Iron sensitizer converts light to electrons with 92% yield - DTU Orbit (08/11/2017)

Iron sensitizer converts light to electrons with 92% yield

Solar energy conversion in photovoltaics or photocatalysis involves light harvesting, or sensitization, of a semiconductor or catalyst as a first step. Rare elements are frequently used for this purpose, but they are obviously not ideal for large-scale implementation. Great efforts have been made to replace the widely used ruthenium with more abundant analogues like iron, but without much success due to the very short-lived excited states of the resulting iron complexes. Here, we describe the development of an iron-nitrogen-heterocyclic-carbene sensitizer with an excited-state lifetime that is nearly a thousand-fold longer than that of traditional iron polypyridyl complexes. By the use of electron paramagnetic resonance, transient absorption spectroscopy, transient terahertz spectroscopy and quantum chemical calculations, we show that the iron complex generates photoelectrons in the conduction band of titanium dioxide with a quantum yield of 92% from the 3 MLCT (metal-to-ligand charge transfer) state. These results open up possibilities to develop solar energy-converting materials based on abundant elements.

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