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Single crystal diffuse scattering–a solution to the phase problem?

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It is well known that the phase problem can be easily solved if oversampled scattering intensities are available [1]. This idea is the foundation of the coherent imaging method, which allows to reconstruct electron density of a separated object using speckle images measured in reciprocal space on a grid which is finer than the Shannon frequency of the object.

It has ben shown that in a special case of translational disorder of solid objects, single crystal diffuse scattering can be used instead of speckle patterns [2]. In such case diffuse scattering is proportional to the molecular form factor and can be phased, in addition it can be measured between Bragg peaks and thus provides Shannon oversampling. However in general it is incorrect to assign phases to raw diffuse scattering, because by definition diffuse scattering at each reciprocal space point is an incoherent average of multiple contributions with different phases.

In the current contribution we propose a new method which allows to overcome this problem in the case of binary disorder. We show how to separate raw diffuse scattering into short range order parameters and a difference molecular form factor. The molecular form factor can then be phased using standard dual phase methods. This allows to investigate the structure of disordered molecules using solely diffuse scattering, without the use of Bragg peaks. The method can be applied to a wide range of disordered solids, including crystals with molecular disorder, charge disproportionation and stacking faults.
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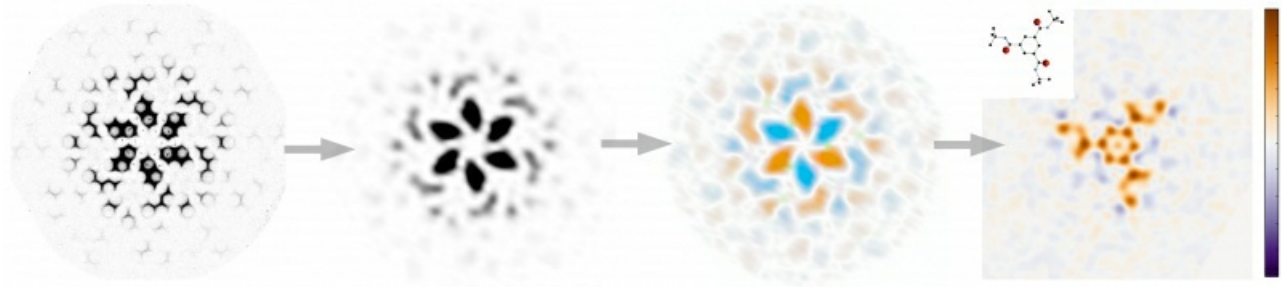

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