Multi-university effort to advance materials, define the future of mobility

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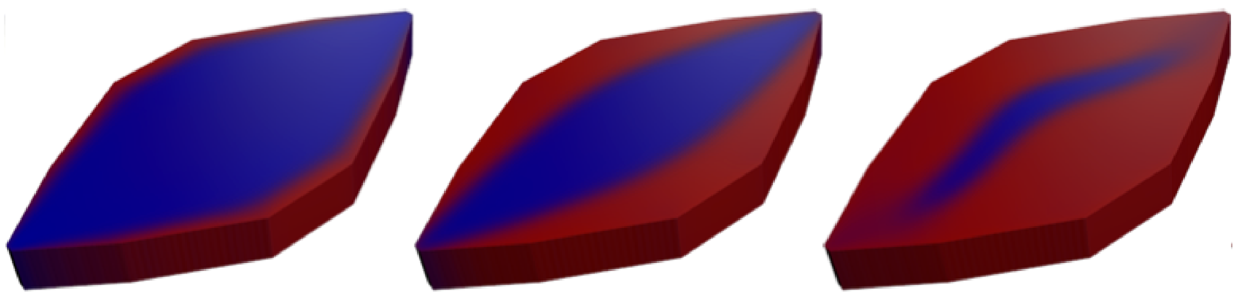


MIT professor Martin Bazant will use funding from TRI to leverage a nanoscale visualization technique that revealed, for the first time, how Li-ion particles charge and discharge in real time (as simulated above). By applying machine learning, he and his collaborators hope to develop a scalable predictive modeling framework for rechargeable batteries. Credit: Martin Bazant.

Three MIT-affiliated research teams will receive about $10M in funding as part of a $35M materials science discovery program launched by the Toyota Research Institute (TRI). Provided over four years, the support to MIT researchers will be primarily directed at scientific discoveries and advancing a technology that underpins the future of mobility and autonomous systems: energy storage.

MIT's Martin Bazant, joined by colleagues at Stanford and Purdue, will lead an effort to develop a novel, data-driven design of lithium-ion (Li-ion) batteries. These energy storage workhorses, used in cell phones and hybrid cars, are practical, but complicated due to the fundamental complexity of their electrochemistry. Leveraging a nanoscale visualization technique that revealed, for the first time, how Li-ion particles charge and discharge in real time, in good agreement with his theoretical predictions, Bazant will use machine learning to develop a scalable predictive modeling framework for rechargeable batteries.

"By applying machine learning methods to these videos of the inner workings of rechargeable batteries—using each pixel and each frame as a measurement—we can tease out models that better fit the experimental data," says Bazant, E. G. Roos (1944) Professor of Chemical Engineering and a professor of mathematics. "The approach has the potential to unify energy materials design by connecting atomistic with macroscopic properties and advance electrochemical materials more generally."

In addition to Bazant's endeavor, which also includes collaborator Richard Braatz, Edwin R. Gilliland Professor, two other MIT-affiliated projects will receive support from TRI. Jeffrey Grossman, Morton and Claire Goulder and Family Professor in Environmental Systems, and Yang Shao-Horn, W.M. Keck Professor of Energy, will lead the largest funded project focused on the design principles of polymer stability and conductivity for lithium batteries. The team also includes Jeremiah A. Johnson, Firmenich Career Development Associate Professor and Adam Willard, assistant professor, both in the Department of Chemistry, and machine learning and optimization expert, Suvrit Sra, principal research scientist in the Laboratory for Information and Decision Systems (LIDS) in the Department of Electrical Engineering and Computer Science.

