

# **AB-INITIO ARPES CALCULATIONS AND THEIR LESS ACCURATE DERIVATIVES**

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Valence band photoemission spectroscopy is theoretically governed by the golden rule which usually is applied at various degrees of accuracy. Here, the one-step model calculation is presented as an ab-initio scheme on an APW basis for the initial bound states as well as for the final outgoing states, and compared with simplified schemes. Thus, the quality of the calculated photoemission spectra is limited only by the accuracy of the band-structure calculation. Computationally more demanding it shows a significantly higher agreement with experiment. Theory seems to close up with experiment in that detailed effects are revealed and explained through associated spectral structures which nowadays are experimentally resolvable. Thus, a basis is prepared to investigate also next order corrections.

For example, modern light sources with high photon intensities might ask for an extension of photoemission codes towards nonlinear field effects, i.e. photocurrent beyond quadratic order. Especially, ballistic behavior competes with multiphoton processes if tuned to suitable photon intensity, photon energy and electron detector parameters.