

## ***Ab Initio* Solution of Incommensurately Modulated Structures by Charge Flipping**

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“Charge flipping” is an algorithm for *ab initio* structure solution from X-ray diffraction data, which is based on alternating modifications of a trial electron density in direct and reciprocal space [1]. This algorithm makes no use of the atomicity of the chemical structure. It is instead based on the observation that the electron density of a crystal consists of a small number of high-density areas separated by large areas with very small electron density. This property is common to both electron densities of periodic structures and superspace electron densities of modulated structures. Therefore, charge flipping can be generalized towards superspace and used to reconstruct the superspace electron densities [2].

Up to now the structure solution of incommensurately modulated structures has been a two-step procedure involving solution of the basic periodic structure followed by the determination of the modulation. Charge flipping offers for the first time the possibility to solve the modulated structures directly in superspace, avoiding the often tedious task to construct and refine the basic structure.

Charge flipping was successfully applied to solve several modulated crystal structures including several organic and organometallic compounds with complex modulations [2].

[1] Oszlányi G., Sütő A., *Acta Cryst.*, 2004, **A60**, 134. [2] Palatinus L., *Acta Cryst.*, 2004, **A60**, 604.

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