

A milestone on the path towards efficient solar cells

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Scientists at Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) are currently working on a joint research project to generate more electricity from solar cells and conduct further research into so-called singlet fission with Argonne-Northwestern Solar Energy Research (ANSER) Center, U.S. 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 increased, and the upward trend is set to continue over the coming years. In a bid to meet demand while protecting the environment, electricity from solar, wind, water and biomass sources is gaining in importance. However, only approximately 6 percent of the gross electricity produced in Germany in 2017 came from photovoltaic systems, and the silicon-based technology currently available is rapidly reaching its limits in terms of potential.

Solar cells are extremely inefficient at converting solar energy to electricity. Their efficiency is currently just 20 to 25 percent. New approaches are required to significantly increase the performance of [solar cells](#) and generate more electricity. The answer may be found in physical-chemical processes that 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. The researchers investigated the so-called singlet [fission](#) (SF) mechanism, in which one photon excites two electrons.

The principle of singlet fission was discovered roughly 50 years ago, but its potential for significantly increasing the efficiency of organic solar cells was only recognised by scientists in the U.S. about 10 years ago. Since then, researchers around the world 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 have now managed to clarify some extraordinarily significant aspects of SF.

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 thereby 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 single fission, 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.

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. Thirdly (and lastly), they proved that SF efficiency clearly correlates to how strongly the two pentacene sub-units are coupled.

The 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.

More information: Bettina S. Basel et al, Evidence for Charge-Transfer Mediation in the Primary Events of Singlet Fission in a Weakly Coupled Pentacene Dimer, *Chem* (2018). [DOI: 10.1016/j.chempr.2018.04.006](#)

Bettina S. Basel et al. Unified model for singlet fission within a non-conjugated covalent pentacene dimer, *Nature Communications* (2017). [DOI: 10.1038/ncomms15171](#)

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