



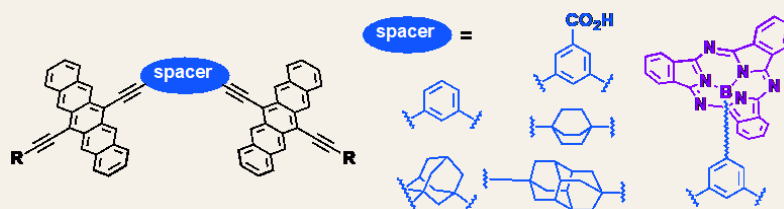
“ACENES AS CHROMOPHORES FOR SOLAR ENERGY CONVERSION”

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21. März 2023, 10.15 Uhr, INF 252, Kleiner Hörsaal

Singlet fission (SF) has the possibility to dramatically increase the efficiency of solar cells. Through the synthesis of specially designed acene oligomers, we are working to understand the fundamental aspects of SF in organic materials. When a molecule absorbs a photon to produce a singlet exciton, the spin-allowed process of SF may produce two triplet excitons if certain energetic and geometric parameters are met, i.e., two charge carriers are produced for each absorbed photon. We hypothesize that dimeric (or oligomeric) acenes would be ideal to study SF. Specifically, the studies are designed to examine intramolecular SF (*i*SF) rather than intermolecular SF. Among other advantages, photophysical studies in solution are greatly simplified for *i*SF since dilute solutions of the acene can be analyzed. Furthermore, the structure of the spacer linking two (or more) chromophores is used to define geometry, as well as the level of communication (coupling) between acene chromophores. Synthetic incorporation of specific spacers allows for tailoring many aspects of chromophore design, and, for example conjugated, cross-conjugated, non-conjugated, or organometallic spacers have been explored and compared. Likewise, spacers can be used to attach chromophores to devices, as well as incorporate antennae that broaden the absorption range. Together, these acene molecules have outlined many of the steps involved in SF. The design and synthesis of selected acene oligomers will be presented in this talk, as well as the resulting characteristics of *i*SF.



- [1] “Pentacene dimers as a critical tool for the investigation of intramolecular singlet fission,” C. Hetzer, D.M. Guldi, R.R. Tykwinski, *Chem. Eur. J.* **2018**, *24*, 8245–8257.
- [2] “Synthesis of unsymmetrical derivatives of pentacene for materials applications,” R.R. Tykwinski, *Acc. Chem. Res.* **2019**, *52*, 2056–2069.