How Metrology can improve Photoemission Tomography

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Photoemission tomography (PT) is a powerful tool to identify the electron orbital structure of mono- and bi-layers of molecules on surfaces. Using angle-resolved photoemission spectroscopy (ARPES) and assuming a basic plane wave as the final state of the measured photoelectrons, the molecular orbital structure can generally be represented by a Fourier Transformation of the resulting impulse maps, respectively in 2D. By stacking several of these maps for different photon energies, an equivalent reconstruction in 3D is possible. Thus, detailed information on electronic properties, geometric structures and molecular orbital densities of different molecular systems on different surfaces, e.g. Sexiphenyl, Pentacene or PTCDA, could be extracted [1], [2].

So far, the PT was successfully applied for molecules aligned on a surface [1], [3]. However, the angular and energy dependent photo emission is a basic property as well for atoms in gas phase. Thus we attempt to investigate if the PT might be generalized. Therefore, already existing datasets for angle-resolved photoemission of atomic systems in gas-phase will be evaluated, regarding the properties of the PT and a possible reconstruction of atomic orbitals.

In a collaborative work between the FZJ, the KFH Graz and the PTB, measurements are conducted, using the radiation of PTB‘s insertion device beamline (IDB) at the Metrology Light Source (MLS). Here, an absolute photon flux can be provided, which showed up to be necessary for a successful normalization of the 3D molecular orbitals. So far, a photo diode is used for the off-line determination of the absolute photon flux. In order to improve the results of the PT in a quantitative manner, a different monitor will be installed, using gas for an on-line calculation of the photon flux.

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[2] *Lüftner, D. et al. (2017). Understanding the photoemission distribution of strongly interacting two-dimensional overlayers. Physical Review B. 96. doi:10.1103/PhysRevB.96.125402.*

[3] *Weiß, S. et al. (2015). Exploring three-dimensional orbital imaging with energy-dependent photoemission tomography. Nat Commun.; 6:8287. Published 2015 Oct 5. doi:10.1038/ncomms9287*