'Artificial leaf' moves closer to reality

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An important step toward realizing the dream of an inexpensive and simple "artificial leaf," a device to harness solar energy by splitting water molecules, has been accomplished by two separate teams of researchers at MIT. Both teams produced devices that combine a standard silicon solar cell with a catalyst developed three years ago by professor Daniel Nocera. When submerged in water and exposed to sunlight, the devices cause bubbles of oxygen to separate out of the water.

The next step to producing a full, usable artificial leaf, explains Nocera, the Henry Dreyfus Professor of Energy and professor of chemistry, will be to integrate the final ingredient: an additional catalyst to bubble out the water's hydrogen atoms. In the current devices, hydrogen atoms are simply dissociated into the solution as loose protons and electrons. If a catalyst could produce fully formed hydrogen molecules (H_2), the molecules could be used to generate electricity or to make fuel for vehicles. Realization of that step, Nocera says, will be the subject of a forthcoming paper.

The reports by the two teams were published in the journals *Energy & Environmental Science* on May 12, and the *Proceedings of the National Academy of Sciences* on June 6. Nocera encouraged two different teams to work on the project so that each could bring their special expertise to addressing the problem, and says the fact that both succeeded "speaks to the versatility of the catalyst system."

Ultimately, Nocera wants to produce a low-cost device that could be used where electricity is unavailable or unreliable. It would consist of a glass container full of water, with a solar cell with the catalysts on its two sides attached to a divider separating the container into two sections. When exposed to the sun, the electrified catalysts would produce two streams of bubbles — hydrogen on one side, oxygen on the other — which could be collected in two tanks, and later recombined through a fuel cell or other device to generate electricity when needed.

"These papers are really important, to show that the catalyst works" when bonded to silicon to make a single device, Nocera says, thus enabling a unit that combines the functions of collecting sunlight and converting it to storable fuel. Silicon is an Earth-abundant and relatively inexpensive material that is widely used and well understood, and the materials used for the catalyst — cobalt and phosphorus — are also abundant and inexpensive.

Putting it together

Marrying the technologies of silicon solar cells with the catalyst material — dubbed Co-Pi for cobalt phosphate — was no trivial matter, explains

Tonio Buonassisi, the SMA Assistant Professor of Mechanical Engineering and Manufacturing, who was a co-author of the PNAS paper. That's because the splitting of water by the catalyst creates a "very aggressive" chemical environment that would tend to rapidly degrade the silicon, destroying the device as it operates, he says.

In order to overcome this, both teams had to find ways to protect the silicon surface, while at the same time allowing it to receive the incoming sunlight and to interact with the catalyst.

Professor of Electrical Engineering Vladimir Bulović, who led the other team, says his team's approach was to form the Co-Pi material on the surface of the silicon cell, by first evaporating a layer of pure cobalt metal onto the cell electrode, and then exposing it to a phosphate buffer solution under an electrical charge to transform it into the Co-Pi catalyst. By using the layer of Co-Pi, now firmly bonded to the surface, "we were able to passivate the surface," says Elizabeth Young, a postdoc who was the lead author of the E&ES paper — in other words, it acts as a protective barrier that keeps the silicon from degrading in water.

"Most people have been staying away from silicon for water oxidation, because it forms silicon dioxide" when exposed to water, which is an insulator that would hinder the electrical conductivity of the material, says Ronny Costi, a postdoc on Bulović's team. "We had to find a way of solving that problem," which they did by using the cobalt coating.

Buonassisi's team used a different approach, coating the silicon with a protective layer. "We did it by putting a thin film of indium tin oxide on top," explains Joep Pijpers, a postdoc who was the lead author of the PNAS paper. Using its expertise in the design of silicon devices, that team then concentrated on matching the current output of the solar cell as closely as possible to the current consumption by the (catalyzed) water-splitting reaction. The system still needs to be optimized, Pijpers says, to improve the efficiency by a factor of 10 to bring it to a range comparable to conventional solar cells.

"It's really not trivial, integrating a low-cost, high-performance silicon device with the Co-Pi," Buonassisi says. "There's a substantial amount of innovation in both device processing and architecture."

Both teams had to add an extra power source to the system, because the voltage produced by a single-junction silicon cell is not high enough to use for powering the water-splitting catalyst. In later versions, two or three silicon solar cells will be used in series to provide the needed voltage without the need for any extra power source, the researchers say.

One interesting aspect of these collaborations, says postdoc Mark Winkler, who worked with Buonassisi's team, was that "materials scientists and chemists had to learn to talk to each other." That's trickier than it may sound, he explains, because the two disciplines, even when talking about the same phenomena, tend to use different terminology and even different ways of measuring and displaying certain characteristics.

Portable power?

Nocera's ultimate goal is to produce an "artificial leaf" so simple and so inexpensive that it could be made widely available to the billions of people in the world who lack access to adequate, reliable sources of electricity. What's needed to accomplish that, in addition to stepping up the voltage, is the addition of a second catalyst material to the other side of the silicon cell, Nocera says.

Although the two approaches to bonding the catalyst with a silicon cell appear to produce functioning, stable devices, so far they have only been tested over periods of a few days. The expectation is that they will be stable for long periods, but accelerated aging tests will need to be performed to confirm this.

Rajeshwar Krishnan, Distinguished University Professor of Chemistry and Biochemistry at the University of Texas at Arlington, says it remains to be seen "whether this 'self-healing' catalyst would hold up to several hours of current flow … under rather harsh oxidative conditions." But he adds that these papers "certainly move the science forward. The state of the science in water photo-oxidation uses rather expensive noble metal oxides," whereas this work uses Earth-abundant, low-cost materials. He adds that while there is still no good storage or distribution system in place for hydrogen, "it is likely that the solar photon-to-hydrogen technology will ultimately see the light of day — for transportation applications — with the hydrogen internal combustion engine."

Meanwhile, Nocera has founded a company called Sun Catalytix, which will initially be producing a first-generation system based on the Co-Pi catalyst material, connected by wires to conventional, separate solar cells .

The "leaf" system, by contrast, is "still a science project," Nocera says. "We haven't even gotten to what I would call an engineering design." He hopes, however, that the artificial leaf could become a reality within three years.

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