

Young Researcher Wants to Change Materials Research Method

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A new method will make the development of previously unknown materials for, e.g., solar cells both faster and more efficient.

By closely combining experimental work with computer modelling, the young talented researcher Andrea Crovetto will create a new method for developing materials.

The method is based on the need for a new material—for example a light absorber for a solar cell—and then determining which material will have the desired properties. This is in contrast with finding a new material and then researching what it can be used for.

The method has been known as inverse design for a while, but Andrea Crovetto will implement it in a significantly different way than previously.

"In my version of inverse design, data from the experiments and computer simulation are gathered in a single, on-demand database of material properties," says Andrea Crovetto.

"This means that the next experiment and the next simulation will be decided based on their likelihood of giving us the data we need. Data from the database are interpreted by both human and artificial intelligence to find trends between different properties in different materials and help us in the inverse design process."

The specific goal is to find a new sustainable material for the top layer of a solar cell that can convert sunlight into energy more efficient than today. Within this project, the search area consists of all materials containing phosphorus and sulphur.

"We don't know much about these materials, even though phosphorus and sulphur are abundant on Earth and although there is evidence that some of them could be excellent photovoltaic materials," says Andrea Crovetto.

World-class research infrastructure

Andrea Crovetto has already made his mark in research circles. Three years ago, he was awarded one of the coveted Marie Curie fellowships, and, this year, he has received both the EU's prestigious ERC starting grant of just over DKK 17 million and a Villum Young Investigator grant of DKK 6 million.

The two grants make it possible for Andrea Crovetto to both purchase the necessary experimental equipment and employ a total of six young PhD and postdoc researchers to assist him.

Andrea Crovetto has chosen to conduct his research at DTU Nanolab.

"There is no doubt that the world-class research facilities we can offer have made it interesting for Andrea Crovetto to look towards <u>Denmark</u> and DTU when choosing where his research will be conducted in the coming years," says Jörg Hübner, Director of DTU Nanolab.

This is not least due to the unique cleanroom at DTU Nanolab and the accompanying opportunities for characterizing materials with atomic resolution.

"In addition, we have both the expertise and the research infrastructure for working with hazardous substances, including handling toxic gases. This is crucial for state-of-the-art nanofabrication and materials synthesis," says Jörg Hübner.

In addition to offering the right research facilities for producing new materials, DTU Nanolab also possesses the necessary expertise to structure and characterize new materials.

"We're therefore interested in building up a couple of material platforms from scratch, where we own the entire food chain—so to speak—and can adapt the material to different applications. A new material of phosphorus and sulphur that Andrea Crovetto is working with is an interesting possibility in this regard," says Jörg Hübner.

With his new research method, Andrea Crovetto expects to have the first material tested already in the first half of next year. This material can hopefully form the basis of a new and better material for solar cells.

"At the same time, my goal is that the whole database that I'm collecting in my upcoming research—where we're testing an incredibly large quantity of compositions of materials with phosphorus and sulphur—will be published at the end of the project. This will give other researchers an opportunity to exploit and build on our work," says Andrea Crovetto.

Read the <u>original article</u> on Technical University of <u>Denmark</u> (DTU).