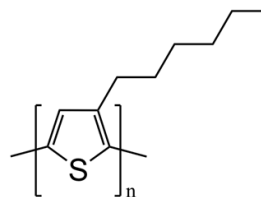


Chem 218: Student Exit Seminar

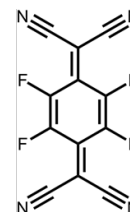
A Tale of Two Doping Mechanisms: Controlling the Formation of Charge Transfer Complexes in Chemically Doped Semiconducting Polymers

By **Dane A. Stanfield**
 Prof. Schwartz Group

Doping of organic semiconductors has emerged as a viable route for the inexpensive fabrication of numerous electronic devices such as light emitting diodes, thin film transistors, and thermoelectric generators. The p-type doping of polymer based semiconductors like P3HT is achieved through the introduction of chemically strong oxidizing agents like F₄TCNQ that usually undergo integer charge transfer, removing an electron from the extended π conjugation network, leaving behind a charged hole in its place that is free to conduct at the bulk level. In contrast, p-type doping of small molecule based semiconductors typically results in formation of charge transfer complexes,



P3HT



F₄TCNQ

where close spatial contact and orbital overlap between the host and guest species cause fractional charge transfer to occur. It has to date remained unclear why polymeric based semiconductors show a preference for doping via integer charge transfer while their small molecule counterparts usually undergo formation of fractional charge transfer complexes. In this talk, we will discuss recent advances in our understanding of the mechanisms that drive these two different types of charge transfer interactions in conjugated polymers. We show that it is possible to exert control over the type and abundance of each type of charge transfer interaction through the simple selection of processing solvent solubility parameters. We are also able to assign two structurally unique packing arrangements that correspond to integer or fractional charge transfer and compare the relative thermal stabilities of these two polymorphs. Finally, we show that the CN groups found on the dopant molecule, F₄TCNQ, can serve as a probe of the local electric field strength and thus the environment of the charge carriers as detected via the vibrational stark effect. Overall, this improved understanding of polymer-dopant interactions allows us to provide new guidelines for enhancing the doping efficiency and limiting the occurrence of fractional charge transfer states in doped semiconducting polymers.



Thursday, February 25, 2021
 12:00 p.m.
 Via Zoom

For questions, please contact: jzabala@chem.ucla.edu