Gerbrand Ceder receives 2016 Materials Theory Award

The Materials Research Society (MRS) has named Gerbrand Ceder, of the University of California, Berkeley, and Lawrence Berkeley National Laboratory, as the recipient of the 2016 Materials Theory Award "for developing methods that enable the field of computationally guided materials design, including the prediction of functional, thermodynamic, and kinetic properties, their integration with experiment, and the field of high-throughput computation." Ceder will be recognized at the 2016 MRS Fall Meeting in Boston. The Materials Theory Award, endowed by Toh-Ming Lu and Gwo-Ching Wang, "recognizes exceptional advances made by materials theory to the fundamental understanding of the structure and behavior of materials."

Ceder has integrated physics, chemistry, mathematics, and materials engineering into approaches that can computationally predict novel materials' behavior and create a virtual laboratory for improved understanding and design of technologically important materials. With his understanding of how to connect the physics side with materials science and engineering, the field of *ab initio* computation has made computationally driven materials design a practical reality.

As an assistant professor at the Massachusetts Institute of Technology in the early 1990s, Ceder made *ab initio* approaches applicable to the complexity of technologically relevant materials, as reflected in his developments on methods to predict the ground states of multi-component cluster expansions, the effects of vibrations in phase diagrams, electronic entropy, and the coupled cluster expansion technique to study coupled disorder in the cation and anion sublattice of oxides and chalcogenides. Most of today's understanding of ionic transport in lithium cathodes is due to his group's early discovery of the divacancy-mediated Li diffusion mechanism in layered oxides and, more recently, the theory for Li percolation in disordered cathode oxides. Between 2008 and 2010, he developed macroscopic models showing that diffusion in materials with one-dimensional channels become slow diffusers at the macroscopic scale. Utilizing the design metrics uncovered by the model, Ceder was able to demonstrate very high rate transport in lithium-ion batteries.

In the early 2000s, Ceder coupled rapidly increasing computing power with the methods he was using, thus spearheading the field of computationally aided materials discovery and design. His groundbreaking efforts in this field were made through development of high-throughput computational methodologies, combined with techniques from the data sciences to mine computational data in the discovery of optimal materials for targeted applications. This area of research has recently become a widespread activity in computational materials science, popularized in part by the creation of the Materials Genome Initiative.

Ceder has led the field by successfully demonstrating the approach on predicting and designing novel or optimized compounds. While "big data" and "data mining" are considered newer ideas in materials science, Ceder's work in this area, which dates back to 2003, showed for the first time how data mining of results from high-throughput density functional theory calculations could be used to predict the energy of unknown compounds.

In 2006, he demonstrated how statistical learning methods trained on large amounts of known crystal structures could drive first-principles computations rapidly toward the correct ground state for a new chemistry, as such integrating data mining and machine learning as new concepts in materials theory. His leadership in computationally driven materials discovery and design inspired the Office of Science and Technology Policy to launch the Materials Genome Initiative.

Ceder's research is currently focused on applying *ab initio* methods and data-driven approaches to better understand and accelerate the synthesis of novel materials. He has published more than 350 manuscripts and has received the TMS Morris Cohen Award, the MRS Gold Award, and the ECS Battery Research Award. He is a MRS Fellow and has been elected to the Royal Flemish Academy of Belgium for Science and the Arts.

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