## Excitons at Organic Semiconductor Interfaces: Approaching or Exceeding the Limit in Solar Energy Conversion

## Prof. Dr. Xiaoyang Zhu

## Department of Chemistry, Columbia University, NY

This lecture aims to explore key mechanistic issues in an emerging photovoltaic technology based on organic and polymeric molecules, i.e., plastic solar cells. While there have been various predictions on whether or when photovoltaic technologies, including plastic solar cells, can be cost-competitive with electric power generation based on fossil fuels, one sometimes neglects the most important outcomes of fundamental research: the serendipity, the unpredictable, and the ground breaking discoveries that can throw the foundation of old predictions out of the window. I will present two examples from recent research in my laboratory on organic photovoltaics. The first example is within the realm of conventional theories and we aim to understand a critical step in charge separation at donor/acceptor interfaces in organic photovoltaics, namely the formation and dissociation of interfacial charge transfer excitons [1]. In particular, we show the critical role of hot charge transfer excitons in setting the fundamental time limit for charge separation in organic photovoltaics [2]. The second example illustrates the serendipity and potentially groundbreaking nature of research. We show how an intriguing physical phenomenon, exciton fission in which a singlet excitons breaks up into two triplet excitons in organic semiconductor materials, may be used to build solar cells with power conversion efficiency exceeding the fundamental limit (the so-called Shockley-Queisser limit) of conventional solar cells. We show how singlet exciton fission can occur in organic semiconductors due to a many electron quantum coherent process [3-4], and how we can efficiently extract two electrons from the quantum superposition [5].

- [1] M. Muntwiler, Q. Yang, W. A. Tisdale, X.-Y. Zhu, "Coulomb barrier for charge separation at an organic semiconductor interface," *Phys. Rev. Lett.* 101 (2008) 196403.
- [2] A. Jailaubekov, A. P. Willard, J. Tritsch, W.-L. Chan, N. Sai, L. Kaake, R. I. Gearba, K. Leung, P. J. Rossky, X.-Y. Zhu, "Hot charge transfer excitons set the time limit for charge separation at donor/acceptor interfaces in organic photovoltaics," *Nature Mater.* 12 (2013) 66-73.
- [3] 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.
- [4] 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.
- [5] 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.