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AIXtal –A Web and now Cross-platform Refinement Platform for First-Time Users

AIXtal is an accessible refinement platform designed specifically for first-time users. It includes a simplified user interface with reduced complexity, tutorials, tooltips and AI helpers for assistance. Currently, AIXtal supports GSAS-II and Fullprof (undergoing a refactoring) refinement of powder X-ray diffraction data. The platform provides visualization of structural, experimental and refinement data, including graphical background selection. The user is supported by on-demand assistance on refinement parameters, either through short tooltips or an AI guide that semi-quantitatively assesses the last refinement result/parameter and recommends next refinement steps. For more in-depth investigation, the user can also access a compact view (web or PDF) of the refinement parameters, including esd's. If unfavorable refinement steps are indicated, the user can rely on the history function to jump back to any point in time. AIXtal also allows the user to export the refinement results in GPX format for further analysis with GSAS-II, if required. The platform AIXtal v1 with this functionality is in alpha state and was tested with students of chemistry lab course in April/May 2024. AIXtal v2 is currently being developed based on the experience from AIXtal v1 and in order to broaden the use case scenarios. With multiple modes of operation, adding an expert mode with full refinement control to the simplified interface, it opens up for future developments of a more universal GUI for Rietveld programs also addressing other common, related crystallographic issues, e.g., a space group prediction. Furthermore, the web interface now runs on WebAssembly, which promises performance gains, and moreover now runs not only in the WebBrowser but also natively on Windows and Linux to allow a local installation as well. The GSAS-II implementation has also been extended to support refinement and visualization of multi-dimensional (angular and wavelength dispersive) data sets.

Current status, AI-helpers and features of AIXtal as well as its technical design principles are shown.

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