Electronic structure of pentacene thin films doped with tetrafluoro-tetracyanoquinodimethane (F4-TCNQ)

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In various studies (in-)organic doping of functional organic materials was reported to lead to significant improvements in the performance of organic electronic devices. Using ultraviolet photoelectron spectroscopy (UPS) we investigated the electronic structure of thin films of the hole-transport material pentacene (PEN) doped via co-deposition with the organic acceptor F4-TCNQ (ratios of 1:1 and 10:1) on SiO_2 and the conducting polymer PEDOT:PSS as substrates.

In all cases we found a severely altered electronic structure of the PEN films upon F4-TCNQ admixture yielding ionization energies larger by at-least 0.3 eV compared to pristine PEN. The low-binding energy onset of the photoemission is well separated from the substrate Fermi level by 0.3 eV indicating entirely filled molecular orbitals in the mixed films. In optical absorption measurements it was observed that this new electronic structure found by UPS is accompanied by a decrease of the optical gap by 0.6 eV. Supporting x-ray diffraction experiments demonstrate almost (PEN:F4-TCNQ ratio 10:1) and entirely amorphous film growth (1:1). In this contribution these results will be discussed in the framework of the models of organic-organic charge transfer and organic doping.