First real time movies of the light-to-current conversion in an organic solar cell

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This film strip contains frames taken from the quantum simulation of a portion of an organic solar cell. The quantity depicted illustrates the wavelike oscillations of an electron after sun light is absorbed at time 0. The time scale is in femtoseconds (fs). [One fs is one millionth of billionth of a second.] The two parts of the system separated by a small space act as the poles of a microscopic sun-operated battery. Each frame depicts a scene about 2 nanometers wide. Credit: Carlo A. Rozzi, Istituto Nanoscienze Cnr

Photovoltaic cells directly convert sun light into electricity and hence are key technological devices to meet one of the challenges that mankind has to face in this century: a sustainable and clean production of renewable energy. Organic solar cells, using polymeric materials to capture sun light, have particularly favorable properties. They are low-cost, light-weight and flexible, and their color can be adapted by varying the material composition. Such solar cells typically consist of nanostructured blends of conjugated polymers (long chains of carbon atoms), acting as light absorbers, and fullerenes (nanoscale carbon soccer balls), acting as electron acceptors. The primary and most elementary step in the light-to-current conversion process, the light-induced transfer of an electron from the polymer to the fullerene, occurs at such a staggering speed that it has previously proven difficult to follow it directly.

Now, a team of German and Italian researchers from Oldenburg, Modena and Milano reported the first real time movies of the light-to-current conversion process in an organic solar cell. In a report published in the May 30 issue of *Science* magazine, the researchers show that the quantum-mechanical, wavelike nature of electrons and their coupling to the nuclei is of fundamental importance for the charge transfer in an organic photovoltaic device.

"Our initial results were actually very surprising", says Christoph Lienau, a physics professor from the University of Oldenburg who led the research team. "When we used extremely short, femtosecond light pulses to illuminate the polymer layer in an organic cell, we found that the light pulses induced oscillatory, vibrational motion of the polymer molecules. Unexpectedly, however, we saw that also the fullerene molecules all started to vibrate synchronously. We could not understand this without assuming that the electronic wave packets excited by the light pulses would coherently oscillate back and forth between the polymer and the fullerene." All colleagues with whom the scientists discussed these initial results, obtained by PhD student Sarah Falke from Oldenburg in close collaboration with the team of Giulio Cerullo from Politecnico di Milano, leading experts in ultrafast spectroscopy, were skeptical. "In such organic blends, the interface morphology between polymer and fullerene is very complex and the two moieties are not covalently bound", says Lienau, "therefore one might not expect that vibronic coherence persists even at room temperature. We therefore asked Elisa Molinari and Carlo A. Rozzi, of the Istituto Nanoscienze of CNR and the University of Modena and Reggio Emilia, for help." A series of sophisticated quantum dynamics simulations, performed by Rozzi and colleagues, provided impressive movies of the evolution of the electronic cloud and of the atomic nuclei in this system, which are responsible of the oscillations found in experiments. "Our calculations indicate", says Molinari, "that the coupling between electrons and nuclei is of crucial importance for the charge transfer efficiency. Tailoring this coupling by varying the device morphology and composition hence may be important for optimizing device efficiency".

Will the new results immediately lead to better solar cells? "Such ultrafast spectroscopic studies, and in particular their comparison with advanced theoretical modelling, provide impressive and most direct insight in the fundamental phenomena that initiate the organic photovoltaic process. They turn out to be very similar to the strategies developed by Nature in photosynthesis.", says Lienau. "Recent studies indicate that quantum coherence apparently plays an important role in that case. Our new result provide evidence for similar phenomena in functional artificial photovoltaic devices: a conceptual advancement which could be used to guide the design of future artificial light-harvesting systems in an attempt to match the yet unrivalled efficiency of natural ones . "

More information: S. M. Falke et al., Coherent ultrafast charge transfer in an organic photovoltaic blend, *Science* 344, 1001 (2014), DOI: 10.1126/science.1249771

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