Overcoming limitations of Li-ion batteries with first-principles calculations
By Dr. Pieremanuele Canepa

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Host: Prof Gong Hao

Abstract
After the rapid expansion of Li-ion in the portable electronics industry over the past decade, Li-ion batteries have now made commercial deployment of electric vehicles an imminent reality. Since advancements at the materials level are approaching a fundamental limit in Li-ion batteries, achieving even higher energy densities has spurred on investigations into the so-called “beyond Li-ion” technologies. In this talk, I will discuss two technologies moving beyond the Li-ion architecture, namely (i) multi-valent ion and (ii) all-solid-state Li-ion batteries. Multi-valent (MV) ion intercalation batteries that replace Li+ ions with MV cations, such as Mg2+, constitute a promising approach to meet the high energy density requirements of the next generation of electrical devices. From the limited experimental studies performed to date, the feasibility of a battery technology based on multivalent intercalation is not yet clear. The cathode and the electrolyte represent the critical components of this technology. One of the most pressing challenges in achieving high energy density MV-ion systems is to develop suitable cathode materials with a high enough voltage and diffusivity for the MV cation. I will present a detailed analysis, based on first-principles density functional theory calculations, of multivalent ion intercalation in a range of promising cathode materials and electrolytes. The discussion will then move to all-solid-state batteries, where the conventional flammable Li-ion liquid electrolyte is replaced by safer solid-electrolytes. The results will demonstrate that computational materials science is a powerful tool for developing and optimizing new materials for energy storage and conversion applications. I will elucidate the crucial role of high-throughput informatics combined with modern computational materials science techniques, to rationalize complex experimental findings, pushing the boundaries of materials science.

Biography of Speaker
Pieremanuele Canepa is an independent Ramsay Memorial fellow at the University of Bath, United Kingdom, and was a postdoctoral fellow at Lawrence Berkeley National Laboratory and the Massachusetts Institute of Technology (MIT) under Prof. Gerbrand Ceder. His research covers the assessment of materials as novel electrode and solid ionic conductors for intercalation batteries as well as the rationalization of the complex structure of liquid electrolytes. In November 2012, he was awarded a Ph.D. in Chemistry from the University of Kent, United Kingdom. He holds a M.Sc. (Hons) and B.Sc. (Hons) in Chemistry from the University of Turin, Italy.