“Structure and energetics of doped organic semiconductors”

Résumé: Doping organic semiconductors (OSCs) for enabling new functionality and improving opto-electronic device performance is done by adding strong molecular acceptors as p-dopants to the OSC host. I will discuss the broad range of phenomena observed upon molecularly p-doping conjugated polymers (CPs) and molecules (COMs), where two different competing scenarios emerged: (i) integer-charge transfer between OSC and dopant forming ion pairs (IPAs), and (ii), partial charge transfer with the emergence of OSC/dopant ground-state charge transfer complexes (CPXs). As prototypical representatives for these two scenarios, IPA formation in F4TCNQ-doped poly(3-hexylthiophene) (P3HT) is juxtaposed to CPX formation found for its parent oligomer, and the respective doping-induced modification of the density of states (DOS) is generally discussed and experimentally assessed by photoelectron spectroscopy. I will further focus on the determination of the thin-film structure of COMs/CPs, its modification through doping and its impact on the degree of charge transfer between OSC and dopant. Correlating Grazing-incidence X-ray diffraction with infrared spectroscopy for thermally annealed films finally provides insight into the complex growth behavior of p-doped P3HT.