

New research findings could lead to safer and more powerful lithium-ion batteries

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Virginia Commonwealth University researchers are working to improve conductivity and safety in lithium-ion batteries, which are used to power many electronic devices around the world, including laptops, iPods,

satellites, artificial hearts and cell phones.

Instability in [lithium-ion](#) batteries due to liquid-state electrolytes that help carry charges from one battery electrode to another is one hazard scientists can prevent, said Puru Jena, Ph.D., a distinguished professor in the Department of Physics in the College of Humanities and Sciences. Despite this instability, liquid-state electrolytes are commonplace in lithium-ion batteries due to their conductive superiority over more stable solid-state electrolytes.

Theoretical studies by Jena and colleague Hong Fang, a postdoctoral fellow in the Department of Physics, show it is possible to design solid-state electrolytes not only to be as conductive as their liquid counterparts but also very stable. Their findings, which were published in the *Proceedings of the National Academy of Sciences* this month, could lead to safer and more powerful lithium-ion batteries.

"Theoretically, you can have your cake and eat it too, when it comes to the stability and conductivity," Jena said.

Electrolytes, which are central to a battery, are salts composed of positive and [negative ions](#). Positive ions are atoms that have more protons than electrons, while negative ions inversely have more electrons than protons.

In a lithium-ion battery, positive lithium ions flow between electrodes via electrolytes. Lithium ions can flow freely through liquid-state electrolytes but are less mobile in a solid-state [electrolyte](#), which adversely affects conductivity.

To improve the conductivity in [solid-state electrolytes](#), the researchers produced a computational model in which a single negative ion is removed. Negative cluster ions—groups of atoms with more electrons

than protons—replace the absent ion.

The scientists conceptualized a twist on a specific solid-state electrolyte previously tested by other researchers. Originally, the electrolyte, which belongs to a family of crystals called antiperovskites, contained positive ions made of three lithium atoms and one oxygen atom. The positive ions were joined with a single chlorine atom that was a negative ion.

In the computational model, the chlorine atom is replaced by a negative cluster ion created by one boron atom and four fluorine atoms joined to the existing [positive ions](#).

Other combinations of negative cluster ions were identified to potentially enhance conductivity.

"Replacing the chlorine ion with cluster ions improves [conductivity](#) because these ions are larger and allow the lithium ions to move quickly, as if they were in a liquid," Fang said.

Jena and Fang are now in search of collaborators to test their computational model in a laboratory setting for eventual [lithium-ion battery](#) applications.

More information: Hong Fang et al, Li-rich antiperovskite superionic conductors based on cluster ions, *Proceedings of the National Academy of Sciences* (2017). [DOI: 10.1073/pnas.1704086114](https://doi.org/10.1073/pnas.1704086114)

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