AI-fueled batteries

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"Otto" is a robotic platform integrated with machine learning to optimize electrolytes for batteries. Credit: College of Engineering, Carnegie Mellon University

Machine learning is increasingly being used as a tool that helps researchers discover new materials and compounds for their unique design requirements. This novel approach cuts down the time researchers spend creating and experimentally testing various materials, so new discoveries can be made faster. At Carnegie Mellon University,

mechanical engineering Ph.D. student and Tata Consultancy Services Presidential Fellow Adarsh Dave applied this approach to batteries and made a surprising discovery.

Dave was motivated by reducing greenhouse gas emissions, he said. Battery innovations are one easy way to reduce emissions. However, these innovations tend to happen very slowly because the chemistry is quite complex, so the team began looking for ways to speed it up. This research focused on aqueous electrolytes, which Dave says are well-suited for storing renewable energy.

"Designing high-performing aqueous batteries is an important process to solve," Dave said. "However, there is a staggering amount of possible formulations here to choose from—that's where our design process comes in."

Dave and his teams built a robotic platform, named "Otto," to characterize battery electrolytes by measuring properties that determine if it will be effective in batteries. The machine learning is integrated with Otto, and together they optimize electrolytes for batteries. The computer tells Otto which electrolytes to test, then Otto tells the computer the properties of those electrolytes. This back and forth between Otto and the computer helps the machine learning run an optimization to find the best electrolyte. Otto can mix and test electrolytes about as fast as a human can, but unlike humans, Otto can run 24/7.

"Most battery labs design electrolytes with legions of graduate students making and testing various electrolytes," said Venkat Viswanathan, an associate professor of mechanical engineering at CMU. "We're just a team of three who've built a robot to do most of this work for us."

The implications of their research are already apparent. In a recently

published paper, Dave and his team present a "non-intuitive, novel electrolyte" that the machine learning revealed. Without their research, this electrolyte could have remained unknown to designers. This shows great promise for the future of machine learning in design processes. Additionally, Otto's automation can speed up the testing and experimentation process, allowing scientists to focus on the big picture research.

"While no robot or algorithm will replace a highly-trained chemist's intuition for innovation, our system certainly automates and accelerates routine science and design tasks," said Jay Whitacre, director of the Scott Institute for Energy Innovation and professor of engineering and public policy and material science engineering. "I hope to see my colleagues in other labs automate away the boring stuff, and really accelerate the pace of battery innovation."

The paper was published in *Cell Reports Physical Science* in November 2020. Other authors include CMU Ph.D. students Kirthevasan Kandasamy, Han Wang, Sven Burke, and Biswajit Paria and Associate Professor Barnabás Póczos. Materials science researcher Jared Mitchell also contributed to the project.

More information: Adarsh Dave et al. Autonomous Discovery of Battery Electrolytes with Robotic Experimentation and Machine Learning, *Cell Reports Physical Science* (2020). DOI: 10.1016/j.xcrp.2020.100264

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