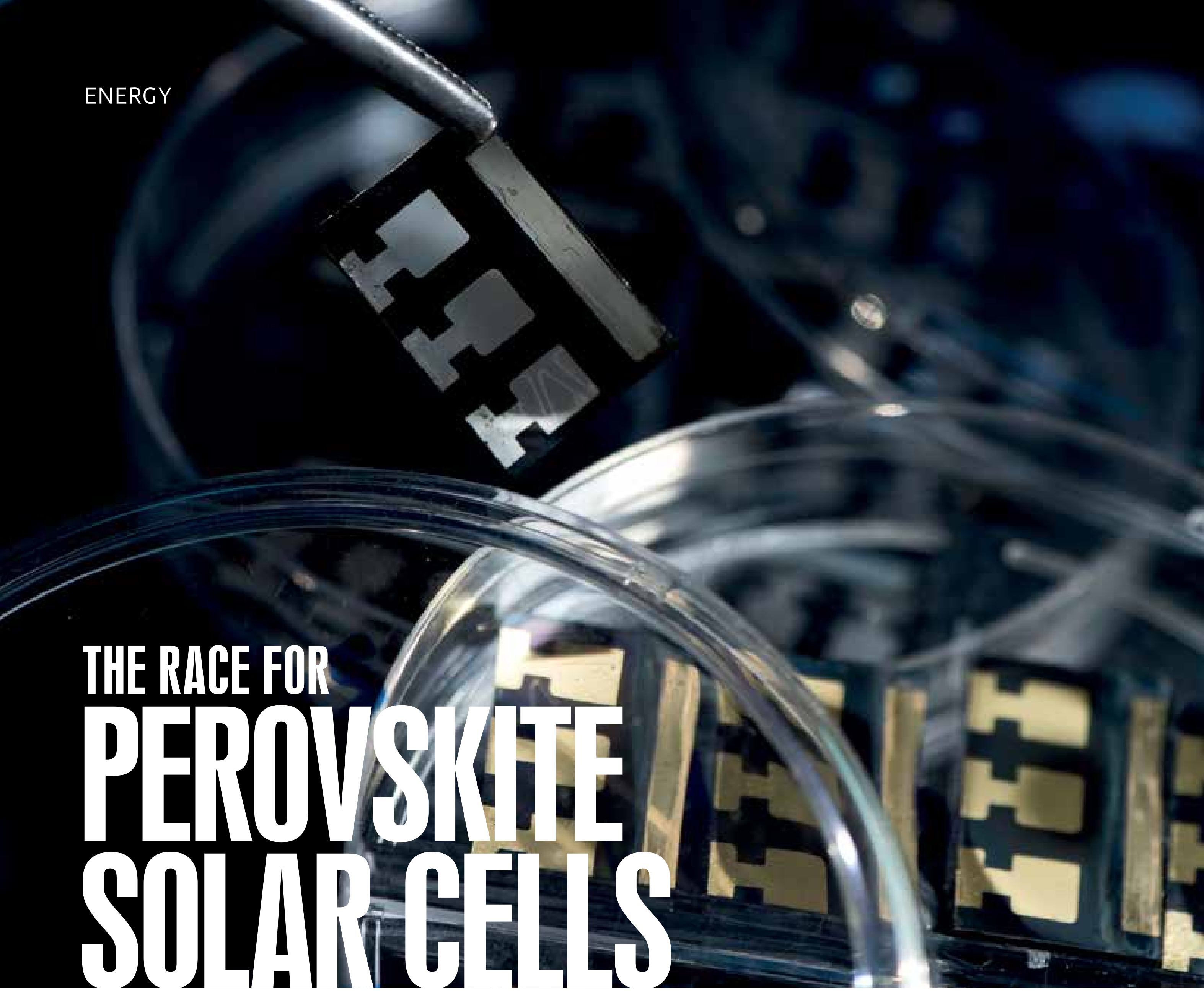


THE RACE FOR PEROVSKITE SOLAR CELLS

Brazilian research groups are helping to advance research on a promising class of materials for photovoltaic applications

Frances Jones

In the global race to develop new materials for clean and cost-effective energy solutions, a crystalline structure has shown promise as a semiconductor; industry experts believe that this semiconductor is set to become a primary raw material for a new generation of photovoltaic solar panels. Perovskite modules developed in laboratories using chemical compounds such as lead bromide, lead iodide, and cesium bromide have proven to be highly efficient in converting photon energy into electricity. The first research exploring the unique properties of perovskites was published in 2009, when a groundbreaking paper in the *Journal of the American Chemical Society* demonstrated their use for the first time as a component in photoelectrochemical solar cells. Since then, research groups worldwide have been studying perovskites.

