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Ph.D. in Chemistry, University of Chicago (2014)

Research Summary:

My Ph.D. research focused on quantum mechanical effects in photosynthesis, seeking to understand if and how quantum mechanics shapes the extraordinarily efficient energy transfer process in photosynthetic bacteria. My work used theory to clarify the interpretation of spectroscopic data, in particular exploring the implications of using coherent laser light to study energy transfer processes that occur under the incoherent light of the sun. Keldysh Green's function models were developed to simulate photosynthetic energy transfer under incoherent illumination. In developing Green's function models for the energy transfer process, various methods for simulating the effects of a noisy biological environment were implemented and compared. My current research interests focus on developing new ways to model charge transport in organic photovoltaics.

Selected Recent Publications:

Pelzer KM, Chan MKY, Gray SK, Darling SB. "Polaron structure and transport in fullerene materials: Insights from first-principles calculations." *Submitted to The Journal of Physical Chemistry C, 2014.*

Pelzer KM, Can T, Gray SK, Engel GS, Morr DK. "Coherent transport and energy flow patterns in photosynthesis under incoherent excitation." *The Journal of Physical Chemistry B 2014, 118: 2693-2702.*

Pelzer KM, Fidler AF, Gray SK, Engel GS. "The dependence of exciton transport efficiency on spatial variation in the radius of correlation." *New Journal of Physics 2013, 15: 095019.*

Pelzer KM, Griffin GB, Gray SK, Engel GS. "Inhomogeneous dephasing masks coherence lifetimes in ensemble measurements." *Journal of Chemical Physics 2012, 136: 164508.*

Pelzer K, Greenman L, Gidofalvi G, Mazziotti DA. "Strong correlation in acene sheets from the active-space variational two-electron reduced-density-matrix method: Effects of symmetry and size." *Journal of Physical Chemistry A 2011, 114: 583-88.*