Applications of 3D-PDF

Oral presentation

Structural complexity on local scale in Prussian Blue Analogues

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In this work, we review structural complexity in the family of Prussian Blue Analogues (PBAs). These porous framework materials are extensively studied for ion trapping, gas storage, gas purification, as well as for rare electronic and magnetic effects like charge transfer and humidity-sensitive magnetism [1,2]. Despite their simple cubic *average* structures, PBAs reveal rich complexity in the *local* structure [3], which manifests in various diffuse features observed in single-crystal diffuse scattering. Using 3D- Δ PDF analysis [4,5], we demonstrate local structure motifs that give rise to observed diffuse scattering.

Our objectives are threefold:

- 1. To classify the different types of disorder observed in synthesized PBA crystals.
- 2. To review synthetic methods to control local structure and crystal symmetry in PBAs.
- 3. To demonstrate "hidden" structural transitions occurring during post-synthetic treatments, such as dehydration, freezing, or gas loading.

We anticipate that the trends discovered in PBAs will be relevant to a wide variety of materials, such as Metal-Organic Frameworks.

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