

# A Shining Example of Collaboration to Advance Solar Energy Technologies

Computational scientists from the Science and Technology Facilities Council (STFC) are working with two UK universities, using real experimentation and high quality computer modelling to accelerate solar cell technology. Improving this technology should push down the price of solar cells and encourage their use as a more accessible and affordable energy solution worldwide.

## The Issue

As the climate crisis intensifies, the switch to renewable energy has become a fundamental need for the future. To meet the UK's ambitious net zero targets and also keep up with modern demands, the research and development of clean energy solutions need to advance quickly.

Solar cells use radiation from the sun to generate the flow of electrons that produce electricity. The solar cell needs two main components – something to absorb the sun's energy and something to transfer the energy from the absorber to an external circuit where it can be used as electrical energy. Absorbers work by capturing the energy from solar radiation and energising electrons that circulate within a transfer material to create a flow of electrons. The transfer component is commonly made from (semi-conducting) materials such as silicon or rare earth metals, both of which have major disadvantages:

- The manufacture of semi-conductors has several negative impacts on the environment; polluting underground water - that ultimately might be used as drinking water and for crop irrigation - and it also generates toxic waste
- The manufacture of rare earth metals has already caused significant damage to agriculture due to pollutants in soil resulting from mining practices. Solar cells produced using these mined materials are expensive to produce and not easy to integrate into roofs and other structures.

## Our Approach

Computational scientists from STFC Scientific Computing are collaborating with researchers at the Universities of Glasgow and Swansea, using computer models to improve the component of solar cells that absorbs energy.

The solar cell type used in this research uses dyes as the absorber of the sun's radiation, and these dyes are adsorbed on the surface of the transfer component – in this case titanium dioxide.

**"Taking advantage of these abundant organic dyes, which are more sustainable and less devastating to the environment than their counterparts, will push us closer and closer to realising the full potential of renewable energy."**

**Dr Ya-Wen Hsiao,  
Senior Computational Scientist  
STFC Scientific Computing**

Titanium dioxide is a common, easily mined crystal that is used safely in all sorts of products, from foods to sun cream and toothpaste. It is abundant worldwide and easy to manufacture using existing processes. The team has identified five dyes that will be good absorbers to match this transfer material, although these still need more testing and research to take full advantage of their properties and ensure they make the best possible solar cells.

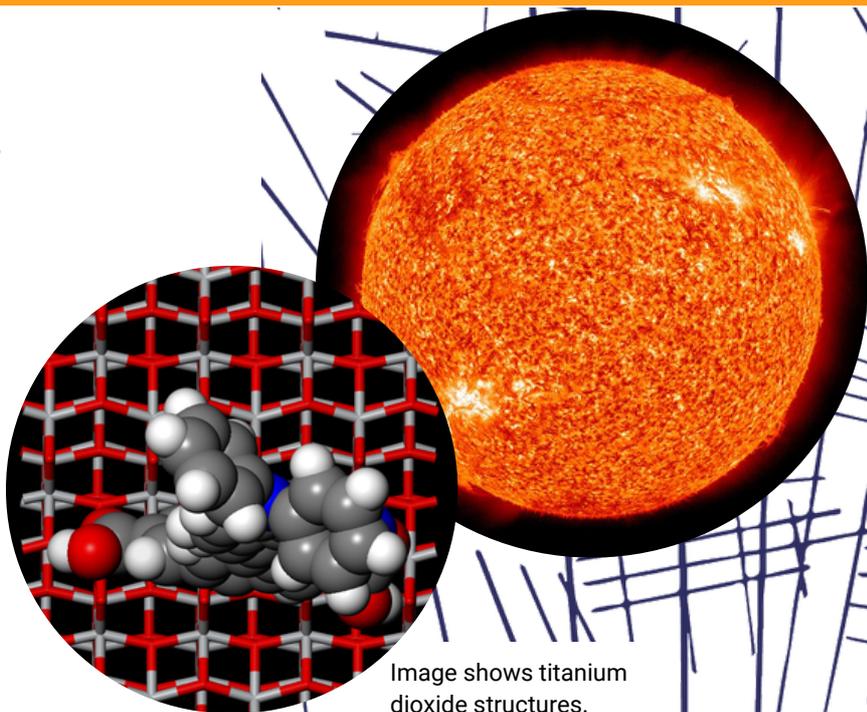


Image shows titanium dioxide structures.

**“The project is a combination of modelling and experimental methods, with our models enhancing the experimental data and the experimental data enhancing our models. This constant feedback loop is a really satisfying and efficient way to carry out research because it leads to faster and better results than doing experiments or theory alone.”**

***Dr Dawn Geatches  
Senior Computational Scientist  
STFC Scientific Computing.***

## The Benefits

Using dyes as opposed to the other alternatives can greatly improve the manufacture of solar cells, making them cheaper to produce and, subsequently, more affordable to consumers. The dyes can be printed onto a large flexible roll instead of the rigid structures you see with solar panels today. This makes the printed sheets much more compatible with existing infrastructures, such as roof tiles, and will make them a cheaper, more favourable way to generate electricity without relying on fossil fuels.

## Extended Projects

The collaborative work with Glasgow and Swansea universities has extended beyond the computational models. The project has been used in outreach programs, such as workshops for A-Level students, and integrated into STFC’s summer schools.

A related project has been developed to extend the life expectancy of solar cell components by introducing recyclability in solar cells.

**STFC Scientific Computing:** Dr Dawn Geatches, Dr Kakali Sen and Dr Ya-Wen Hsiao; (and previously Dr Sebastian Metz now at Fraunhofer ISE, Freiburg)

**Swansea University (College of Engineering):** Prof. Peter J. Holliman, Dr Christopher P. Kershaw, Dr Diana Meza-Rojas, and extended team

**Glasgow University (School of Chemistry):** Prof Graeme Cooke and team

