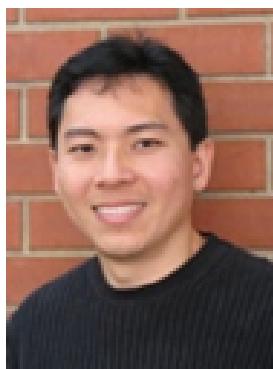


## CBC SEMINAR ANNOUNCEMENT



**Associate Professor Tak W. Kee**  
**University of Adelaide**

### **Making Two Triplets from One Singlet Exciton – Singlet Fission Yield of TIPS – Pentacene in a Polymer Matrix**

Singlet fission is a process by which a singlet exciton is dissociated to form two triplet excitons through a spin allowed process within a pair of molecules.<sup>1</sup> Singlet fission is attracting significant interest in renewable energy research because it addresses a critical issue in single-junction solar cells, of which the efficiency is limited to ~33%.<sup>2</sup> Singlet fission solar cells can potentially minimize thermalization of the initially prepared exciton, leading to a theoretical efficiency limit of 45%.<sup>3-4</sup> The accepted mechanism of singlet fission involves converting a singlet exciton to a correlated triplet pair (<sup>1</sup>TT), which further dissociates to form two separated triplet excitons.<sup>1</sup> Owing to the requirement of proximity of the two molecules for singlet fission, the intermolecular distance is expected to play a significant role in the quantum yield of triplet excitons. We have developed an aqueous nanoparticle system in which TIPS-pentacene, a compound that is known to undergo efficient singlet fission, in an inert, amorphous host polymer matrix. We have employed a combination of femtosecond transient absorption and time-resolved fluorescence spectroscopy to study the TIPS-pentacene/host polymer nanoparticles. The relaxation dynamics of excited state TIPS-pentacene exhibit a strong dependence on intermolecular distance, indicating a control of processes including singlet migration and singlet fission. Kinetic modelling of the time-resolved spectroscopic results indicates that only half the <sup>1</sup>TT population undergoes dissociation to form triplet excitons whereas the other half relaxes to the ground state. Our most recent work involves a combination of molecular dynamics simulation and Monte Carlo simulation to model the time-resolved fluorescence and polarization anisotropy experimental results. This work reveals the roles of singlet fission, singlet migration and aggregation of TIPS-pentacene in the host polymer matrix, contributing to further understanding of singlet fission mechanism.

#### References

1. M. Smith, and J. Michl, *Chem. Rev.* **2010**, 110, 6891.
2. W. Shockley and H. J. Queisser, *J. Appl. Phys.* **1961**, 32, 510.
3. M. J. Y. Tayebjee, A. A. Gray-Weale and T. W. Schmidt, *J. Phys. Chem. Lett.* **2012**, 3, 2749.
4. M. C. Hanna and A. J. Nozik, *J. Appl. Phys.* **2006**, 100, 074510.

**Date:** 8<sup>th</sup> February 2019 (Friday)  
**Time:** 2.00pm to 3.30pm  
**Venue:** SPMS Research & Graduate Studies  
Office Conference Room  
**Host:** Associate Professor Tan Howe Siang