

## Rechargeable Solid-State Batteries – Millisecond Ion-Transport in Solid Electrolytes

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Rechargeable Li-ion batteries have performed admirably as the linchpin technology enabling today's mobile electronics industry, currently powering hundreds of millions of laptops, cameras, and phones worldwide. However, the energy density required for stationary energy storage devices and electric vehicles are quickly exceeding the limits of what can be achieved by commercial Li-ion batteries. Finding alternatives to the Li-ion battery is a crucial priority in the diversification and modernization of energy storage technologies. Indeed, when life-cycle analysis is examined in the design of batteries, sodium (Na) appears attractive because it can be "harvested" directly from seawater, making Na ~50 times lower in cost than Li.

An important class of phosphate electrodes and electrolytes discovered by Hong and Goodenough is the Natrium Super Ionic CONductors (NaSICONs), with chemical formula  $\text{Na}_x\text{MM}'(\text{XO}_4)_3$ , where M and M' are transition metals and X = Si, P and/or S. NaSICON electrode materials and electrolytes typically display significant Na-ion mobility. In this talk the speaker will show that computational materials science, in particular first-principles methodologies, can guide the design of better NaSICON electrode and electrolyte materials, with superior energy densities and improved ion transport. For example, the speaker and his team's predictions indicate that suitably doped NASICON compositions, especially with high silicon content, can achieve high  $\text{Na}^+$  mobilities.

These findings are relevant for the optimization of mixed polyanion solid electrolytes and electrodes, including sulfide-based polyanion frameworks, which are known for their superior ionic conductivities.



### Introduction of speaker

Pieremanuele (Piero) Canepa is an Assistant Professor in the Department of Materials Science and Engineering at the National University of Singapore. Piero is part of the Singapore-MIT Alliance. Previously, he was a Postdoctoral fellow under the guidance of Prof. Gerbrand Ceder initially at the Massachusetts Institute of Technology and later at Lawrence Berkeley National Laboratory. He received his bachelor's and master's degrees in Chemistry from the University of Torino (Italy) and his Ph.D. from the University of Kent (United Kingdom). His research contributes to the rational design of new materials for clean energy technologies, such as electrode materials for batteries, ionic conductors, and liquid electrolytes for sustainable energy storage devices. In March 2020, Piero was awarded the National Research Fellowship and equivalent to NSF CAREER in the US (or the ERC in Europe). In 2021 he was elected Fellow of the Royal Society of Chemistry and in 2022 a Materials Au Rising Star from the American Chemical Society.

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