Contribution ID: **117** Type: **Poster**

Data driven models for structure determination from powder diffraction measurements

The structure determination pipeline of a polycrystalline sample from its powder diffraction measurement has several adjunct steps, which are as follows: background removal, peak finding, indexing, database matching, extinction and space group(s) determination, atom type and position determination, and finally Rietveld refinement. Experienced users employ various well-established algorithms—available in software tools such as EXPO2014, Match!, GSASII, and FullProf—at different stages of the pipeline. At each step, they must apply their expertise to interpret results, evaluate candidate solutions, and make informed decisions to advance the structure determination process effectively. Our research focuses on (1) leveraging data-driven models as alternatives to various steps in the aforementioned pipeline and (2) developing a broader universal AI framework to directly propose candidate solutions. In the first direction, we have achieved state-of-the-art results in symmetry prediction tasks, with our model outperforming well-known indexing algorithms, such as those in EXPO2014, when used independently. We analyze our models in terms of robustness to noise and experimental effects, generalizability, and scalability, with a focus on their applicability to our broader goal of developing an automated AI for structure solution. From a user-focused software standpoint, we aim to integrate our most robust models into our AIXtal platform, as AI helpers.

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Session Classification: Poster