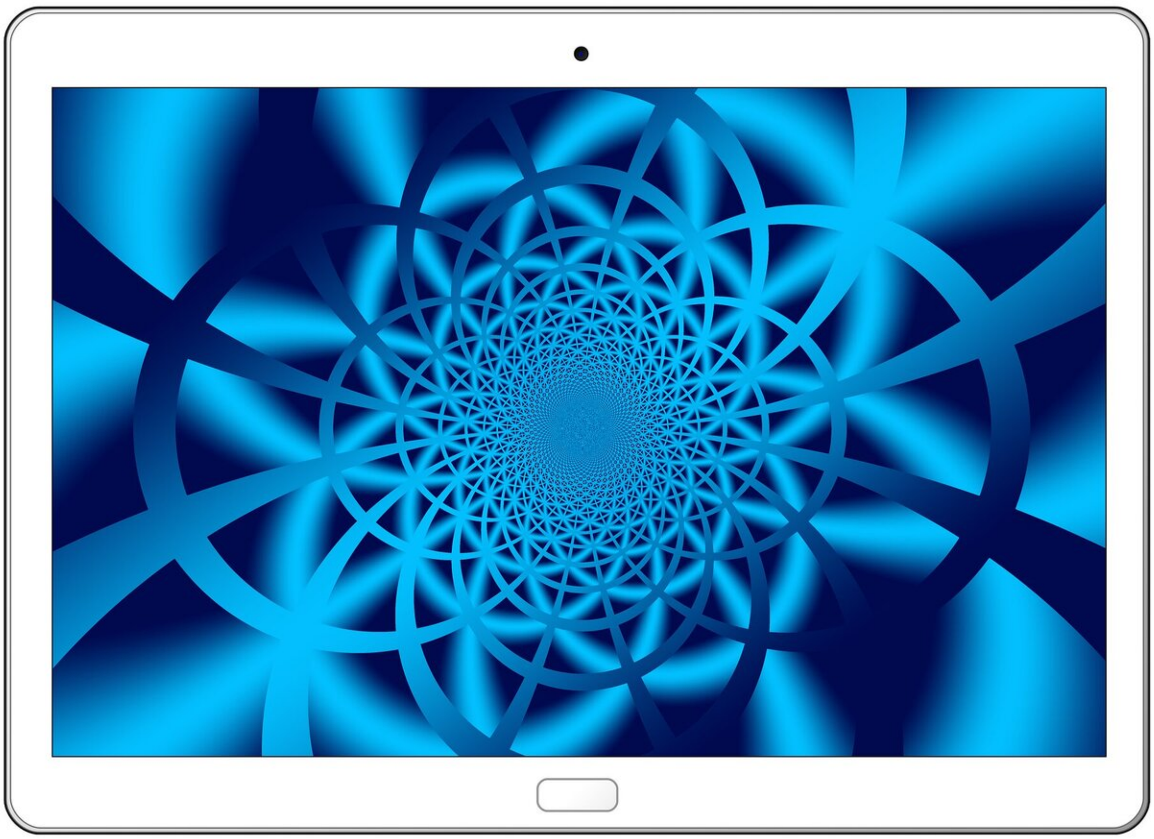

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A collaborative investigation has revealed new insight into how room temperature ionic liquids (RTILs) conduct electricity, which may have a great potential impact for the future of energy storage.

The research focuses on the debate surrounding the physical mechanism of the electrical conductivity of RTILs. Their charged positive and negative organic ions lead them to be good conductors, but the conductivity seems paradoxical. Their high conductivity arises from their high density of charged ions within the liquid, but this density should also mean that the positive and negative ions are close enough to neutralise one another, creating new, neutral particles which cannot support an electrical current. The modelling attempts to identify how conductivity is maintained in RTILs in light of these contradictory factors.

The research involved an international group of researchers, including Professor Nikolai Brilliantov of the University of Leicester and led by Professor Alexei Kornyshev of Imperial College London and Professor Guang Feng of the Huazhong University of Science and Technology.

Researchers elaborated special numerical methods and theoretical approaches to trace the dynamics of particles in RTILs. They discovered that, most of the time, positive and negative ions reside together in neutral pairs or clusters, forming a neutral substance which cannot conduct electricity. From time to time however, positive and negative ions emerge by pairs as charged particles in different parts of the liquid, making the liquid conductive.

The emergence of these ions is caused by thermal fluctuations. Suddenly and randomly the ions receive a portion of energy from the surrounding fluid, which helps them to release themselves from the "paired" neutral state and become free charged particles. This state is only temporary, however: after some time, they will return back to their paired neutral state as they join with another ion of opposite charge.

As this happens, another ionic pair elsewhere in the liquid is splitting into free charged particles, thereby sustaining the conductivity of the liquid and its electrical current in a kind of ongoing "relay race" of charges. This is similar to the behaviour observed in crystalline semiconductors, where the positive and negative charge carriers also emerge in pairs due to thermal fluctuations. It is therefore expected that a rich variety of physical phenomena observed in semiconductors might also be revealed in RTILs in the future.

Just as these phenomena in semiconductors are exploited for many applications, this research reveals that there may be potential too for RTILs to be exploited in new and innovative ways, with possible uses ranging from supercapacitors, fuel cells and batteries to various power devices.

Professor Brilliantov, Chair in Applied Mathematics and the University of Leicester's lead on the project, said: "Understanding of the conductivity mechanism of RTILs seems to open new horizons in designing ionic liquids with the desired electrical properties."

More information: Guang Feng et al. Free and Bound States of Ions in Ionic Liquids, Conductivity, and Underscreening Paradox, *Physical Review X* (2019). DOI: 10.1103/PhysRevX.9.021024

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