Challenges in Developing Next-Generation Battery Technology

Gerbrand Ceder
Massachusetts Institute of Technology

I will present the principles of chemical energy storage and highlight the challenges and opportunities to develop storage with significantly higher energy and power density. While in principle most reversible chemical reactions could be used to store electrical energy, Li-ion cells have the particular advantage of combining high energy density with good kinetics and reversibility. This makes Li the technology to beat for future energy storage systems. Many of the critical performance metrics of battery material can be traced back to fundamental physics or materials science phenomena, such as electron transfer and correlation, ion diffusion, and phase transformation kinetics. Unless these are better understood and controlled so that materials can be designed rather than discovered, progress will only occur at the slow pace that has been characteristic of most historic materials developments. Such a pace is likely to be too slow to have any impact on climate change.

Lithium cells with double or triple the energy density of current batteries can however be conceived and I will demonstrate what the essential building blocks of such cells would be. In the search for better energy storage materials and systems, computational modeling may play a significant role. It can lead to the fundamental understanding of battery materials that is needed to rationally design novel materials.

Because of its scalability, computational design and searching can be performed in a large-scale, high-throughput fashion, unlike experimental approaches. Using some basic statistics, I will demonstrate that a large fraction of the possible compounds in nature can reasonably be scanned for their energy storage characteristics using computational ab initio methods.