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Tuning local structure in Prussian blue analogues (PBAs)

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Prussian Blue analogues, $M[M'(CN)_6]_{1-x}$ n·H_2O, which we abbreviate here as M[M'] (M and M'=transition metal ions), is a diverse family of cyanide materials, which is intensely investigated for its potential application for hydrogen storage, as catalysts and as electrode materials. Applications that require efficient mass transport utilize the ability of the structure to accommodate a large number of $M'(CN)_6$ vacancies, which create a highly connected porous network. It was theoretically shown that the connectivity and the accessible volume of such a network depend on the local structure[1]. Therefore, to optimize mass transport properties not only the number of vacancies but also their distribution must be precisely controlled. In this work we show how to tune the local structure of Mn[Co] Prussian Blue analogues grown in gel by varying the crystallization parameters: the type of gel, the crystallization temperature, the concentration of reactants, and the concentration of chelating agents. We probe the defect distribution by single-crystal x-ray diffuse scattering, which allows quantitative characterization of the local structure. All of the above-mentioned parameters allow smooth continuous control of diffuse scattering and thus of the local order in Mn[Co] crystals.

[1] A. Simonov, et. al., Nature 578.7794, 256-260 (2020).

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