Non-covalent functionalization of carbon nanotubes:
Controlling Chirality Selectivity via Alkyl Groups of Conjugated Co-Polymers

Braden Weight, Brendan Gifford, and Svetlana Kilina

Department of Chemistry and Biochemistry, North Dakota State University, ND

Carbon nanotubes (CNTs) play an important role in nanotechnology, including electronics, chemical sensors, and solar cells. Their electronic and optical properties depend on the size and geometry (chirality) of the nanotube. However, one main concern regarding nanotube application in optoelectronic devices is the difficulty of separating them based upon chirality after synthesis, as all known synthesis methods produce more than one chirality simultaneously. To get around this, one method is the functionalization of the CNTs via non-covalent bonding of co-polymers by wrapping them around the tube. We use force field simulations to explore the effects of various structural manipulations to the co-polymer 9,9-dialkylfluorenyl-2,7-diyl bipyridine (PFO-BPY) to find the preferential mechanisms of selective interactions between the PFO-BPY and CNTs of various chiralities. In particular, we focus on the effect of the branching in alkyl side-groups of PFO-BPY on their binding to the CNT surface. We have observed correlations between the side-group structures and their wrapping morphology on the CNT-Polymer interactions. Our calculations demonstrate that the branching in the position closest to the conjugated backboned results in the strongest interaction with all CNT.