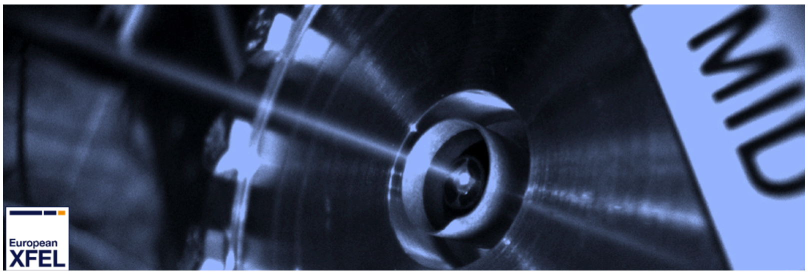

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Towards pump–probe single-crystal XFEL refinements for small-unit-cell systems

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X-ray crystallography on macromolecular compounds has seen significant progress through X-ray free electron laser (XFEL) studies (Chapman et al., 2011, 2014; Schlichting, 2015). This is, among other things, because the short pulse durations of serial femtosecond crystallography essentially remove all effects of beam damage and atomic motion, and because the extreme brilliance reduces the crystallite size required for sufficient scattering intensity.
Recently, a dedicated pipeline for small unit-cell systems (Figure 1) has been published (Støckler et al. 2023) capable of handling of all steps of data reduction from spot harvesting to merged structure factors and has successfully solved the structure of K4[Pt2(P2O5H2)4] 2(H2O). There are still challenging aspects for which a higher energy might be the answer. Particularly the partiality correction critically relies on the accurate determination of the crystal orientation which is complicated by the low number of diffraction spots for small-unit-cell systems. Here, the compressed reciprocal space for higher energies allows for the observation of more diffraction spots per shot, improving the performance of the orientation refinement and generally making more data available. As of now, the impact of systematic errors such as absorption and extinction on the structure remain buried under the larger errors introduced by the partiality correction and the inter-shot scaling. Again, the application of a high energy XFEL will minimize systematic errors, facilitate more accurate structures and is expected to enable investigations of excited states and reaction intermediate chemistry.

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