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EXPO Software: Advances Tools for Structural Analysis of Crystalline Materials by X-ray Powder Diffraction

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Background and State of the Art

In recent years, the number of crystal structures solved from powder X-ray diffraction (PXRD) data has been increasing, as proved by the number of crystallographic information files (CIFs) deposited in the various crystal structure databases. Even though still not comparable to the single-crystal case, structure solution of microcrystalline powders has become widespread, especially in the case of small-size molecules. This success is well supported by the availability of software, among which we mention DASH,[1] FOX,[2] SUPERFLIP,[3] and EXPO,[4] the software developed by the Institute of Crystallography. This latter is able to solve crystal structures from powder diffraction data by using reciprocal- (Direct Methods) as well as real-space methods (Simulated Annealing). It is able to carry out the full pathway of the solution process: indexing, space group determination, estimation of the integrated intensities, structure solution and Rietveld refinement. Over the past few years, EXPO has been enriched with new powerful computing tools for enhancing the structure solution process and facing challenging cases.[4] Our research activity is focused on developing advanced crystallographic methodologies that are implemented in EXPO for making the solution process successful and more easily accessible also to not experts in crystallography.

Results[5,6]

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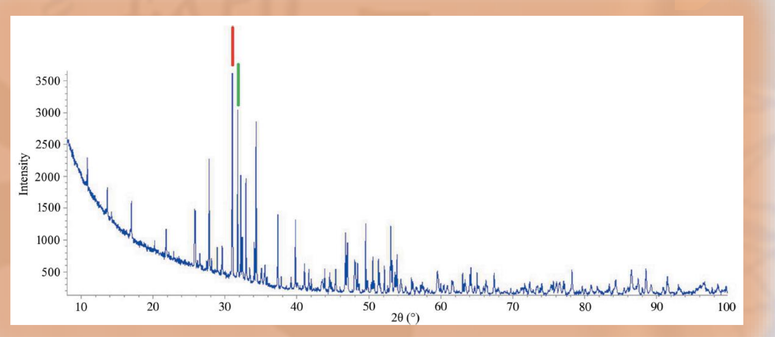
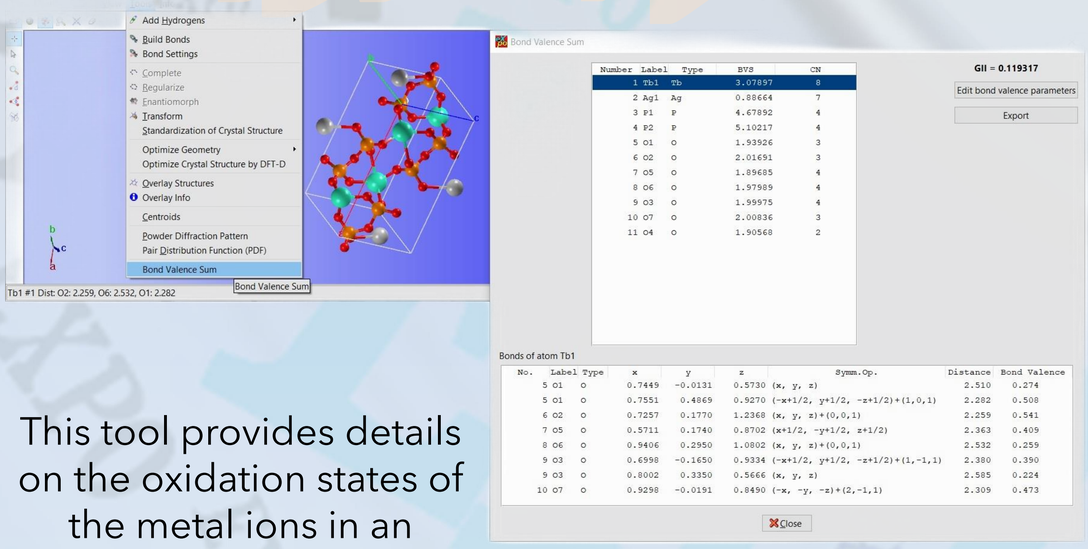
Additional Tools

