Neutron reflectivity has been used to take a look at buried interfaces in solar cells, to see how their structure could impact their performance.

Dye-sensitised solar cells (DSCs) are a special type of photovoltaics that are transparent and flexible. This gives them huge potential for applications such as solar-powered windows or wearables. To understand how their performance can be improved, the structure of the interfaces between the component layers inside a DSC needs to be investigated.

Each DSC is made up of three interfacial layers: an electrolyte, a dye and a top layer of titanium dioxide. In this study, published in *Langmuir* [1], a group of researchers studied the interfaces between these layers inside a working DSC. Their multi-continental endeavor used data from two neutron institutes, sample cell development that originated from a third and complementary experiments at laboratories in the USA and the UK.

Initially, the team, led by Professor Jacqui Cole, deposited atomically flat layers of amorphous TiO₂ onto a silicon substrate using atomic layer deposition at the Center for Nanoscale Materials, Argonne National Laboratory. Creating this ultra-flat film set the foundations for the scattering geometry needed for the reflectometry experiments that were to come.

They then brought this TiO₂/Si substrate to the Research Complex at Harwell, where they added the dye layer to the system to produce a working electrode. To check their fabrication technique, they used X-ray photoelectron spectroscopy (XPS) and Fourier transform infra-red spectroscopy at the Research Complex alongside X-ray reflectometry at the Materials Characterisation Laboratory at the ISIS Neutron and Muon Source.

Continuing their investigations into the working electrode, the researchers used *ex situ* neutron reflectometry at the China Spallation Neutron Source, being among the first international users. They were able to benchmark their results against the X-ray reflectometry data collected at the ISIS Materials Characterisation Laboratory.

The next stage was to embed the working electrode into a fully assembled DSC. Because neutrons can penetrate into the deep interior of a sample, the scientists were able to study how the layered structures of a DSC device interact *in situ*, while the cell was fully assembled.

These *in situ* experiments were carried out on the Inter beamline at ISIS. Figure 1 shows the fully assembled cell set upside down on a custom sample stage, so that the incident neutrons can approach from above while simulated solar light can come from below.

The cell used was a development on a prototype designed as part of a previous project [2] between Professor Cole and the Australian Centre for Neutron Scattering at the Australian Nuclear Science and Technology Organisation (ANSTO). The custom set up was transferred to ISIS, with ANSTO’s agreement, in order to take advantage of its much higher neutron flux for future experiments.

![Figure 1. Photograph of the fully assembled solar cell, set upside down on a custom sample stage (image credit: Jacqueline Cole).](image-url)
To study the interaction between the layers of the DSC device, the team was able to exploit the fact that neutrons interact differently with distinct isotopes of the same element. By changing the isotope of hydrogen present in the solvent of one of the layers to deuterium, and comparing the two experiments, the team was able to build a contrast picture of the system.

They used these contrast pictures to highlight different layers of the DSC, enabling them to see the different structural features present. Their experiments gave an unique insight into the how the different layers interact with one another, as illustrated in Figure 2.

In addition to the expected monolayer of dye molecules formed on the titanium dioxide (TiO₂) layer, the researchers observed, for the first time, that the electrolyte was disturbing this monolayer. This was, in turn, affecting the interactions between the dye and the TiO₂.

The fact that the electrolyte changes the interactions at the dye/TiO₂ interface could influence the operation of a DSC. This structural finding is therefore crucial to consider when determining how they could be made in the future.

References
1. K. Deng et al., Langmuir 37, 1970 (2021). doi:10.1021/acs.langmuir.0c03508
2. J. McCree-Grey et al., Nanoscale 32 (2017). doi:10.1039/C7NR03936K

Figure 2. Illustration of the in situ measurement of a layered DSC using neutron reflectometry. Reprinted with permission from Langmuir 2021, 37, 5, 1970–1982. © 2021 American Chemical Society.