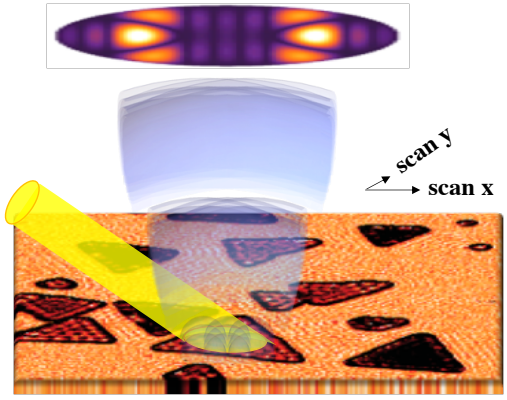
Master Arbeit: Wave Function Imaging

Angle resolved photoemission spectroscopy (ARPES) is a powerful *photon-in – electron-out* technique that efficiently measures the electronic band structure of long range ordered solid state. With the advent of modern electron spectrometers and powerful light sources (like third generation synchrotrons), ARPES has become a *must have* electronic structure probe in the field of experimental surface science and is heavily employed by several research groups here in Würzburg.



What only few people know, however, is that ARPES in principle can be also used to image electronic wave-functions (see figure to the left).[1] In order to do this properly, we need powerful but simplistic models to *reconstruct the wave-function amplitude and phase from the distribution of photoelectrons* measured by the detector.

Very recently, we developed an intuitive but powerful analytic model to describe ARPES based on effective Hamiltonians derived from DFT in combination with input from the experimental setting (We will start with simple tight binding models, however.). This formalism shall now be implemented into a code that interfaces state-of-the art DFT codes and allows us to routinely provide ARPES simulations (e.g., to EP4, EP7) based on their DFT or model band structures. In the second step, we will then invert this formalism to allow for a ***lens-less imaging of Bloch waves directly from the photoemission signal***. In the scope of this master project, the student thus will work at right at the interface between theory and experiment to

1) refine our photoemission model and properly but simplistically describe the ARPES process.
2) to invert the model for a direct imaging of the wavefunction from ARPES data.
3) to test this formalism for real 2D quantum materials, such as graphene

If you are interested to put your **mathematical and numerical skills** to life and get a direct glance at electronic wave-functions, then please contact:

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References

1. Puschnig, P. *et al.* Reconstruction of Molecular Orbital Densities from Photoemission Data. *Science (80-.).* **326**, 702–706 (2009).