



## Recent advancements in laboratory PDF data quality

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Although the very first laboratory-based X-ray pair distribution function (PDF) analysis had been carried out in the 1930s [1], laboratory PDF studies have been pretty uncommon till a few years back. [2] Limited momentum transfer vector  $Q_{\max}$ , insufficient instrumental resolution and very long measurement times impeded a routine use for structural refinements. A few years ago, we have significantly pushed instrumental resolution of PDF data in the laboratory by reducing air scattering and optimizing beamstop positioning for a diffractometer in transmission geometry, using a MYTHEN2 4K module to cover a large angular range. [3] The use of monochromatic Ag  $K\alpha_1$  radiation permitted laboratory PDF data to be fitted over interatomic distance ranges of several dozens of Angstroms, e.g. to refine PDF data of 7 nm  $TiO_2$  nanoparticles with a goodness-of-fit  $R_w$  as low as 0.222 over 70 Å. Since then and as very specialized PDF setups are not available in many laboratories, more diverse attempts to optimize laboratory PDF analysis have been carried out. Diffractometers using Goebel mirrors provide  $K\alpha_{1,2}$  mixtures, which results in overlap of PDF peaks beyond about 20 Å. However, recent advanced data processing evolved and, for instance, TOPAS can nowadays deconvolute the instrumental contributions such as wavelength mixtures, emission profiles or axial divergence, yielding less instrumentally dampened PDF data [4] – in particular for crystalline materials. This approach is showcased and compared to monochromatically measured laboratory PDF data. To conclude, and in light of recent pushes in high-energy X-ray detectors such as the HyPix-Arc series (Rigaku) or Photon III (Bruker) combined with high-flux microfocus sources, single crystal diffractometers can accomplish very decent PDF data in only about two hours. This approach is based again on  $K\alpha_2$  stripping, necessary for data fitting beyond 30 Å, and highlighted for poorly crystalline powders and solutions of polynuclear lanthanide complexes. [5]

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