UFRGS study changes the paradigm of clean energy production from photocatalysts

Researchers propose a different path that increases the efficiency of the technique of obtaining hydrogen as a source of chemical energy

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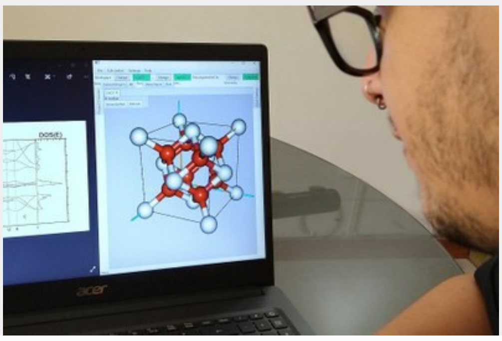
by Thiago Soria



The search for alternative energy sources is one of the biggest challenges in the world to reduce dependence on fossil fuels. In order to find these alternative energy sources, a study developed at the Laboratory of Physics of Nanostructures of the Institute of Physics at UFRGS showed how to increase the energy efficiency of photocatalysts to obtain chemical energy from photocatalysis. The process consists of breaking water molecules (H2O) with solar energy in order to get hydrogen, an atom with a high energy density that could be used as fuel in car engines, for instance, with no emission of CO2, one of the gases responsible for global warming. The research group increased the efficiency of the technique by decreasing the solar energy needed for the reaction to take place and increasing the production of hydrogen by about ten times. For this, due to its electronic structure suitable for the objectives of the study, ceria nanoparticles (also called cerium oxide) were used as photocatalysts. Ceria presents a microscopic mesoporous structure, unlike the commonly used titanium, which has a microporous structure. This structural change goes on the counter-intuitive path to what has been established in the literature.

Fabiano Bernardi, coordinator of the Laboratory and also professor at the Graduate Program in Physics at UFRGS, reports that two articles were written based on the findings of the studies *[see below]*, which began in 2018 and were developed in the chemistry and physics laboratories at UFRGS, and also in a physics laboratory at the Federal University of Minas Gerais (UFMG). Bernardi points out that a different way to increase the efficiency of the photocatalyst was possible due to the influence of oxygen on the reactions. Photocatalysis uses metallic oxide materials, which, therefore, are made up of oxygen. In microporous materials, such as titanium photocatalysts, the greater the absence (vacancy) of oxygen in the material, the greater the production of hydrogen. "However, we realized that this is a half-truth. In mesoporous materials like ceria, the exact opposite happens. The less vacancy, the greater the efficiency in producing hydrogen," he reports, explaining why the study shows a different path from what the literature has pointed out, in addition to being another reason for choosing ceria.

According to Fabiano, global energy consumption doubled from 1973 to 2015 and is expected to double again by 2050, if not before. "In a global energy crisis, the need to change the energy matrix is evident. Much of our energy production is based on fossil fuels, finite and pollutants. From that comes the idea of using solar energy," he explains. According to the professor, the annual global energy consumption is approximately equal to the energy that the Sun delivers to Earth in one hour. However, this problem is simply not resolved because, nowadays, the way this energy is managed is very inefficient. "It takes a small percentage [of the emitted solar energy], which is then transformed and very little is left over," he highlights.

The efficiency of photocatalysis

Wallace Figueiredo, one of the PhD students who participated in the study, declares that the group worked a lot with the water molecule's break to obtain hydrogen. He explains that the water molecule could be broken without a catalyst, but it would take a lot of energy, and the catalyst makes the breakage easier. In the case of the photocatalyst, the energy needed to break it comes from the Sun, a light source.

During the experiment, the water is placed in a sort of beaker, under a strong light that simulates the Sun. Ceria, which is a powder – colored from white to very light yellow tones – is dissolved directly in water and promotes a chemical reaction. There is also a sacrificial agent, another metal, so that oxygen is deposited there, while hydrogen (in this case, in the H2 form) is suspended in the air inside the container. The reaction goes on, and every thirty minutes, the concentration of hydrogen in the system can be measured. From the photocatalysis process comes the chemical energy that is the objective of the study. As Fabiano explains, for a water molecule to break, an electron-hole pair is needed: a "hole" where the particle was and the particle itself. This pair manages to keep breaking more and more molecules, releasing more hydrogen electrons. "The photocatalyst needs minimal energy coming from the sunlight or a similar energy source to generate the electron-hole and obtain hydrogen," he explains. However, the professor adds that one of the problems with the method is precisely in the photocatalyst material, because the minimum energy needed for this to happen is located at a high value within everything that the Sun delivers to Earth. The spectrum of sunlight has three levels, infrared (IR), visible light and ultraviolet (UV), each with an energy value. What happens is that these levels come in different proportions, such as: 50% IR, 40% visible light and 10% UV. Common photocatalysts need energy in the UV range to act. "As presented in the first article, we reduced the energy needed for the material, reaching the visible light range," Fabiano explains – based on a large atomic instability in the photocatalyst, possible due to the electronic properties of ceria.

Finally, besides requiring less energy, by using ceria, the group was also able to increase the production of hydrogen by about ten times – producing, therefore, more, with less energy. "It is important to emphasize that ceria is not the best material for photocatalysis. Usually an 'x' material is used, but we chose a 'y' material, not used, and realized that it is promising, and this is the way to optimize it. The course literature is taking is not quite right. The paradigm changes with what must be done to improve the efficiency of a material", concludes the professor.

National science

The articles were published in the international relevance *Journal of Materials Chemistry A*. According to Fabiano, the research group has about a dozen masters, PhD or undergraduate research students, working directly in the laboratories, in addition to other participations. "It is Brazilian-based scientific work, produced a little in each laboratory according to the potential that each one presents", explains the coordinator. He points out that the research was very efficient, as it was able to theoretically explain everything that was done experimentally, in addition to the fact that many techniques were studied. "We took a material and analyzed it in different ways: the surface part, the optics, the structure, the electronics… The result was efficient, internationally expressive, and it's all Brazilian scientific work," he says.

In view of the scientific challenge posed by the generation of clean and renewable energy, the group continues working to produce better materials in the direction of what was discovered with ceria and also materials to store H2, another problem involved in the issue of solar energy. "For some applications, producing H2 is not enough; it also has to be stored efficiently," concludes Fabiano, envisioning new scientific advances that are ecologically and efficiently promising.

JOURNAL ARTICLES

Thill, Alisson *et al.* **New horizons in photocatalysis: the importance of mesopores for cerium oxide.** Journal of Materials Chemistry A, 2020.

Thill, Alisson *et al.* **Shifting the band gap from UV to visible region in cerium oxide nanoparticles.** Applied Surface Science, 2020.

Translated into English by Júlia Moraes Alves, under the supervision and translation revision of Elizamari R. Becker (PhD) – IL/UFRGS.