Ab-initio Structure Solution without the Use of Atomicity

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Charge flipping [1] is an amazingly simple ab-initio structure solution method that is based on the existence of extended zero regions in the electron density, but not directly on atomicity. The algorithm is iterative: the real-space modification simply changes the sign of electron density below a threshold, while in reciprocal space observed moduli are prescribed without any weighting. It was tested using synthetic data for a wide range of structures [1], and was shown to work on real data of both normal [2] and modulated [3] crystals. Recently, we have found an efficient modification of the charge flipping algorithm [4] that complements the phase exploration in reciprocal space. In the modified algorithm weak reflections are treated separately, their calculated moduli are let to change freely and their calculated phases are shifted by $\pi/2$. Paradoxically, it is better not to use observed moduli of weak reflections, in the search for a solution they create only unwanted constraints. The improvement is drastic, in some cases the success rate is increased by a factor of ten, in other cases a previously unsolvable structure becomes solvable by the modified algorithm.

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