Oral presentation

Characterising the local structures of metal halide clusters in MOFs using deep learning

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Constraining the size, shape and dimensionality of inorganic structures can lead to enhanced optical, electronic, magnetic, and catalytic properties [1]. One synthetic approach is to grow metal halide nanostructures inside single crystal MOFs [2]. Understanding the links between synthesis and the resulting structures, including how they are arranged on a local scale, is vital for establishing precise control over the desired properties. Diffuse scattering is one technique that can provide this insight. For simple substitutional disorder, the analysis can be simplified under assumption that the scattering is a product of two components: I_{FF} and I_{SRO}, arising from the form factor difference between the disordered atoms A and B, and the compositional short-range correlations, respectively [3]. We recently showed that this factorisation can be performed rapidly and accurately using deep learning methods.[4] Our neural network, DSFU-Net, was trained on a dataset of ~200000 planes of simulated diffuse scattering and demonstrated its efficacy on the solved disordered structure of tris-tert-butyl-1,3,5-benzene tricarboxamide, producing outputs at sufficient quality to be useful for quantitative analysis and the extraction of structural information.

Here, we further test and develop this method by applying it to a series of MOF frameworks with metal halide clusters residing in the pores. By modelling I_{FF}, we deduce that the diffuse scattering is largely due to whether or not a cluster is present within the pores, with the exact form of I_{FF} being sensitive to the shape of the clusters. We characterise the local correlations between clusters in terms of SRO parameters refined from the I_{SRO} and find a range of local configurations depending on the cluster. The workflow for an example system is illustrated in Fig. 1. These materials provide excellent experimental case studies to streamline our deep learning approach and the insight gained could provide the basis for relating the disorder in these materials to the synthetic conditions, ultimately enabling synthetic control over disorder, and providing another design parameter to be exploited.

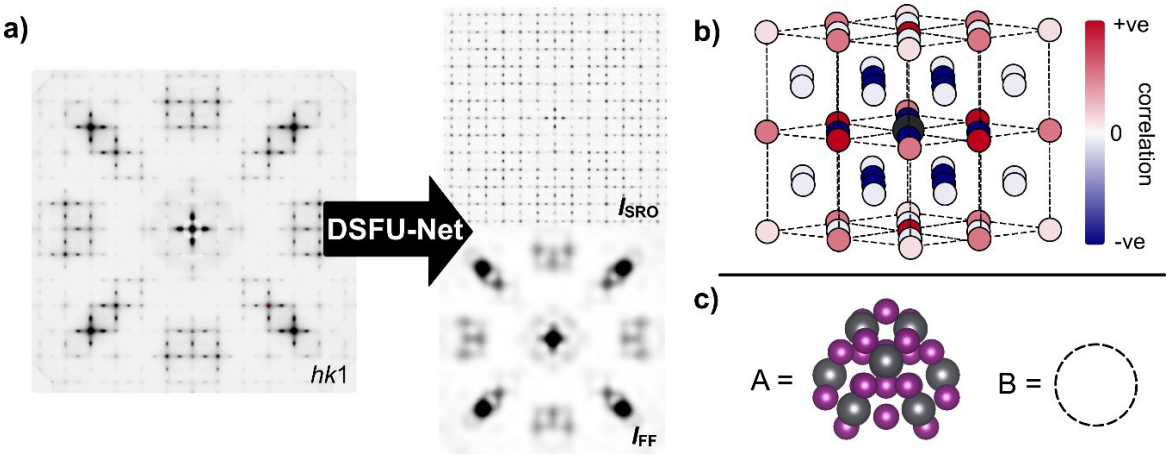

Figure 1. **a)** The reconstructed *hk*1 plane is factorised into its constituent I_{FF} and I_{SRO} by DSFU-Net. **b)** A visualisation of the SRO parameters refined from I_{SRO}. The colour represents the sign and strength of the correlations between the metal halide clusters at that position relative to the central cluster in grey. c**)** The structure of a metal halide cluster and a vacancy, illustrating the occupational disorder responsible for the diffuse scattering.

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