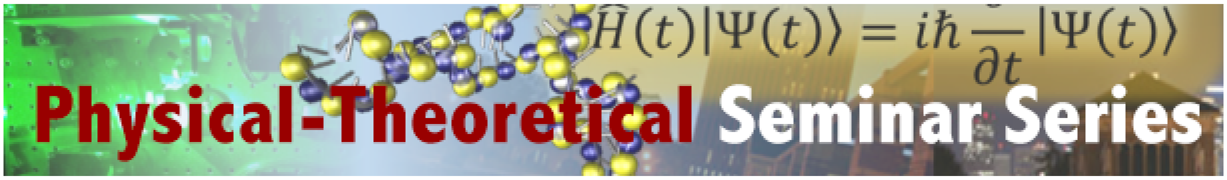

Monday, February 26, 2018, 12:00 pm
Seaver Science Library, Room 150
SSC Auditorium next to the library

Professor Sean Roberts

Department of Chemistry
University of Texas

Manipulating Energy and Spin in Molecular Semiconductors

The negligible spin orbit coupling in many organic molecules creates opportunities to alter the energy of excited electrons by manipulating their spin. In particular, molecules with a large exchange splitting have garnered interest due to their potential to undergo singlet fission (SF), a process where a molecule in a high-energy spin-singlet state shares its energy with a neighbor, placing both in a low-energy spin-triplet state. When incorporated into photovoltaic and photocatalytic systems, SF can offset losses from carrier thermalization, which account for ~50% of the energy dissipated by these technologies. Likewise, compounds that undergo SF's inverse, triplet fusion (TF), can be paired with infrared absorbers to create hybrid structures that upconvert infrared into visible light. However, integrating materials that undergo SF or TF with existing electronics remains challenging as the efficacy of these processes depends strongly on how molecules order in the solid state. I will summarize work aimed at identifying critical structure-function relationships that guide SF within perylenediimide (PDI) films. By adding functional groups at key locations along the PDI backbone, we can force these molecules to adopt different structures in the solid state. Guided by electronic structure calculations, we have used this approach to optimize the electronic coupling between PDIs such that they undergo SF with near quantitative efficiency. In addition, I'll describe recent work whose goal is to understanding energy transfer pathways that operate in hybrid organic:inorganic structures that use TF to upconvert infrared light into the visible range.

<u>References:</u>

Aaron K. Le, Jon A. Bender, Dylan H. Arias, Daniel E. Cotton, Justin C. Johnson, and Sean T. Roberts. Singlet Fission Involves an Interplay between Energetic Driving Force and Electronic Coupling in Perylenediimide Films. Journal of the American Chemical Society 2018 140 (2), 814-826. DOI: 10.1021/jacs.7b11888

Bender, J. A.; Raulerson, E. K.; Li, X.; Goldzak, T.; Van Voorhis, T.; Tang, M. L.; Roberts, S. T. Surface States Mediate Triplet Energy Transfer in Nanocrystal-Acene Composite Systems. ACS Nano.

Hosted by Professor Anna Krylov
The scientific community is invited

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