Valence band tomography and the reconstruction of molecular orbitals from angle resolved photoemission

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With examples of chain- and plate-like molecules it will be shown that the combination of studies of conjugated molecules with modern electron energy spectrometers has led to advances in understanding valence band photoemission in general and the electronic structure of "organic semiconductors" in particular. Angle resolved valence band photoemission will be focused upon and it will be shown that the hitherto apparently complex angular distribution can be simply understood making it a very powerful tool. Examples of intra- and inter-band dispersion will demonstrate how a simple Fourier transform of molecular orbitals predicts the angular/momentum distribution of emitted photoelectrons. For adsorbate monolayers it will be shown how this can be used to reconstruct orbitals in real space, determine molecular geometries and gain insight into the nature of the surface chemical bond. Finally we show that momentum maps allow the orbital energy ordering to be unambiguously determined providing important bench marks for the selection of functionals for DFT calculations. Acknowledgment: This work was supported through the Austrian Science Foundation FWF national research network: Interface controlled and functionalized organic films.