Small-scale perovskite solar modules developed in a laboratory at the USP Institute of Chemistry

PHOTO LÉO RAMOS CHAVES / PESQUISA FAPESP MAGAZINE

Due to the rapid progress in the research and development of perovskite cells, their commercial viability has been the focus of researchers and startups (*see* Pesquisa FAPESP *issue no. 260*). In under 15 years, the conversion efficiency of these solar cells—which have the advantage that they can be made flexible, lightweight, and transparent—has increased from 3.8% to 26.1%. These levels were achieved using modules with relatively small surface areas. In comparison, the efficiency of commercial silicon-based solar panels, which currently dominate the market, ranges from 15% to 20%.

A more recent technology known as tandem solar cells—in which a perovskite solar cell is overlaid on a silicon cell—has recently demonstrated an efficiency of 33.7% in the laboratory. The new world record was set in June 2023 at the King Abdullah University of Science and Technology (KAUST) in Saudi Arabia. The U.S. government's National Renewable Energy Laboratory (NREL) maintains a chart of the highest confirmed conversion efficiencies achieved at various research centers worldwide over the past few years.

Companies and startups in China, the US, and Europe are set to start large-scale production of perovskite solar modules in the upcoming months. One example is British-based Oxford Photovoltaics; this is a spin-off from the University of Oxford that operates a state-of-the-art manufacturing line for perovskite-on-silicon tandem solar cells in Germany. In the US, Caelux is building a facility to upscale its production of perovskite photovoltaic glass, and the first deliveries for building solar modules are anticipated within the year. In 2023, Chinese-based GCL-SI revealed that a 320-watt perovskite solar module had an efficiency of 16% and that it is currently being produced at the pilot scale.

In Brazil, the organization closest to a commercially viable perovskite cell model is Oninn; this is a nonprofit, private organization based in Belo Horizonte, formerly named CSEM Brazil until 2022 (*see* Pesquisa FAPESP *issue no. 247*). The initiative is a collaboration between researchers from São Paulo State University (UNESP) and the Center for Innovation in New Energies (CINE); CINE is an Engineering Research Center (CPE) established in 2018 by FAPESP and Shell Brazil. However, further improvements are still needed for the commercial-scale production of technically and economically viable perovskite cells.

Leveraging its experience from developing solar panels via organic photovoltaic cell technology, Oninn is currently working to scale up its perovskite-based cells from the laboratory scale—no larger than a few square millimeters or centimeters (cm²)—to larger modules measuring hundreds of cm², as needed for commercial applications.

"We've successfully produced our first prototype perovskite panel with an area of 800 cm². But our standard panel, which is still under development, is slightly smaller at 500 cm²," explains Diego Bagnis, an Italian physicist and scientific director at Oninn, who has been involved in the research effort in Brazil over the past nine years. "We're still in the prototyping phase, testing our first real-world applications to validate the technology." Bagnis hopes to have a pilot manufacturing line set up by 2026 and to go to market in 2028, initially targeting small-scale applications.

Oninn is not currently developing tandem cells. "We are focusing on what is known as a single-junction solar cell, or a cell with only one layer of perovskite," says Bagnis. "Making tandem cells—with perovskite overlaid on silicon—makes sense in Europe as silicon technology is well-established there and they have local production facilities to produce these cells. But this is not the case in Brazil." Local producers in Brazil import the silicon-based materials used to make solar panels and assemble the modules locally.

Despite recent advancements and promises of soon-to-be-launched commercial models, Brazilian researchers interviewed for this article say they are still far from understanding the properties of this emerging material, especially their relationship to cell stability—and their ability to retain their mechanical integrity over an extended period—and the process to replicate the energy efficiency achieved in the lab with larger-scale modules.

"There are still scientific and technological hurdles that will require investment, time, and expert personnel to overcome," says physicist Carlos Frederico de Oliveira Graeff from the UNESP School of Sciences, Bauru campus.

Graeff, who is developing perovskite solar cells and is a member of Oninn, explained: "From a physics and engineering standpoint, silicon is a relatively simple material with a known crystal arrangement, whereas perovskite is physically and chemically complex. It is generally composed of both organic and inorganic components, consists of multiple elements, and exhibits high ionic mobility." One of Graeff's most recent projects, with funding from FAPESP, is investigating the stability of these solar cells.

