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Multidimensional Photoemission Spectroscopy: proposal & demonstration of data (infra)structure

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The complexity of photoemission data is rapidly increasing, as new technological breakthroughs have enabled multidimensional parallel acquisition of multiple observables. Most of the community is currently using heterogeneous data formats and workflows.

We propose a new data format based on NeXus, a hierarchically organized hdf5 structure. The aim is to immediately enable preprocessed data and metadata shareability according to FAIR principles, employing the existing storage and archiving infrastructure such as Zenodo, OpenAIRE and Nomad/FAIRmat. Ultimately, the multidimensional photoemission spectroscopy (MPES) format is designed to allow high-performance automated access, providing experimental databases for high-throughput material search.

The MPES format is based on the creation of a standardized set of classes that univocally identify experimental observables and metadata. Such dictionary is complemented by "application definitions", i.e. ontologies that constrain the existence of specific elements in a file.

Our approach involves reaching out to the community using a website with a wiki structure. By this medium, we wish to favour acceptance, to avoid conflict with different low-level preprocessing workflows, and to create continuously updated documentation.

As a demonstrator of the potential of our approach, we present the workflow we developed for our data pipeline, originating from time-resolved angularly-resolved photoemission spectroscopy.

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