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SINGLE CRYSTAL TOTAL SCATTERING USING IN-HOME DIFFRACTOMETERS

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Single crystal diffraction analysis is largely considered the gold standard for atomic structure determination. This is surely due to an ever-advancing automation of software and instruments, but a more fundamental reason is that single crystals provide 3D-resolved data, where structural information along different crystallographic directions is not averaged out by a broad distribution of crystallite orientations. If, on the one hand, crystal structures can be reliably determined by using appropriately indexed powder diffractograms, real structure features such as defects, disorder and their local arrangement produce broader inter-Bragg intensities, whose 3D features can only be analyzed using single crystal data. The interpretation and use of these intensities, combined with the determination of the average crystal structure, is known as 'single crystal total scattering analysis'.

This lecture serves as an introduction and a welcome to this technique. We will explore why a total scattering mindset is important to approach crystallography with better awareness and summarize useful rules of thumb for interpreting diffuse scattering reconstructions. Most importantly, we will analyze key aspects for the acquisition of informative single crystal total scattering data with in-home instrumentation, thereby showing how this analysis can be conducted reliably also without synchrotron-grade data.