Gustavo Dalpian, a physicist at the University of São Paulo (USP) Institute of Physics, noted that many fundamental properties of the material's crystalline structure are still not effectively understood. "It's quite different from what we see in other materials. In crystalline silicon, for example, atoms tend to stay in well-defined positions, but in perovskites, they move a lot. This is believed to be one of the reasons they are so unstable."

Perovskite has an instability, which causes it to degrade much faster than silicon; this instability is one of the major barriers in its commercial production. While silicon modules can last up to 30 years with minimal loss of efficiency, cells made of the perovskite can barely last over a year. Early cell models degraded within hours or days. Moisture, heat, oxygen, and even sunlight could easily degrade them.

"Once we understand the structural properties of these materials and their flaws, we can develop or think of ways to prevent them from degrading as fast as they do today," says Dalpian. The research group he leads specializes in computational modeling of materials using big data and machine learning.

He recently visited Colombia as part of a FAPESP Sprint project, where he spoke with *Pesquisa FAPESP*. "We are discussing new projects involving perovskites, and researchers from two universities in Medellín are expected to join the initiative," says Dalpian. Dalpian is also collaborating with an experimental group at the Federal University of ABC (UFABC), where he lectured until receiving tenure at USP in 2023.

SYNCHROTRON LIGHT AND PEROVSKITE

During an in-depth investigation of perovskite properties, a team at CINE was the first to observe its properties using a synchrotron light source at Sirius, operated by the Brazilian Synchrotron Light Laboratory (LNLS) at the Brazilian Center for Research in Energy and Materials (CNPEM). CINE brings together researchers from the University of Campinas (UNICAMP), USP, and the Institute for Energy and Nuclear Research (IPEN).

"Studies into the use of perovskite in photovoltaic applications have been among the fastest-growing energy research niches globally, and our experiments with synchrotron light have allowed us to gain a foothold in an extremely competitive research environment," says chemist Ana Flávia Nogueira, CINE's director and a professor at the UNICAMP Institute of Chemistry. She has been researching emerging photovoltaic materials since 1996, and in 2015, she began investigating perovskite materials.

With the scientific instruments available at the CNPEM, researchers are able to analyze materials at the nanoscale in real time. "We brought the equipment used to produce the perovskite film—a rotating disk called a spin-coater, which resembles a CD burner—to the X-ray beamline," says Nogueira. This was the first experiment of this kind. But why is this kind of experiment—known as *in situ* X-ray diffraction—particularly useful? "As the perovskite film was forming, X-rays struck the sample, providing useful information about

HOW SOLAR CELLS WORK

A solar cell is composed of semiconductor materials that convert sunlight into electrical current

1. LIGHT ABSORPTION

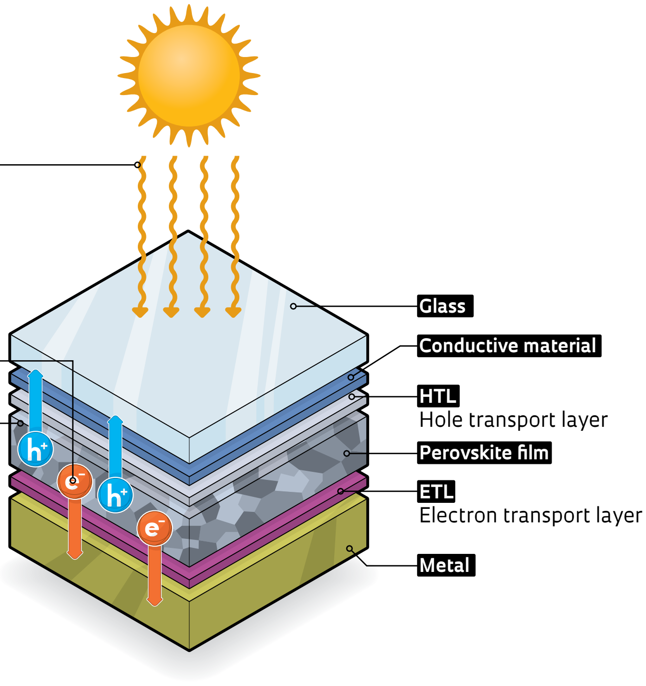
Sunlight passes through the glass substrate and is absorbed by the perovskite film

2. CHARGE SEPARATION

The energy from the absorbed light (photons) separates the electric charges: the ETL layer transports the **electrons** (negative charges), and the HTL layer transports the **holes** (positive charges)

