Dipole Modulation of Charge Transfer in Anthranilamides

Molecular-level control of charge transfer is paramount for organic electronics and solar-energy conversion. 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. We have demonstrated the utility of anthranilamides as suitable candidates for a bioinspired approach in the design of molecular electrets. Anthranilamides comprise non-native beta amino acids, and much like protein helices, they 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 providing pathways for highly efficient electron and hole transfer.\textsuperscript{1,2} 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.\textsuperscript{2} The dipole of even a single anthranilamide residue can rectify the kinetics of charge separation and charge recombination.\textsuperscript{4} That is, the rates of electron transfer along the dipole are different from the rates against the dipole, and for an anthranilamide residue with an electron acceptor, that difference can be as large as an order of magnitude. Indeed, dipoles are key components for charge transfer rectification. The reports on dipole effect on charge transfer focus on the driving forces and the Franck-Condon component of the kinetics. Recently, we have examined the effects that electron-density distribution, affecting the electronic coupling, has on charge-transfer electrets. We determined that optimization of the initial photoinduced charge separation between the sensitizer and the first electret residue is key for efficient long-range charge transfer occurring via hopping mechanism. The synergy between the dipole effects on the Franck-Condon and the electronic-coupling components of the kinetics provides new unexplored paradigms for design and development of charge-transfer systems.

References