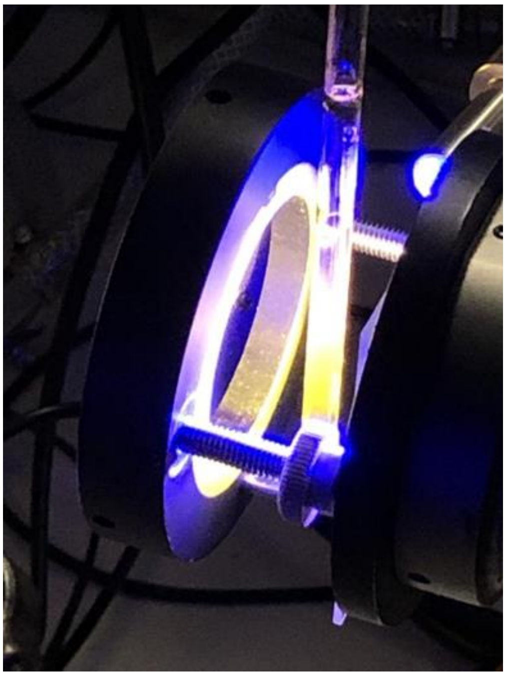
August 2021

Hurdle race to hydrogen - PhD student discovers a new type of H_2O splitting at LIKAT

Regine Rachow *Press Office*

It sounds simple, and nature shows us how: Green plants store solar energy by splitting water into hydrogen and oxygen - using light and chloroplasts. Researchers are excited to arrive at hydrogen gas (H_2) in a similar way, because produced "green" it is considered a protagonist of a sustainable energy and basic materials economy.

Jacob Schneidewind from the Leibniz Institute for Catalysis in Rostock has shown a way to achieve this with his dissertation. He uncovered the mechanism of a new type of water splitting that can make photolysis possible at low cost. The report on this appeared in the specialist journal ENERGY & ENVIRONMENTAL SCIENCE.



Excited by light in the blue and yellow spectral range: catalyst-water mixture during photolysis in the laboratory at LIKAT. (J. Schneidewind, LIKAT)

Green hydrogen can be produced in different ways. Electrolysis using a catalyst and electricity from the wind or sun is currently being used technically. More elegant and possibly more cost-effective, however, is photolysis, in which sunlight directly causes the splitting of water with the help of a catalyst - without a diversion via electricity from wind or solar plants. Under the keyword "artificial photosynthesis", chemistry is currently intensively exploring this photocatalytic path.

What it needs: Water, light source, catalyst

12 years ago, a team from the Weizmann Institute, Israel, reported in SCIENCE magazine on a chemical reaction in which a novel catalyst used light to split water. "But no one understood in what way this happened," says Dr Jacob Schneidewind. "The only thing that was clear was that no one had ever seen or described this type of water splitting. It is also completely different from natural photosynthesis."

Here was something fundamentally new to learn about water splitting. And to explore a new way to use these processes technically. For three years, Jacob Schneidewind studied the original reaction of his Israeli colleagues using water, a light source and a ruthenium catalyst for his doctorate at LIKAT. The goal was to elucidate the processes at the molecular level and to simulate the processes on the computer.

Four hurdles for photons

A short reminiscence of secondary school biology lessons: during photolysis in green plants, an oxygen molecule (O_2) is created from every two H_2O molecules, as well as exactly four protons of hydrogen (H^+) and four electrons (e^-). Jacob Schneidewind explains: "The energy for the release of the four electrons also comes from four absorbed light particles, the photons. To obtain enough photons, nature uses several absorbing centres."

You can think of the reaction as an energetic hurdle race, says Jacob Schneidewind. "There are then four hurdles to overcome before reaching the goal, i.e. the splitting of water. If even one of them is broken, photolysis fails - at least for this molecular bond." So much for the process in nature.

Original leaves questions unanswered

In the laboratory at the Weizmann Institute, however, photolysis did not occur at several absorbing centres, but only at a single point. "That seemed strange," says Dr Schneidewind. "That one catalytic centre alone would absorb four photons is extremely unlikely." Nor would the energy of a single photon be sufficient to jump all four hurdles. There was no meaningful explanation for this.

As a PhD student, Jacob Schneidewind worked his way into quantum chemistry and the kinetics of chemical reactions, which he used to model reactions on the computer. In the lab, he recreated the Israeli experiment with changing light sources, from short-wave, high-energy blue light to the low-energy red range. Colleagues at the University of Rostock took over the analyses using high-speed spectroscopy.

The solution: two hurdles are enough

"It surprised us all to see what was happening in the system," says Jacob Schneidewind. In fact, the photocatalytic pathway to hydrogen gets by with two photons instead of the usual four. And both the absorption of the photons and the actual fission reaction take place at a single centre, which consists of a pair of ruthenium atoms. "Once the first photon has cleared its hurdle, a new compound is formed that absorbs the second photon. And this requires even less energy for the second hurdle than was needed for the first hurdle." Thus, a wider bandwidth of light can be used, which can significantly improve efficiency.

Structurally, everything seems to be cleared up. What follows technically from this? "You could, for example, fill transparent plastic tubes with a suspension or solution of water and catalyst and expose them to the sun over a large area," says Dr Schneidewind. With the right catalyst, this approach would be three to four times cheaper than combining solar cells and an electrolyser. Starting in autumn, Jacob Schneidewind plans to develop a suitable catalyst for this with his own junior research group at RWTH Aachen University, where he moved after completing his doctorate.

Sustainable energy concepts assume, among other things, that in future green hydrogen will be produced in sunny regions and imported to Europe. The knowledge from LIKAT will help to develop appropriate technologies.

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Original publication:

DOI: 10.1039/d1ee01053k