Close Contact penalty Functions in direct Space Methods and energetic Considerations in Structure Refinement

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When solving crystal structures from powder diffraction data using direct space methods, all available information such as molecular structures and space group symmetry is used to limit the number of degrees of freedom. When limited quantity of information is available from a powder diffraction pattern (e.g., broad peaks, preferred orientation, positions of weak scatters) and/or the number of degrees of freedom is large, it may be necessary to add extra chemical information in order to obtain a solution. This chemical information can be that the generated structures should be energetically stable, where the potential energy contributes to a combined figure of merit alongside the powder pattern similarity, R_{wp}.

Considering the fact that viable solutions should not contain overlapping atoms, adding a simple close contact penalty that prevents solutions with non-viable intermolecular interactions from being generated is adequate for the global optimization process, which aims at locating a rough, refinenable solution.

During Rietveld refinement an accurate description of the potential energy should be used in combination with the R_{wp} in a weighted optimization process. The a priori determination of the weighting factor might not be intuitive; in such cases a Pareto optimization (a posteriori preference articulation) can be used to obtain an appropriate value so as to ensure that structures that are both chemically viable and in close agreement with the experimental powder pattern.

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