

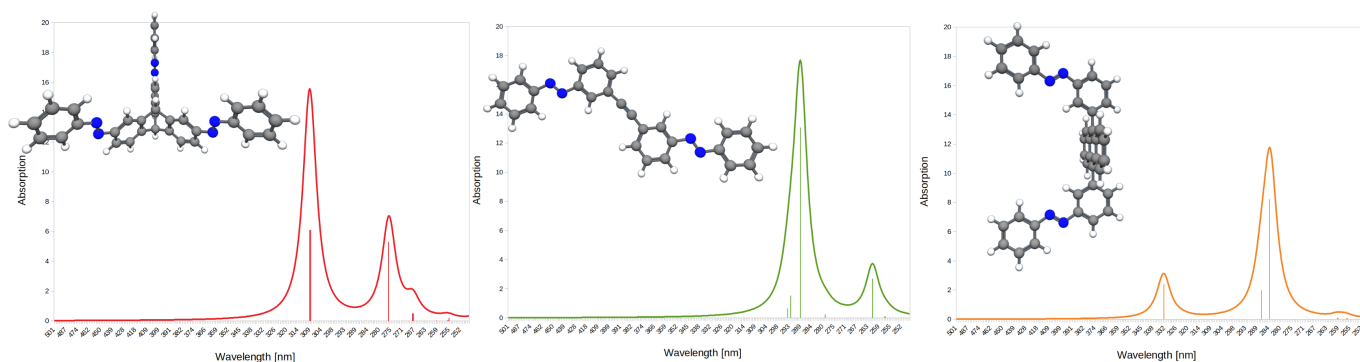
# COUPLED BUT INDIVIDUAL: MULTIPLE AZOBENZENES IN ONE MOLECULE

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A theoretical perspective on a small variety of different linking strategies for combining azobenzenes (AB) in a single molecule is given. AB is the most studied photoswitch with a variety of applications in energy and information storage, molecular machines, photobiology and photopharmacology as well as many other areas of research.

Herein the switching units were separated either via a  $sp^3$  center<sup>[1]</sup>, a geometrically orthogonal photosystem or following the “meta-rule” with an additional spatial separator. These three linking strategies show promising electronic separation of the photoactive switches. Due to their close proximity the photosystems interact predictably through excitonic coupling, with their switching ability still intact. The connectivity pattern can be used to align the transition dipole moments of the  $\pi \rightarrow \pi^*$  excitations, in turn leading to slightly altered absorption spectra. These insights allow for the development of new design parameters for the combination of multiple AB photoswitches in one molecule, which potentially find application in energy and information storage as well as in molecular machines or supramolecular chemistry.



**Fig 1.** Depiction of the three different linking strategies for multiple azobenzenes in one molecule with their respective calculated absorption spectra.

## References

- [1] Kunz, A., Oberhof, N., Scherz, F., Martins, L., Dreuw, A., Wegner, H. A., *Chem. Eur. J.*, **2022**, e202200972.

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