- *Crystal structure solution in case of a mixture of chemical phases*



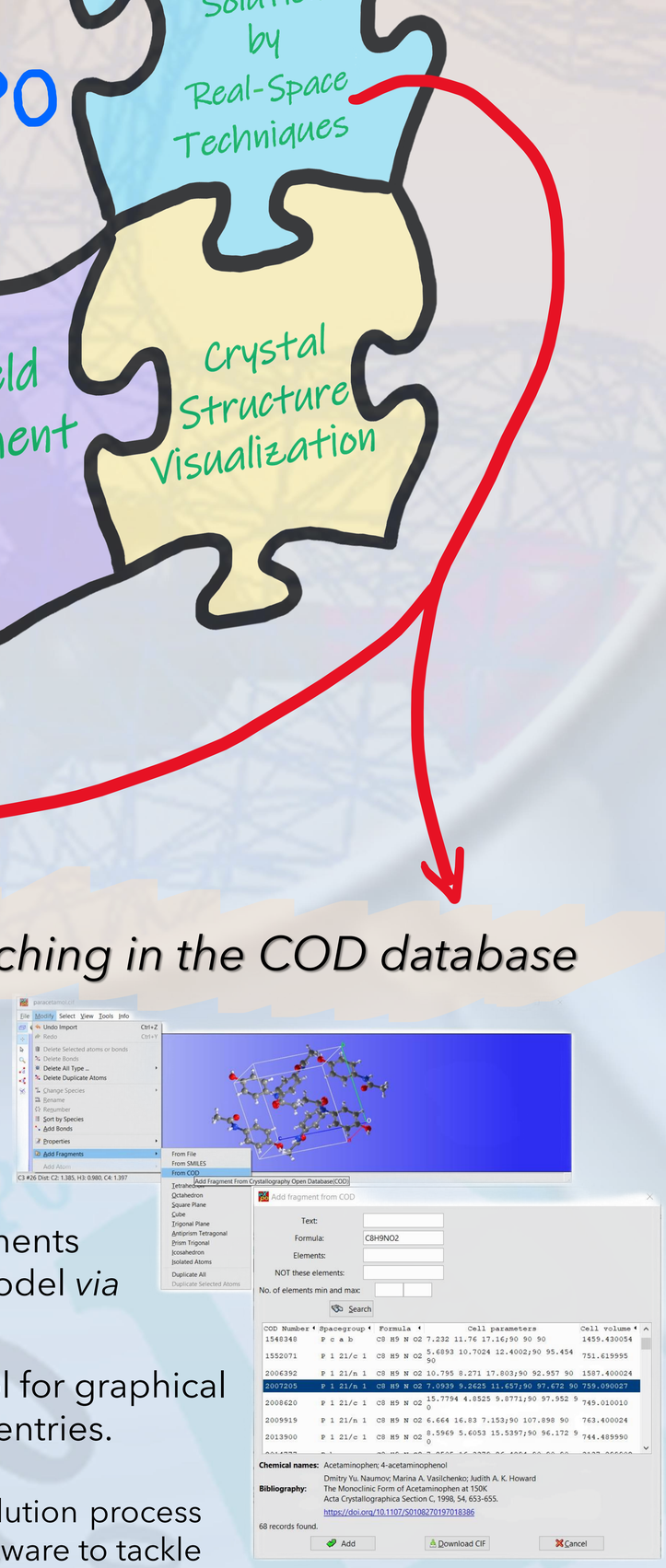
Capability to solve an UNKNOWN structure from a mixture composed of one UNKNOWN structure and one or more KNOWN structures

- *Bond Valence Sum (BVS) Tool*



This tool provides details on the oxidation states of the metal ions in an inorganic compound and serves as an additional support for the accuracy of the corresponding crystal structure.

- *EISM Tool for searching in the COD database*



This tool enables to import CIF files from the COD database[7] by allowing the user to provide the chemical formula or the chemical elements contained in the structure model *via* the graphical interface.

The EISM is also a handy tool for graphical visualization of COD entries.

Conclusions

Innovative computational and graphical tools have been implemented for advancing the crystal structure solution process from powder diffraction data using the EXPO software. These tools enabled to improve the capacity of the software to tackle challenging solution cases and make the structural analysis of microcrystalline materials more user friendly.

References

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