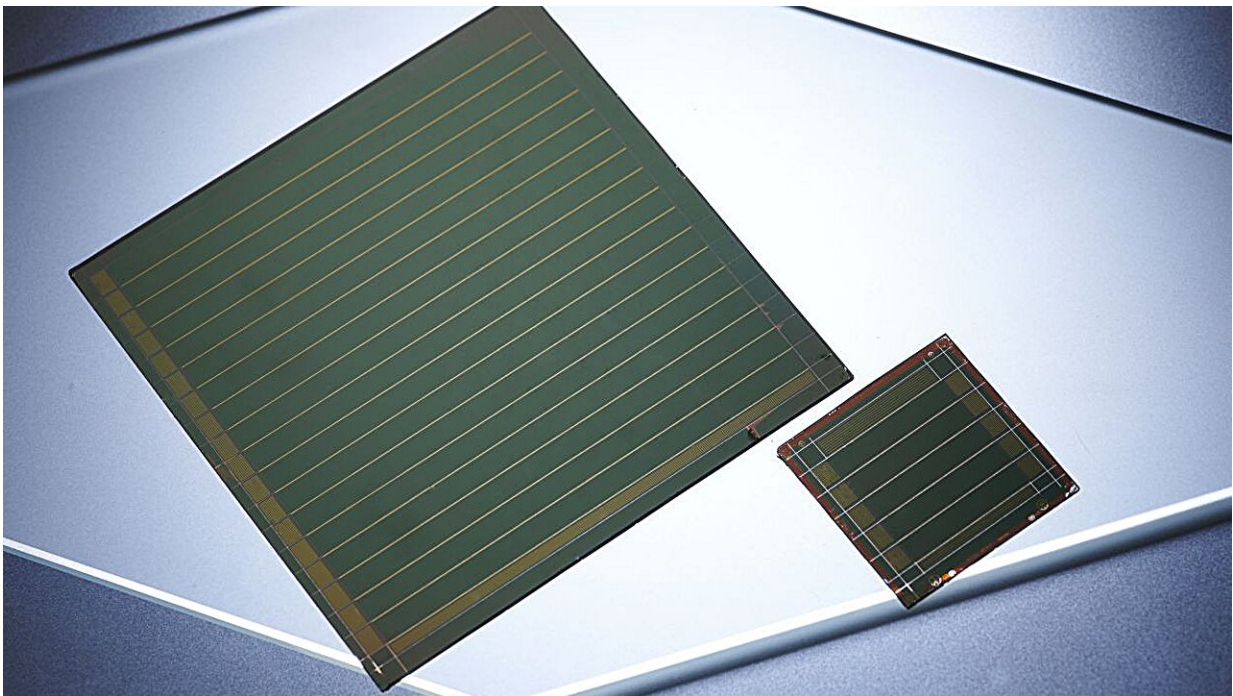


Using AI as a guide for the better manufacturing of perovskite solar cells

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Assisted by AI methods, researchers are striving to improve the manufacturing processes for highly efficient perovskite solar cells. Credit: Amadeus Bramsiepe, KIT

Tandem solar cells based on perovskite semiconductors convert sunlight to electricity more efficiently than conventional silicon solar cells. In order to make this technology ready for the market, further improvements with regard to stability and manufacturing processes are

required.

Researchers of Karlsruhe Institute of Technology (KIT) and of two Helmholtz platforms—Helmholtz Imaging at the German Cancer Research Center (DKFZ) and Helmholtz AI—have succeeded in finding a way to predict the quality of the perovskite layers and consequently that of the resulting [solar cells](#). Assisted by [machine learning](#) and new methods in [artificial intelligence](#) (AI), it is possible to assess their quality from variations in light emission already in the manufacturing process.

[The results](#), which can be used to derive better manufacturing processes, have been published in *Advanced Materials*.

Perovskite tandem solar cells combine a perovskite solar cell with a conventional solar cell, for example, based on silicon. These cells are considered a next-generation technology: They boast an efficiency of currently more than 33%, which is much higher than that of conventional silicon solar cells. Moreover, they use inexpensive raw materials and are easily manufactured. To achieve this level of efficiency, an extremely thin high-grade perovskite layer, whose thickness is only a fraction of that of human hair, has to be produced.

"Manufacturing these high-grade, multi-crystalline thin layers without any deficiencies or holes using low-cost and scalable methods is one of the biggest challenges," says tenure-track professor Ulrich W. Paetzold who conducts research at the Institute of Microstructure Technology and the Light Technology Institute of KIT.

Even under apparently perfect lab conditions, there may be unknown factors that cause variations in semiconductor layer quality. "This drawback eventually prevents a quick start of industrial-scale production of these highly efficient solar cells, which are needed so badly for the energy turnaround."

AI finds hidden signs of effective coating

To find the factors that influence coating, an interdisciplinary team consisting of the perovskite solar cell experts of KIT has joined forces with specialists for Machine Learning and Explainable Artificial Intelligence (XAI) of Helmholtz Imaging and Helmholtz AI at the DKFZ in Heidelberg. The researchers developed AI methods that train and analyze [neural networks](#) using a huge dataset. This dataset includes [video recordings](#) that show the photoluminescence of the thin perovskite layers during the manufacturing process.

Photoluminescence refers to the radiant emission of the semiconductor layers that have been excited by an external light source. "Since even experts could not see anything particular on the thin layers, the idea was born to train an AI system for machine learning (Deep Learning) to detect hidden signs of good or poor coating from the millions of data items on the videos," Lukas Klein and Sebastian Ziegler from Helmholtz Imaging at the DKFZ explain.

To filter and analyze the widely scattered indications output by the Deep Learning AI system, the researchers subsequently relied on methods of Explainable Artificial Intelligence.

A blueprint for follow-up research

The researchers found out experimentally that the photoluminescence varies during production and that this phenomenon has an influence on the coating quality. "Key to our work was the targeted use of XAI methods to see which factors have to be changed to obtain a high-grade solar cell," Klein and Ziegler say.

This is not the usual approach. In most cases, XAI is only used as a kind

of guardrail to avoid mistakes when building AI models. "This is a change of paradigm: Gaining highly relevant insights in materials science in such a systematic way is a totally new experience."

It was indeed the conclusion drawn from the photoluminescence variation that enabled the researchers to take the next step. After the neural networks had been trained accordingly, the AI was able to predict whether each solar cell would achieve a low or a high level of efficiency based on which variation of light emission occurred at what point in the manufacturing process.

"These are extremely exciting results," says Ulrich W. Paetzold. "Thanks to the combined use of AI, we have a solid clue and know which parameters need to be changed in the first place to improve production. Now we are able to conduct our experiments in a more targeted way and are no longer forced to look blindfolded for the needle in a haystack. This is a blueprint for follow-up research that also applies to many other aspects of energy research and materials science."

More information: Lukas Klein et al, Discovering Process Dynamics for Scalable Perovskite Solar Cell Manufacturing with Explainable AI, *Advanced Materials* (2023). [DOI: 10.1002/adma.202307160](https://doi.org/10.1002/adma.202307160)

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