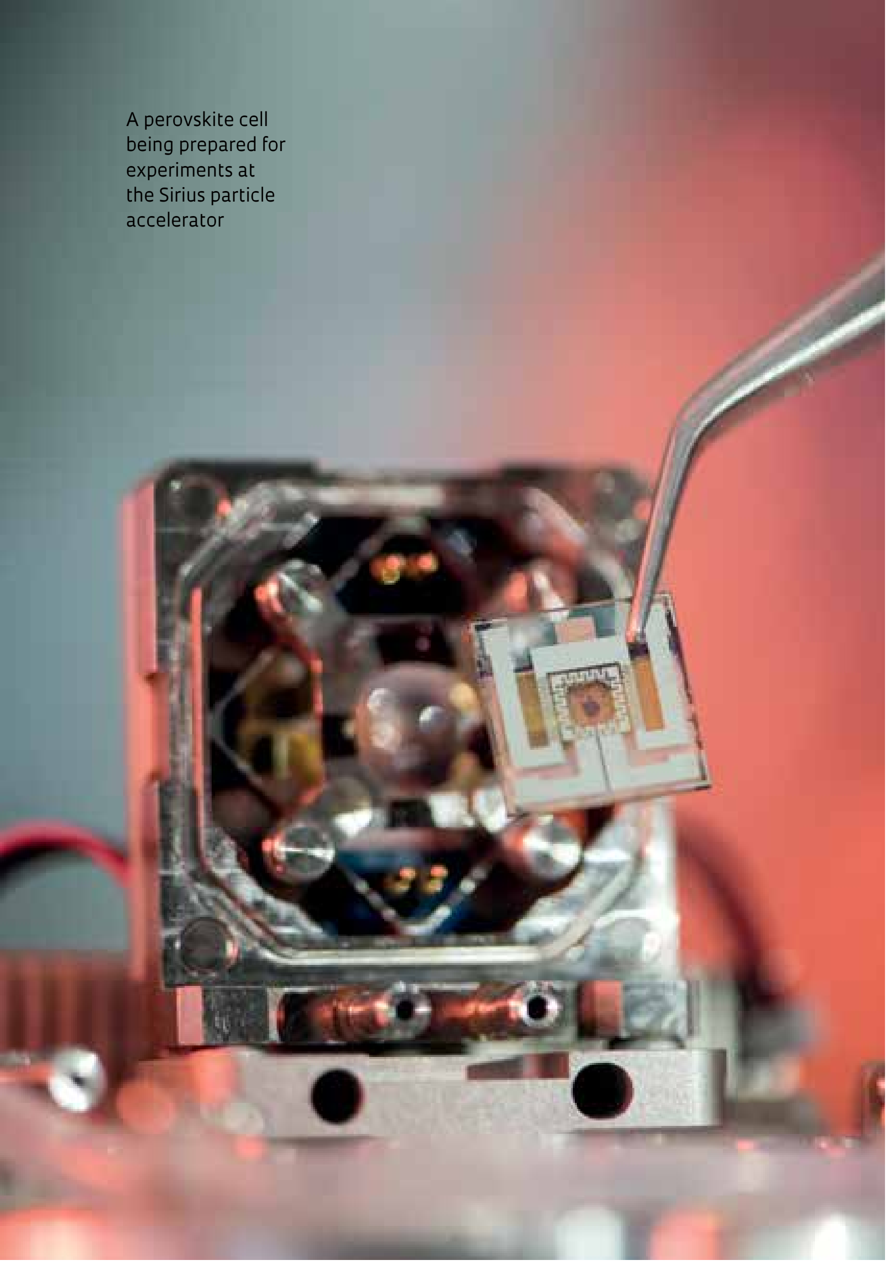
3. CURRENT GENERATION

Holes migrate to the conductive material of the cell, while the electrons are captured by the metal, generating an electrical current



SOURCE MURILLO HENRIQUE DE MATOS RODRIGUES

PHOTO LÉO RAMOS CHAVES / PESQUISA FAPESP MAGAZINE **INFOGRAPHIC** ALEXANDRE AFFONSO / PESQUISA FAPESP MAGAZINE



A perovskite cell being prepared for experiments at the Sirius particle accelerator

the structure and how the film crystallized at each stage," explains Nogueira.

Due to this research and other studies analyzing the degradation of perovskites and employing *in situ* techniques at Sirius, the researchers at CINE became well known in this field and were invited to write a review on this subject for the journal *Chemical Reviews*. The 77-page article was published in early 2023. "The invitation to author a review article for a high-impact journal crowns the work we have been doing in recent years," says Nogueira. In addition to investigating the use of perovskites to make solar cells, this group is also exploring applications for materials in light-emitting devices, such as LEDs and lasers.

