

## **Extending the Lifetime of Nitrated Poliaromatic Hydrocarbons for Photoinduced Hole Transfer Systems**

**Eli M. Espinoza**

University of California, Riverside

Efficient solar-energy conversion relies on molecular-level control of charge transfer for organic electronics. Electromagnetic interactions, originating from the second strongest fundamental force in the universe, occur between charged particles. As electrostatic analogues of magnets, molecular electrets are dielectrics that contain ordered electric dipoles. Much like protein helices, anthranilamides, composed of non-native beta amino acids, possess intrinsic dipole moments originating from ordered amide and hydrogen bonds. Unlike the protein helices, however, anthranilamides have a backbone of directly linked aromatic moieties comprising pathways for highly efficient electron and hole transfer. The distal sites, i.e., the fourth and fifth position in the aromatic rings, provide a means for tuning the electronic properties of the electrets via chemical modifications. The dipole-generated local fields of the bioinspired molecular electrets rectify the kinetics of charge separation and charge recombination. That is, the rates of electron transfer along the dipole are different from the rates against the dipole. Because our focus is on hole-transfer electrets, we need a suitable electron acceptor for photoinitiating long-range charge transfer, providing the motivation for the design and development of such light sensitizers. To be able to harvest the energy from the sun, we choose sensitizers that absorb in the red, green and blue region of the spectrum, i.e., corroles, diketopyrrolopyrrole and fluorescent nitropyrenes. Such broad use of the light across the visible region of the electromagnetic spectrum will open avenues toward tandem light harvesting devices. In this presentation I will focus on our newly discovered fluorescence from nitropyrenes. Pyrenes are the most used organic photoprobes. Upon nitration, pyrene exhibits a shift in its absorption to the visible spectral region. While the nitro group makes it a better electron acceptor, the nitropyrene is non-fluorescent due to efficient triplet formation. Amidating the nitropyrene to produce  $\text{NO}_2\text{-Py-C(O)-NH-R}$  did not eliminate the intersystem crossing. Recently, we discovered that inversion of the amides suppresses triplet formation and makes nitropyrene fluorescent. However, is an amide bond needed for efficient fluorescence? Converting the  $(\text{NO}_2)_2\text{-Py-C(O)-NH-R}$  to  $(\text{NO}_2)_2\text{-Py-C(O)-NH}_2$  revealed a unique solvatochromism effect where the quantum yields was as high as 0.75 and lifetime of 5.6 ns in nonpolar toluene. Understanding what makes nitrated pyrene amines/amides fluoresce is necessary to create new novel chromophores for organic electronics.