MS38-P02 | PUSHING DATA QUALITY FOR LABORATORY PAIR DISTRIBUTION FUNCTION EXPERIMENTS

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Although the very first laboratory X-ray pair distribution function (PDF) measurement was carried out in the 1930s [1], laboratory PDF studies are rare. Only few studies emerged during the last decade [2], but limited Q_{max} or insufficient instrumental resolution impeded a routine use for structural refinements. Based on a STOE STADI P powder diffractometer in transmission geometry, we designed a novel PDF diffractometer with monochromatic Ag $K\alpha_1$ radiation covering a Q-range of 0.3 - 20.5 $Å^{-1}$ (144° 2θ). Four MYTHEN2 silicon strip detectors are arranged as a MYTHEN2 4K module on one detector arm, providing high instrumental resolution and low background. PDF data is collected in a moving mode within 6 hours for powders. For benchmarking, we measured and refined LaB_6 standards with goodness-of-fits R_w = 0.14 over 80 Å, and ca. 7 nm TiO_2 nanoparticles over 30 Å with R_w = 0.18. While all previous lab PDF studies did not show or refine any data for distances > 30 Å – due to a PDF peak overlap beyond ca. 25 Å due to a lack of monochromatization - we can readily refine our TiO_2 PDF data with an R_w as low as 0.22 over 70 Å. [3] Further data on ionic liquids and metal organic frameworks will be presented.

[1] B.E. Warren, et a., *Physical Review* **46** (1934) 368
[2] J.T. Nijenhuis, et al., *Z. Kristallogr.* **2009** (2009) 163
[3] S.L.J. Thomä, et al., *Rev. Sci. Instr.* (2019)*, accepted*