Scientists harness machine learning to lower solar energy cost

By David Nutt

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A Cornell-led collaboration received a $3 million grant from the U.S. Department of Energy to use machine learning to accelerate the creation of low-cost materials for solar energy.

The three-year project, "Formulation Engineering of Energy Materials via Multiscale Learning Spirals," is led by principal investigator Lara Estroff, professor of materials science and engineering in the College of Engineering, in partnership with co-PI John Marohn, professor of chemistry and chemical biology in the College of Arts and Sciences, as well as researchers at University of Virginia, Johns Hopkins University, Lawrence Livermore National Laboratory (LLNL), National Renewable Energy Laboratory (NREL) and Pacific Northwest National Laboratory (PNNL). Those researchers include co-PI Paulette Clancy, the Samuel and Diane Bodman Chair of Chemical Engineering Emerita, now at Johns Hopkins University, and alumni Josh Choi, Ph.D. '12, with University of Virginia and David Moore, Ph.D. '14, of NREL.

The collaboration originated in an earlier project, funded by the Cornell Center for Materials Research (CCMR), which brought together a team that included Estroff's expertise in crystallization and structural characterization and Clancy's computational modeling of semiconductor materials, to explore a class of materials called hybrid organic-inorganic perovskites – crystal structures that can efficiently convert light into electricity.

This type of perovskite is especially noteworthy because it has the potential to be grown from solution, rather than processed with high temperature, and so can be manufactured via low-cost methods, such as inkjet printing and slot-die coating, on a wide range of substrates, Estroff said.

This makes perovskites bright candidates for photovoltaic cells. The reason the material is still in the lab and not in the solar panels on your roof is threefold: perovskites are difficult to scale up, they are unstable, and they are challenging to reproduce reliably.

"We think we can solve all of these problems," Marohn said. "This is like the dream team for solving them. You have people who have made breakthroughs in various areas. And now we get to put all of these breakthroughs together."

Estroff's lab, which has done extensive work in biomineral growth, previously observed how the crystalline precursors develop, which gave the researchers the idea that they might be able to steer how perovskites crystallize into a stable form that can operate better. The lab's work with Clancy found they could compute how the precursors form in different solvents, which suggested a possible role for large-scale machine learning to predict material synthesis. Marohn's group showed, by measuring the material's electronic properties, that when light is shined on perovskites, not only are electrons knocked loose, triggering electronic conductivity, but so are ions. The ionic conductivity could be one reason why the material has been unstable.

The role of machine learning is particularly crucial for growing perovskites that will have optimal performance in devices.

"If you start writing down the number of different combinations of atoms, and allow for substitutions, you very quickly reach half a million different compounds that you could make. And then if you add all the different solvents that you could use to make them, it just explodes," Estroff said. "Experimentalists like myself could never make all of the different materials that are possible. The diversity of compositions and processing routes makes this a problem waiting for machine learning and data science."

Equally important, Estroff said, is the continuous feedback loop that exists between the data scientists and the experimental scientists. The team's interdisciplinary model will not only advance knowledge of perovskites, but will also enable the researchers to apply their machine-learning framework to other solution-grown materials, such as hybrid Ruddlesden-Popper phases, also known as "2D perovskites."

The project is one of 10 that the Department of Energy is funding through a $26 million initiative to leverage cutting-edge research tools for clean energy solutions.

"Data science, and especially AI/ML, provides unique opportunities to leapfrog to novel capabilities for understanding fundamental properties and processes in physical and chemical systems," Steve Binkley, acting director of DOE's Office of Science, said in a press release. "This research will take advantage of the rapid growth of AI/ML to accelerate the discoveries needed for more efficient energy generation, storage, and use, while eliminating or reducing the emission of greenhouse gases and the use of critical resources."

The project team includes co-PI Rigoberto Hernandez from Johns Hopkins University, and co-investigators Rebecca Lindsey with LLNL and Jinhui Tao with PNNL.

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