NANYANG TECHNOLOGICAL UNIVERSITY SINGAPORE

Seminar Topic:
Engineering Cavity Singlet Fission in Rubrene

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Abstract
Hybridization of light and matter states creates unprecedented potential for molecular and materials sciences that greatly benefits organic and hybrid photovoltaics. Quantum light also opens up an entirely novel venue for nonlinear spectroscopy. By employing the numerically exact multiple Davydov D_2 ansatz, we study cavity-manipulated singlet fission that is mediated by polaritonic conical intersections for both 1- and 2-molecule systems. Population evolution of the TT state and the cavity photons is carefully examined in search for a high fission efficiency via cavity engineering. Several interesting mechanisms have been uncovered, such as photon-assisted singlet fission, system localization via a displaced photon state, and collective enhancement of the fission efficiency for the 2-molecule system. It has been demonstrated that the cavity-controlled singlet fission process can be switched on and off by controlling the average pumping photon number. Highly accurate methodology has also been developed for the simulation of nonlinear spectroscopic signals of cavity-assisted, conical-intersection-controlled singlet fission systems.*

*Research Articles:

- K. Sun, M.F. Gelin and Y. Zhao (2022) Engineering Cavity Singlet Fission in Rubrene. *Journal of Physical Chemistry Letters*, 13(18), 4090-4097. DOI: https://pubs.acs.org/doi/full/10.1021/acs.jpclett.2c00801
- K. Sun, M.F. Gelin and Y. Zhao (2022) Accurate Simulation of Spectroscopic Signatures of Cavity-Assisted, Conical-Intersection-Controlled Singlet Fission Processes. *Journal of Physical Chemistry Letters*, 13(19), 4280-4288. DOI: https://pubs.acs.org/doi/10.1021/acs.jpclett.2c00989#

Biography
Dr. Zhao was selected from the best of Chinese physics students to pursue PhD studies in the US by the prestigious CUSPEA program (sponsored by Nobel Laureate Tsung-Dao Lee). His Bachelor of Science was awarded by the Zhejiang University , and his PhD degree, University of California at San Diego. Following a brief stay in the International Center for Theoretical Physics in Trieste, Dr. Zhao took up a postdoctoral appointment at the Rochester Theory Center in University of Rochester, where he worked with Prof. Shaul Mukamel in Chemistry and Prof. Bob Knox in Physics. Prior to joining the Nanyang Technological University in 2007, he also held positions in the University of Hong Kong that include Research Assistant Professorship and Honorary Assistant Professorship. Upon arrival in NTU, Dr. Zhao received as PI over 11 million SGD of research funding.

Wednesday, 26 October 2022 ǁ Time: 2:00 pm - 3:00 pm ǁ
Venue: MSE Meeting Room (N4.1-01-28)
Hosted by: Nanyang Asst Prof Chae Sanghoon

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