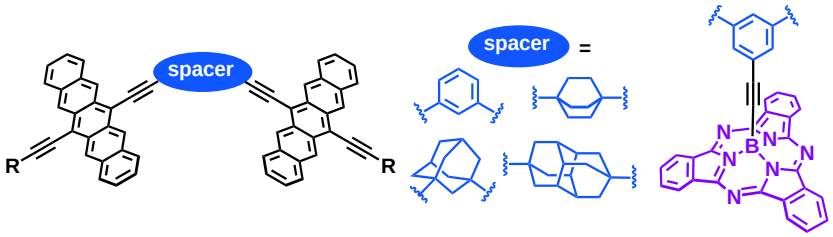
TAMING SINGLET FISSION WITH PENTACENE DIMERS AND OLIGOMERS

Rik R. Tykwinski

Department of Chemistry, University of Alberta, Edmonton, Alberta, Canada T6G 2G2.
rik.tykwinski@ualberta.ca

Singlet fission (SF) has the possibility to dramatically increase the efficiency limit of solar cells. Through the synthesis of special designed pentacene 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 hypothesized that dimeric or oligomeric pentacene molecules would be ideal to study SF. Specifically, the studies were designed to examine intramolecular SF (*i*SF) rather than intermolecular SF.[1,2] Furthermore, the structure of the group linking two (or more) pentacene chromophores is used to define geometry as well as the level of communication (coupling) between pentacene chromophores. Among other advantages, photophysical studies in solution are greatly simplified for *i*SF, since dilute solutions can be analyzed. Synthetic incorporation of specific linkers allows for tailoring many aspects of the chromophore design, and conjugated, cross-conjugated, non-conjugated, and organometallic groups have been explored and compared. Together, these molecules have outlined many of the steps involved in SF. The design and synthesis of selected pentacene oligomers, as well as the resulting aspects of *i*SF, will be presented in this talk.



[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, *Acct. Chem. Res.* **2019**, *52*, 2056–206