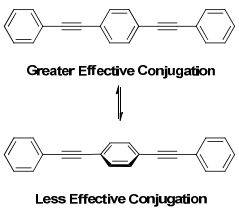
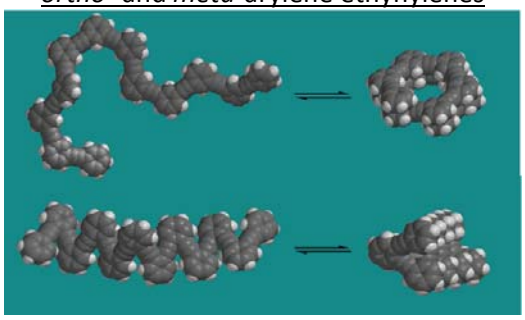
Research Overview: The main focus of our research is developing novel unsaturated compounds in which we can install unique molecular features that give us the ability to control the properties of not only individual molecules but also potential materials made from those molecules.

Rotation around single bonds is an important consideration in all arylene ethynylene research. In *para* systems, bond rotation leads to changes in the effective conjugation and therefore electronic properties of the unsaturated system. Similarly, rotation around single bonds in *ortho* and *meta* systems is necessary for the equilibrium between random coil and helical arrangements. The ability to manipulate *para*-phenylene ethynylene structures provides an opportunity to optimize functionality of organic substrates in next-generation electrical conductors, optical devices, sensors, and an array of other novel organic materials. Similarly, controlling the dynamics of helix formation in the isomeric *ortho*- and *meta*-phenylene ethynylenes provides an avenue for designing higher order molecular structures with valuable functions, such as host-guest chemistry.

para-arylene ethynylenes

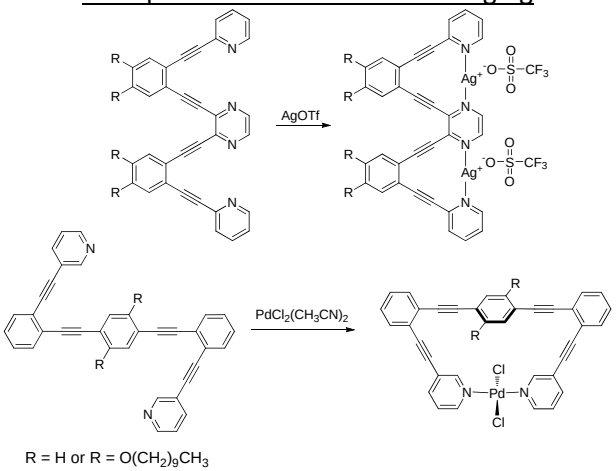


ortho- and *meta*-arylene ethynylenes



Our primary tools for controlling arylene ethynylene conformation are transition metal coordination and halogen bonding. With coordination, transition metals bridge two different regions of a molecule via attractions to nitrogen lone pairs. These bridges can result in significant changes in electronic properties. Similarly, halogen bond bridges can link two different regions of an arylene ethynylene compound via attractions of halogen atoms to nitrogen lone pairs. In the latter, the arylene ethynylene serves as a framework that allows us to study this lesser known intermolecular/intramolecular force.

Examples of Transition Metal Bridging



Examples of Halogen Bond Bridging