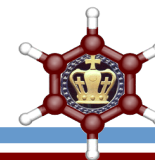




Columbia University Department of Chemistry
Fall 2017 Colloquium Seminar Series



Charge Transfer Dynamics, Excited State Energetics, and Organic Photovoltaics

Presented by Nandini Ananth, Cornell University

Addressing the challenge of designing efficient organic photovoltaics requires a detailed understanding of both the low-lying electronic excited states of molecular systems and the coupled nuclear-electron dynamics that drive exciton diffusion and dissociation. In the first part of this talk, we focus on our work towards developing novel path-integral based methods for approximate quantum dynamics that employ only classical trajectories to simulate condensed phase charge and energy transfer reactions. In the second part, we turn our attention to Singlet Fission (SF), a phenomenon that may hold the key to increasing the efficiency of organic solar cells. In SF, a singlet exciton formed by photon absorption spontaneously splits to form two longer-lived triplet excitons that can, in turn, dissociate to generate two free charges for every photon absorbed. Using accurate electronic structure to characterize excited states, orbital and normal mode analysis to identify vibronic couplings, and quantum dynamic simulations, we uncover two distinct mechanistic pathways for ultrafast SF in pentacene based materials. We then identify design rules for molecules with enhanced SF efficiency, and working with our experimental collaborators we verify them.



Hosted by
**Luis Campos and
David Reichman**

Thursday, September 14, 2017

1:30 – Meet the Speaker in room 328 Havemeyer

4:00 – Tea & Cookies in room 328 Havemeyer

4:30 – Seminar in room 209 Havemeyer



COLUMBIA UNIVERSITY
IN THE CITY OF NEW YORK

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All lectures take place on Thursdays at 4:30pm in room 209 Havemeyer, unless otherwise indicated. Tea and cookies will be served prior to each lecture at 4:00pm in room 328 Havemeyer.

Please check our website for updates. If you would like to be added to our email list, please email your request to d.farrell@columbia.edu.