Self-organization gives rise to more efficient organic solar cells

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Organic solar cells have the potential to convert sunlight into electrical energy in an economical and environmentally friendly fashion. The challenge is that they still work less efficiently than inorganic semiconductors. Ultrafast measurements on hybrid cells now reveal a route to double their efficiency.

The use of organic photovoltaics for the production of electricity from sunlight offers an attractive and promising basis for an innovative and environmentally friendly means of energy supply. They can be manufactured quite economically and, because they are as bendable as plastic wrap, they can be processed flexibly. The problem is that they are yet markedly less efficient than conventional inorganic semiconductor cells. The most crucial process in the conversion of light into electric current is the generation of free charge carriers. In the first step of photoconversion, upon absorption of light one component of the organic solar cell, usually a polymer, releases electrons that are taken up by the second component of the cell - in this case silicon nanoparticles - and can then be transported further.

"The mechanisms and the timescale of charge separation have been the subject of controversial scientific debate for many years," says LMU physics professor Eberhard Riedle. In cooperation with investigators at the Technical University in Munich and at Bayreuth University, Riedle and his group have now been able to dissect the process in detail. To do so, the researchers used a novel hybrid cell type containing both organic and inorganic constituents, in which silicon serves as the electron

acceptor. Based on the insights obtained with this system, they developed a processing strategy to improve the structural order of the polymer - and found that this enhances the efficiency of charge separation in organic semiconductors by up to twofold. Their findings provide a new way to optimize the performance of organic solar cells.

The key to this breakthrough lies in a unique, laser-based experimental setup, which combines extremely high temporal resolution of 40 femtoseconds (fs) with a very broadband detection. This allowed the team to follow the ultrafast processes induced by photon absorption in real time as they occur. Instead of the fullerenes used in typical organic cells, the researchers used silicon as the electron acceptor, a choice that has two major advantages.

"First, with these novel hybrid solar cells, we were able to probe the photophysical processes taking place in the polymer with greater precision than ever before, and secondly through the use of silicon, a much larger segment of the solar spectrum can be harnessed for electricity," says Riedle.

It turns out that free charge carriers – so called polarons – are not generated immediately upon photoexcitation, but with a delay of about 140 fs. Primary photoexcitation of a polymer molecule first leads to the formation of an excited state, called an exciton. This then dissociates, releasing an electron, which is then transferred to the electron acceptor. The loss of electrons leaves behind positively charged "holes" in the polymer and, as oppositely charged entities are attracted to one another by the Coulomb force, the two have a tendency to recombine.

"In order to obtain free charge carriers, electron and hole must both be sufficiently mobile to overcome the Coulomb force," explains Daniel Herrmann, the first author of the new study. The team was able to show, for the first time, that this is much easier to achieve in polymers with an

ordered, regular structure than with polymers that are chaotically arranged. In other words, a high degree of self-organization of the polymer significantly increases the efficiency of charge separation.

"The polymer that we used is one of the few known to have a tendency to self-organize. This tendency can be inhibited, but one can also increase the polymer's intrinsic propensity for self-organization by choosing appropriate processing parameters," Herrmann explains. By cleverly optimizing the processing of the polymer P3HT, the researchers succeeded in doubling the yield of free charge carriers – and thereby significantly enhancing the efficiency of their experimental solar cells.

More information: "Role of Structural Order and Excess Energy on Ultrafast Free Charge Generation in Hybrid Polythiophene/Si Photovoltaics probed in Real Time by Near-Infrared Broadband Transient Absorption" D. Herrmann, S. Niesar, C. Scharsich, A. Köhler, M. Stutzmann, E. Riedle *J. Am.Chem. Soc.* online, 21. September 2011 dx.doi.org/10.1021/ja207887q

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