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Addressing the photoinduced mechanism of visible operated molecular photoswitches

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Molecular photoswitches are light responsive chemical structures allowing reversible optical control of a number of systems with applications in chemistry, material science and biology. Most of the commonly used photoswitches, such as azobenzene, diarylethene or spiropyran only absorb in the UV range. Achieving a selective switching using visible light is crucial for several applications, such as those related to the emerging field of photopharmacology, but it is still a major challenge. A key step for the design and optimization of new systems is a clear understanding of their photoswitching mechanism.

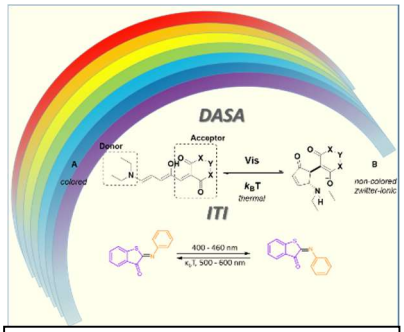

Figure 1: Structure and photoreactions of DASA and ITI

Here we show that a combined multidisciplinary approach based on ultrafast spectroscopy, quantum chemical computations and chemical synthesis allows to disentangle important details of the photoinduced relaxation pathways of several recently developed visible absorbing photoswitches, paving the way for their optimization. Examples will be provided regarding different classes of switches, such as Donor Acceptor Stenhouse Adducts (DASA)[1] or Iminothioindoxyl (ITI),[2] and the influence of a second external stimulus, such as protonation,[3] on their operation will be discussed.

[1] *M. Di Donato et al. J. Am. Chem. Soc., 139 (2017) 15596-15599;* [2] *M. W. H. Hoorens et al. Nat. Commun. 10 (2019) art. N. 2390;* [3] *M. Medved' et al. Chem. Sci, 12 (2021) 4588-4598;*

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