MS17-2-6 Tuning local structure in Prussian blue analogues (PBAs)
#MS17-2-6

Y. Kholina [1], A. Simonov [1]
[1]ETH Zurich - Zurich (Switzerland)

Abstract
Frontier research seeks to control the local structure of disordered crystals to optimize their functional properties. We apply this approach to the Prussian Blue Analogue (PBA) system with the chemical formula Mn[Co(CN)6]2/3*xH2O, which we abbreviate as Mn[Co]. The structure of this material contains 33% of Co(CN)6 vacancies. These vacancies create a highly connected porous network, making PBAs attractive for hydrogen storage applications. It was theoretically shown that the connectivity and the accessible volume of such a network depend on vacancy distribution [1]. Therefore, to optimize mass transport properties, we need to grow material with a particular local structure. In this work, we show how to tune the local structure of PBA crystals grown in gel by varying the crystallization parameters: type of gel, crystallization temperature, the concentration of reactants, and concentration of chelating agents. We probe defect distribution by measuring the single crystal X-ray diffuse scattering, which allows quantitative characterization of local structure. All above-mentioned parameters allow smooth continuous control of diffuse scattering and thus of local order in Mn[Co] PBA crystals.