UNDERSTANDING HOW IT WORKS

At Sirius, the current focus of experiments is understanding how perovskite solar cells work and not just the material itself. These experiments are termed "*operando*" experiments. One of the challenges in this type of analysis is that synchrotron radiation can induce undesired changes in the material.

"We are investigating the effects of the radiation dose required to study these devices and how to mitigate them. We've already developed devices to simulate the operating conditions of photovoltaic solar cells and have produced some initial results," says physicist Helio Cesar Nogueira Tolentino, head of the Division of Heterogeneous and Hierarchical Matter at LNLS. "We're working on fine-tuning the optimal working conditions for obtaining information using synchrotron light without degrading the photovoltaic material, or if degradation occurs, to ensure it is in a controlled manner."

Tolentino explained that a perovskite's crystalline structure typically resembles a cube but can vary depending on the preparation method or synthesis route. In their first *operando* experiment, the researchers observed the impact of sunlight on the material's atomic structure. "While we have not yet come to a definitive interpretation, there is evidence suggesting that varying light levels alter the material's structure."

Brazilian researchers are investigating a number of potential solutions to prevent the material from developing undesirable properties for the intended application; these solutions include additives, new molecules, modifications to the film production process, and even a two-dimensional (2D) perovskite film overlayed on a three-dimensional (3D) layer. However, the material instability is just one of many technological challenges. Sustaining the energy efficiency achieved with lab-scale cells on a larger scale is also a complex issue.

"The scaled-up cells are often not homogeneous," explains Nogueira from UNICAMP. "The crystallization process that occurs as perovskite forms differs from that of other materials used in photovoltaics."

According to Graeff, researchers are currently working to develop formulations and processes to produce economically viable technology. "We need robust production processes that can be used on a large scale. In the meantime, we're learning a lot about the fundamental physics and chemistry. These materials are complex, and their use in electronic devices is fairly incipient," says Graeff. "The electronics used for current solar panels are designed for silicon, a very simple and stable material. Now we are dealing with a material composed of different chemical elements and with a complex structure."

Research in this field provides good examples of successful collaboration between the theoretical and experimental scientists. Using computer modeling, theorists can design structures that have never been created in the lab or save time and costs in selecting elements to be tested in experiments.

"We analyze different materials and try to infer or learn about their properties," says Dalpian, who has coauthored at least five papers with the experimental group at UFABC. "Our collaboration has been highly productive. Typically, experimental researchers make requests, and we oblige, but in our case, they also listen to our input. For instance, we once suggested that introducing iron into perovskite could impart useful magnetic properties. They tried it, and the results led to an interesting article," recounts Dalpian.

At the CINE, theoretical and experimental researchers are collaborating on multiple research fronts. One project is working to develop alternatives to lead (a toxic substance) in the composition of perovskites. "There are obvious benefits from reducing or completely eliminating lead content in these structures," says Juarez L. F. da Silva, a physicist at the USP Institute of Chemistry in São Carlos (IQSC) and coordinator of the Computational Materials Science program at CINE.

"Computational modeling can be used to simulate a large number of materials to replace a given element in low-dimensional perovskites—such as tin, germanium, or combinations of two chemical species," explains Da Silva. The material needs closely match a particular set of parameters. "We use experimental information to identify materials that can meet these specifications."

Another research program led by experimental researchers at the CINE involves the exploration of how molecules interact with perovskite surfaces. The team uses computer modeling to discover mechanisms that could contribute to cell degradation, says Da Silva. "In a solar cell, the metal wire used to carry electrical current interacts with the perovskite, causing chemical species to be carried from one side to the other. In some circumstances, they can destabilize the cell structure."

According to Dalpian, perovskite solar cells can be used in a wide range of applications; however, for this to occur, a breakthrough in cell stability is needed. "By today's standards, a solar cell is expected to last 20 to 25 years. But it doesn't necessarily have to be that way. If cells are considerably cheaper, they can be replaced when they become less efficient, as we do today with light bulbs," says Dalpian. "But there would need to be an ecosystem in place to recycle end-of-life panels, minimizing their environmental impact." The goal of current perovskite cell research is not necessarily to completely replace silicon modules but to provide an additional material with useful properties and characteristics for solar energy. ■

The research projects and scientific articles consulted for this report are listed in the online version.

A tandem solar cell production line at the Oxford Photovoltaics facility in Germany

PHOTO OXFORD PV