Exploration of Orbital Characters and Symmetries in Correlated Materials using Cross-Sections in (Angle Integrated) Photoemission Spectroscopy

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To understand the electronic structure of correlated and complex materials, it is crucial not only to have theoretical models, but also the experimental evidence that guide and validate them. For that, one of the most direct approaches is the photoemission spectroscopy, a technique that has for decades been considered the workhorse for electronic structure studies and is by now a well-established, highly widespread tool.

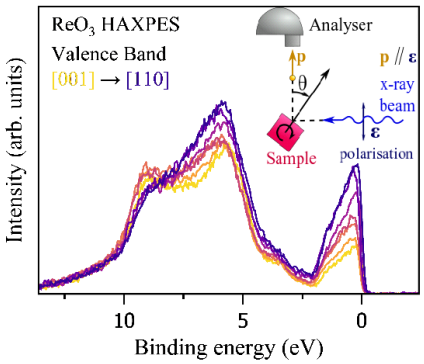

Figure 1. Angle integrated valence band spectra of ReO_3 at different crystallographic orientations [2].

While many novel and promising approaches based on the photoemission principle are being developed with state-of-the-art technologies, its most *vanilla* form of angle integrated photoemission is by now often considered by many rather limited and old-fashioned.

However, in this presentation, we show how by using the (often underappreciated) photoionization cross-sections, a wide range of new possibilities and understanding is enabled. The choice of geometry allows or facilitates comparisons to theory by selectively suppressing or enhancing the orbital contributions of interest [1] and can even provide complete novel capabilities such as directly obtaining from the experiment the symmetries of the different states in the valence band [2]. We will also show that such considerations are also key to preventing misidentifications [3] that could and have resulted in wrong leads. We thus show that for the study of correlated materials, there is still plenty to learn from and about photoemission spectroscopy.

References

[1] D. Takegami *et al*, Phys. Rev. X **12**, 011017 (2022)

[2] D. Takegami *et al*, Phys. Rev. Research **4**, 033108 (2022)

[3] D. Takegami *et al*, Phys. Rev. B **99**, 165101 (2019)