

Materials Engineering Program Texas Center for Superconductivity at Univ. of Houston Center for Integrated Bio and Nano Systems 10:00 am, Friday, Sept. 8, 2023

This seminar will be held in hybrid mode: in person at HSC 102 Online: zoom link: <u>https://uh-edu-cougarnet.zoom.us/j/97136580701</u> Meeting ID: 971 3658 0701

The Rise of Sodium-ion Batteries

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Abstract: Powering hundreds of millions of laptops, cameras, and phones worldwide, rechargeable Lithium(Li)-ion batteries have performed admirably as the linchpin technology enabling today's mobile electronics industry. However, the energy density required for stationary energy storage devices and electric vehicles is quickly exceeding the limits of commercial Li-ion batteries. Finding alternatives to the Li-ion battery appears a crucial priority in the diversification and modernization of energy storage technologies. Indeed, when the 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) and chemical formula Na_xMM' (XO₄)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, I 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, our predictions indicate that suitably doped NASICON compositions, especially with high silicon content, can achieve high 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.

Bio: Dr. Pieremanuele Canepa is an Assistant Professor in the Department of Materials Science and Engineering at the National University of Singapore. Pieremanuele is part of the Singapore-MIT Alliance. Previously, he was a Postdoctoral fellow under the guidance of Prof. 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, Pieremanuele was awarded the National Research Fellowship, which is equivalent to the ERC Starting grant in Europe. In 2021, Pieremanuele was elected Fellow of the Royal Society of Chemistry, and, in 2022 a Materials Au Rising Star from the American Chemical Society.