Rational design of conjugated triazole-based polymers for organic solar cells based on structure-property relationships

Jeromy Rech[1] and Wei You[1]

1. University of North Carolina at Chapel Hill

With the recent remarkable advances in the efficiency of organic solar cells, the need to distill key structure–property relationships for semiconducting materials cannot be understated. The fundamental design criteria based on these structure–property relationships will help realize low-cost, scalable, and high-efficiency materials. In this talk, we will systematically explore the impact of a variety of functional groups, including nitrogen heteroatoms, fluorine substituents, and cyano groups, along the conjugated polymer backbone. Each functional group and can modify the optoelectronic, photovoltaic, and morphological properties of the resulting solar cell, and we highlight the strengths and weaknesses of the functional groups and location of functionalization. Interestingly, amongst this library of polymers, there are limits to the improvements which can be made to the conjugated polymers, and a delicate balance is required to achieve the best organic solar cell. Overall, this work highlights some of the benefits, thresholds, and limitations for functionalization of conjugated polymers for organic solar cells.