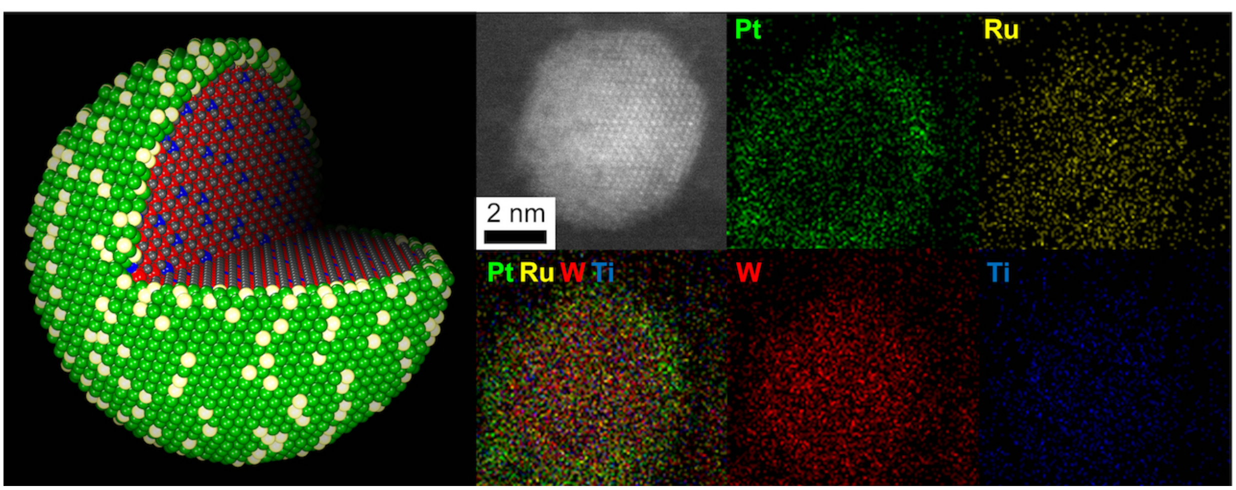
As part of a $35 million materials science discovery program The Toyota Research Institute (TRI) will support three MIT-affiliated projects directed at scientific discoveries and advancing a technology that underpins the future of mobility and autonomous systems, energy storage, such as rechargeable batteries used in hybrid and electric cars. Credit: Photostock.

Sra is excited about the research because it "brings together diverse expertise and offers a remarkable opportunity to develop machine learning models tuned to the problem, as well as large-scale discrete probability and optimization algorithms, topics that lie at the heart of my research." The long-term impact that machine learning, and more, broadly AI techniques, will have on materials discovery, he adds, extends well beyond this one project. Sra expects that in addition to accelerating materials discovery the methods he develops will lead to fundamental progress in machine learning too.

In addition to these lithium battery projects, Yuriy Román, associate professor in chemical engineering, will serve as co-lead investigator with Shao-Horn to explore the design principles of nanostructured, non-precious-metal-containing catalysts for oxygen reduction and evolution. Leveraging a novel synthesis route to create nanostructured catalysts with minute precious metals developed in the Roman lab, Roman and Shao-Horn will develop a predictive framework for catalytic activity. The researchers aim to identify new classes of stable, highly active electrocatalysts—essential components in renewable energy technologies like fuel cells, metal-air batteries and solar fuels—that are less expensive to produce and commercialize.

A nimble, flexible approach

While backed by a company known primarily for its cars, TRI's priorities are expansive, including artificial intelligence and computer science, home robotics and assistive technologies, and materials design and discovery.



With support from TRI, MIT faculty members Yuriy Román and Yang Shao-Horn will explore the design principles of nanostructured, non-precious-metal-containing catalysts for oxygen reduction and evolution. The researchers aim to identify new classes of stable, highly active electrocatalysts that are less expensive to produce and commercialize. Credit: Yang Shao-Horn

Bazant has been impressed by the flexibility TRI provides and by their comfort with backing fundamental science, practical application, as well as blue-sky ideas. "It's an unusual institute in terms of funding, unlike most government and industry avenues. We can set up teams that are not too big and more nimble, and each year we can revise our plan rather than be focused on a specific technology," he says.

Not bound to the typical "trial and error approach to product development and commercialization" Bazant and other faculty can focus on theory and simulation using data or explore the basic design principles of materials. In his case, that means the possibility of contributing to the design of a future hybrid car as well as advancing machine learning techniques for materials that go well beyond batteries.

"I'm confident we will push boundaries in basic scientific discoveries, nanomaterials, catalysis, and energy systems that go beyond just new innovation a few years down the road," adds Shao-Horn. All of the research findings supported by TRI will remain open and publishable in scientific journals.

"Accelerating the pace of materials discovery will help lay the groundwork for the future of clean energy and bring us even closer to achieving Toyota's vision of reducing global average new-vehicle CO2 emissions by 90 percent by 2050," said TRI Chief Science Officer Eric Krotkov in a prior press release.

Provided by Massachusetts Institute of Technology