CORE-CM SEMINAR
Michigan State University — Department of Chemistry

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Exciton Fission & Solar Energy Conversion Beyond The Limit

The absorption of one photon by a semiconductor material usually creates one electron-hole pair, but this general rule breaks down in a few organic semiconductors, such as pentacene and tetracene, where one photon absorption may result in two electronhole pairs in a process called singlet exciton. Recent measurements in our group by time resolved two-photon photoemission (TR-2PPE) spectroscopy in crystalline pentacene and tetracene provided the first spectroscopic signatures in singlet fission of a critical intermediate known as the multiexciton state. More importantly, population of the multiexciton state is found to rise concurrently with that of the singlet state on the ultrafast time scale upon photo excitation. This observation provides an experimental foundation for a quantum coherent mechanism in which the electronic coupling creates a quantum superposition of the singlet and the multiexciton state immediately following optical excitation. We demonstrate the feasibility of harvesting the multiexciton state for multiple charge carriers or the triplets. We outline a set of design principles for molecular materials with high singlet fission yield and for the implementation of singlet fission in solar cells with power conversion efficiency beyond the Shockley-Queisser limit.

[1] W.-L. Chan, M. Ligges, A. Jailaubekov, L. Kaake, L. Miaja-Avila, X.-Y. Zhu, "Observing the Multi-Exciton State in Singlet Fission and Ensuing Ultrafast Multi-Electron Transfer," *Science* 334 (2011) 1541-1545.
[2] W.-L. Chan, M. Ligges, X.-Y. Zhu, "The energy barrier in singlet fission can be overcome through coherent coupling and entropic gain," *Nature Chem.* 4 (2012) 840-845.
[3] W.-L. Chan, J. R. Tritsch, X.-Y. Zhu, "Harvesting singlet fission for solar energy conversion: one versus two electron transfer from the quantum mechanical superposition," *J. Am. Chem. Soc.* 134 (2012) 18295–18302.
[4] W.-L. Chan et al. "The quantum coherent mechanism for singlet fission: experiment and theory," *Acct. Chem. Res.* 46 (2013) 1321-1329.
[5] J. R. Tritsch, W.-L. Chan, X. Wu, N. R. Monahan, X.-Y. Zhu, "Harvesting singlet fission for solar energy conversion via triplet energy transfer," *Nature Commun.* 4 (2013) 2679.

Thursday, April 3, 2014
12:00 PM
Room 1400 – BPS
Professor Marcos Dantus – Host

Accommodations for persons with disabilities may be requested by calling the Chemistry Department at (517) 355-9715, X345 two days prior to the event to ensure sufficient time to make arrangements. Requests received after this date will be met when possible.