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Direct observation of charge separation in an organic light harvesting system by femtosecond time-resolved XPS

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Organic semiconductors constitute an important novel class of electronic materials, especially for applications requiring low power consumption and lightweight, flexible materials. The large variety of these compounds paired with relatively low cost and ease of processing as well as the possibility to design and modify them using synthetic organic chemistry have created high expectations for the development of new functional materials. In particular, their potential application in organic photo-electronic devices such as organic photovoltaic cells (OPVs), solar fuel generation or artificial photosynthesis has motivated numerous investigations. Preferential conductivity for electrons or holes in OPVs is usually achieved by mixing molecular compounds with different electronic functionalities. For example, adding C60 to an organic semiconductor improves the photoconductivity by orders of magnitude.
Here we present the first femtosecond time-resolved XPS (tr-XPS) measurement of charge transfer dynamics in a CuPc/C60 bi-layer system using the Free-Electron Laser FLASH at DESY. Tr-XPS offers the unique opportunity to investigate the dynamics underlying the charge transfer process with exquisite site-specificity by monitoring the time-resolved C 1s XPS from the CuPc/C60 system following optical excitation of the chromophore (Pc). We observe an energy-shifted C 1s XPS line of the C60 electron acceptor after optical excitation, which can be seen as a direct indicator for the electron transfer to the C60. A previously unobserved channel for interfacial charge-transfer (ICT) state separation into mobile charge carriers with an efficiency of 22% is identified, providing a direct measure of the internal quantum efficiency of the heterojunction for this channel.

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