O 12: Invited Talk (Achim Schöll)

Time: Monday 15:00–15:45 Location: TRE Phy

Invited Talk O 12.1 Mon 15:00 TRE Phy

Uncovering Molecular Orbitals by ARPES — •Achim Schöll — Experimentelle Physik VII, Universität Würzburg, 97074 Würzburg, Germany — Karlsruher Institut für Technologie (KIT), Gemeinschaftslabor für Nanoanalytik, 76021 Karlsruhe, Germany

Electrons are responsible for the structural, chemical and physical properties of materials. As one of the fundamental concepts of quantum mechanics, electrons in molecules are described by molecular orbitals. Consequently, visualizing these wave functions experimentally has been highly desired ever since quantum mechanics was established.

I will demonstrate how Angle Resolved Photoelectron Spectroscopy (ARPES) can provide unprecedented information on molecular orbitals by mapping the angle dependent intensity patterns of photoelectrons with a Photoelectron Emission Microscope (PEEM). The full potential of this tomographic technique becomes obvious by providing three-dimensional images of orbitals in real space. While this has already been proposed theoretically, I will demonstrate how 3D-imaging of molecular orbitals is feasible for the first time by momentum mapping with a PEEM and synchrotron radiation. This allows reconstruction of the molecular orbital in momentum space from the hemispherical k-space tomograms. The phase information, which is usually lost in the experiment but mandatory for the Fourier transformation of the orbital data into real space, can be derived from experiments with circular light polarization. In consequence, the full molecular orbital can be uncovered in 3D in real space, thus providing fascinating insight into the properties of electrons in molecules.