Converting renewable electricity into stable molecules could provide long-term energy storage

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For renewable energy and energy storage technologies, variation is the name of the game.

The intensity of the natural resources that provide renewable energy varies from day to day, as well as season to season. Spring brings high winds to scour the deserts and fills rivers with snowmelt. Summer is synonymous with long sunlit hours before the days shorten as fall transitions into winter.

We need a multitude of ways to store renewable energy that match how we use it, from batteries to fuel cells. Batteries work well for shorter duration storage, on the order of hours to days. Of the different methods for storing renewable energy, one stands out for providing a way to hold on to energy for months at a time: storing energy in the chemical bonds of molecules such as hydrogen.

Through decades of fundamental research, scientists at Pacific Northwest National Laboratory (PNNL) have contributed detailed information about how catalysts help convert energy into molecular bonds, storing the energy by making bonds and releasing it by breaking bonds.

Now, a team led by chemist and Laboratory Fellow Tom Autrey is working to turn chemical energy storage into practical setups that could one day help power neighborhoods, infrastructure, and industry. To do that, the team is studying entire systems, from catalysts to reactors to end products—and everything in between.

"Our work considers everything from electrons to dollars," said chemist Mark Bowden, a longtime contributor to the project. The interdisciplinary team combines knowledge in chemistry, engineering, technoeconomics, and theoretical calculations to examine the practical viability of chemical energy storage systems for large-scale storage.

The team will have a supportive home in PNNL's Energy Sciences Center, scheduled to open later this year. The building will host over 250 staff members and a suite of advanced scientific instruments previously scattered around campus, fostering a collaborative environment to build on the team's long history of progress. Research at the Energy Sciences Center will also include work focused on developing new catalysts for converting electricity into chemical bonds through the Center for Molecular Electrocatalysis.

Hydrogen as the starting point

Discussions involving chemical storage often revolve around hydrogen as the most promising molecule of all possibilities, noted Autrey. It can be produced by splitting water into hydrogen and oxygen gases before being used as a carbon-free energy source. In a fuel cell, hydrogen combines with oxygen to produce electricity and water.

However, storing pure hydrogen as a gas or liquid is logistically difficult, requiring either large, high-pressure tanks or very low temperatures. Researchers are developing a variety of alternative storage solutions to hold hydrogen in molecules or materials.

At PNNL, Autrey and the team are developing hydrogen carrier systems that harness chemical reactions to add and remove hydrogen from stable molecules on demand. An entire subfield of chemistry studies the catalysts that perform hydrogen addition and removal. PNNL researchers specialize in designing catalysts that facilitate storing hydrogen in molecules such as formic acid, methylcyclohexane, and butanediol, among others.

PNNL chemist Ba Tran led work testing the suitability of hydrogen-rich ethanol, combined with an established catalyst, to cycle with ethyl acetate for long term storage. Hydrogen remains bonded to the ethanol until needed, when it can be released for use and the ethanol converted into ethyl acetate. The catalyst can add two molecules of hydrogen to a single ethyl acetate molecule, producing two stable ethanol molecules that store the hydrogens.

Analysis beyond the lab

In addition to understanding the fundamental chemistry of adding and releasing hydrogen from other molecules, Tran and his colleagues incorporated data from experimental measurements and advanced molecular simulations into studies of larger-scale systems. "We want to see how the process of storing hydrogen in ethanol—and other forms of chemical energy storage—would behave in an application-scale system," said theoretical chemist Samantha Johnson.

In the ethanol study, for example, the team analyzed a reactor design at a scale relevant for seasonal energy storage in a neighborhood. The chemistry of the reactions worked well and the project taught the team valuable lessons about the engineering needed for a practical system, taking them in new directions to explore different hydrogen carriers.

Grounding research in reality

Whether studying the molecular details of how a hydrogenation catalyst works or engineering a neighborhood-scale storage system, the researchers are always asking questions that will help move research from the lab into the world. The team takes a cyclical approach to problem solving, where different portions of their research inform one another and create a more complete picture of how an energy storage system works. And bringing together researchers with diverse technical backgrounds allows the team to identify solvable problems or challenges for the broader energy storage field.

The collaborative atmosphere and additional instrumentation of the new

Energy Sciences Center fits with the work the team performs. Their project is part of the wide range of energy-related research at PNNL that will be accelerated by the presence of the new building. The Energy Sciences Center brings together researchers with different specialties to encourage collaboration. Said Autrey: "We want to help move our society towards a future focused on renewable energy."

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