# 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

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