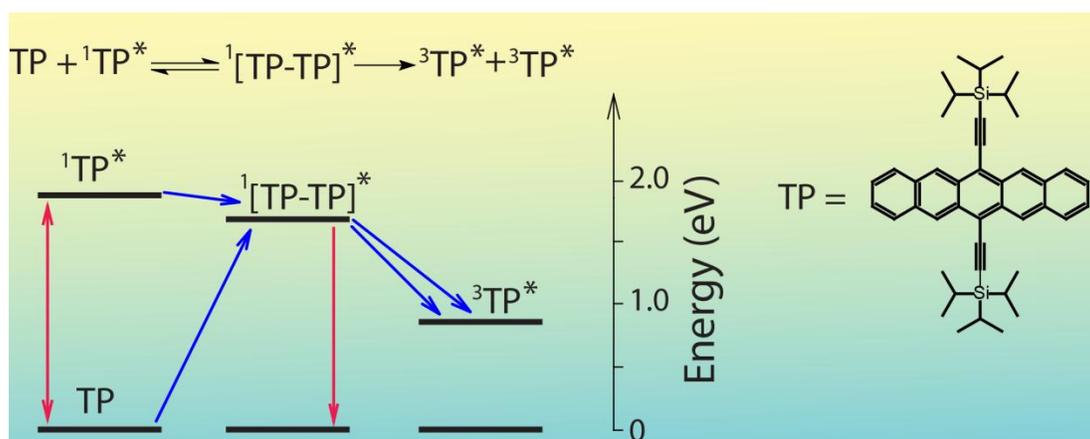


Singlet Exciton Fission: Applications and Mechanistic Insight

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Singlet fission is a spin-allowed process by which a chromophore in a singlet excited state gives rise to a pair of triplets. When paired with a small band gap semiconductor, singlet fission has the potential to reduce the thermalization losses in photovoltaic devices, thus exceeding the Shockley-Queisser limit with a single junction. We have designed singlet fission-sensitized solar cells using pentacene and infrared semiconductor nanocrystals, and we can use the nanocrystals both to increase the overall efficiency as well as characterizing the energetics of the pentacene triplet.

From a molecular perspective, the mechanism of singlet fission is not well-understood, in particular the degree of order required to promote coupling between molecules. I will show that complete singlet fission occurs for fully disordered molecules in solution. Specifically, two triplets are formed from a single molecule in the excited state and occurs with near-unity quantum efficiency, leading to ~200% triplet yield. We observe an intermediate whose geometry can be mapped using excited state electronic structure calculations. The resulting molecular picture of singlet fission suggests new design rules for chemists and new means to harvest light beyond the Shockley-Queisser limit.

Biography:

Dr Brian Walker is from the state of Maryland and received his undergraduate degree in chemistry with highest honours from Cornell University. He completed his PhD in physical chemistry at the Massachusetts Institute of Technology with Mounqi Bawendi, where he studied the chemical, and optoelectronic coupling between molecular aggregates and semiconductor nanocrystals. At Cambridge, Brian is the Herchel Smith Research Fellow in Materials for Sustainable Energy and a research fellow in Clare Hall. His research in the Cavendish is on the photovoltaic applications and fundamental mechanism of singlet exciton fission.