A milestone on the path towards efficient solar cells

Generating more electricity from solar cells and conducting further research into so-called singlet fission. This is what scientists at Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) are currently working on as part of a joint research project conducted in collaboration with Argonne-Northwestern Solar Energy Research (ANSER) Center at Northwestern University in Evanston, USA. Singlet fission could considerably boost the efficiency of solar cells – and thanks to the latest research it is one step closer to becoming possible. The findings have been published in the scientific journal ‘Chem’.

Global energy consumption has rocketed, and the upward trend is set to continue over the coming years. In a bid to meet demand whilst protecting the environment, electricity from the renewable energy sources solar, wind, water and biomass is gaining in importance. However, only approximately six percent of the gross electricity produced in Germany in 2017 came from photovoltaic systems and the technology we currently have available – based on silicon – is rapidly reaching its limits in terms of potential.

Generating more electricity from solar cells

Solar cells are extremely inefficient at converting solar energy to electricity. Their efficiency currently lies at just 20 to 25 percent. New approaches are called for to significantly increase the performance of solar cells and generate more electricity. The answer may be found in physical-chemical processes which significantly boost the efficiency of solar cells. Scientists at FAU and the ANSER Center have been exploring a promising approach as part of their joint research project within the Emerging Fields Initiative (EFI) ‘Singlet fission in novel organic materials – an approach towards highly-efficient solar cells’. The researchers investigated the so-called singlet fission (SF) mechanism, in which one photon excites two electrons.

Gaining a better understanding of singlet fission

The principle of singlet fission was discovered roughly fifty years ago now, but its potential for significantly increasing the efficiency of organic solar cells was only recognised by scientists in the USA just under ten years ago. Since then, researchers across the globe have been working on gaining a more detailed understanding of the fundamental processes and complex mechanisms behind it. Together with Prof. Michael Wasielewski from the ANSER Center, the researchers from FAU – Prof. Dr. Dirk Guldi from the Chair of Physical Chemistry I, Prof. Rik Tykwinski from the Chair of Organic Chemistry I (since moved to University of Alberta, Canada), Prof. Dr. Michael Thoss from the Chair of...
Theoretical Solid State Physics (since moved to Albert-Ludwigs-Universität Freiburg) and Prof. Dr. Tim Clark from the Computer Chemistry Center (CCC) have now managed to clarify some extraordinarily significant aspects of SF.

Detailed insights into the process

When a photon from sunlight meets and is absorbed by a molecule, the energy level of one of the electrons in the molecule is increased. By absorbing a photon, an organic molecule is therefore converted into a state of higher energy. Electricity can then be generated within solar cells from this energy which is stored temporarily within the molecule. The optimal scenario in conventional solar cells is that each photon generates one electron as a carrier for the electricity. If, however, dimers from selected chemical compounds are used, two electrons from neighbouring molecules can be converted into a state of higher energy. In total, one photon generates two excited electrons, which in turn can be used to produce electrical current – two are made out of one. This process is known as SF and in the ideal scenario can considerably boost the performance of solar cells. Chemists and physicists at FAU and the ANSER Center have investigated the underlying mechanism in more detail, leading to a considerably more extensive understanding of the SF process.

Three important findings

As the first step in their research, the scientists produced a molecular dimer from two pentacene units. This hydrocarbon is considered to be a promising candidate for using singlet fission in solar cells. They then exposed the liquid to light and used various spectroscopic methods to investigate the photophysical processes within the molecule.

This gave the researchers three far-reaching insights into the mechanism behind intra-molecular singlet fission. Firstly, they succeeded in proving that coupling to a higher charge transfer state is essential for highly efficient SF. Secondly, they verified a model for singlet fission they recently created and published (doi:10.1038/ncomms15171). Thirdly (and lastly), they proved that SF efficiency clearly correlates to how strongly the two pentacene sub-units are coupled.

The researchers’ findings indicate the importance of carefully planning the design of SF materials. This is an important milestone on the way towards using SF-based photovoltaic systems to generate electricity. Further basic research is still required, however.

The study was published under the title ‘Evidence for Charge-Transfer Mediation in the Primary Events of Singlet Fission in a Weakly Coupled Pentacene Dimer’ in: *Chem (2018), 4, 1092-1111.
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