“Open-Shell Molecules: A Radical Design for Organic Optoelectronic Materials”

Friday, March 4, 2022, 11:30 AM
Life Science Center II, Room 130

Abstract: Open-shell molecules possess unpaired electron density (radical character), which makes them intriguing candidate materials for many optoelectronic applications. Air-stable structures have been reported, but most require lengthy synthetic sequences with limited generality. Our lab has developed a concise strategy for rapidly accessing a variety of bisphenalenyls from commercial starting materials. We used this method to synthesize a neutral biradicaloid, Ph$_2$s-IDPL, and several novel heteroatom-substituted, π-radical cations. One such molecule is O-substituted (Ph$_2$-PCPL)(OTf), which displays electrostatically-enhanced, intermolecular covalent-bonding interactions that impart remarkable charge transport properties. Specifically, we have discovered that mixing soluble PCPL derivatives with polystyrenesulfonate (PSS) enables the formation of water-processable, n-type conductive organic films that demonstrate high optical transparency (>94% transmission), electrical conductivity ($\sigma_{rt} < 117$ S/cm), and electron mobility ($\mu_e < 322$ cm$^2$ V$^{-1}$ s$^{-1}$). In these composites, PSS not only serves as a counterion, but also promotes n-doping and solution-phase aggregation, which leads to molecular ordering in solid-state. We have also discovered a N-substituted, red emissive, π-radical cation [(Ph$_2$-PQPL)(OTf)] that is structurally distinct from all other luminescent radicals, and achieves rare antiambipolar charge transport in field-effect transistors. N-substituted bisphenalenyls also display self-sensitized and reversible reactivity with dioxygen that shows potential for use in colorimetric oxygen sensors and for on-demand singlet oxygen release.

Biographical sketch: Mark Chen is an Assistant Professor in the Department of Chemistry at Lehigh University. He received his B.A. and Ph.D. in Chemistry from Harvard University with M.-Christina White developing catalytic C-H bond oxidation methodologies. As a Dreyfus postdoctoral fellow in the lab of Jean Fréchet at U. C. Berkeley, he led a team developing polymeric and molecular materials for organic electronic devices. Since coming to Lehigh University, the Chen Lab has investigated the synthesis of open-shell organic molecules and their application to optoelectronic materials and devices. Mark is the recipient of several awards, including a Kaufman Foundation New Investigator Award (2015) and NSF CAREER Award (2021).