Realization of Common Platform Technology, Facilities, and Equipment that creates Innovative Knowledge and Products

Upgrading of the Fourier and global optimization techniques used in material structure analysis

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Summary :

In the analysis of experimental data based on nonlinear optimization methods, it is generally considered that very time-consuming procedures are required for concluding that the true solution has been obtained.

However, for example, magnetic structure analysis and acquisition of occupancies or chemical species in crystal structure analysis belong to the type of problem for which the framework of convex relaxation can be used to ensure the obtained solution in very short time. In this project, various new techniques such as removal of truncation errors in the Fourier analysis will be also applied, in order to open up new capabilities of mathematical data analysis.