Poster Presentation

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Stacking faults type disorder in layered double hydroxides

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Layered double hydroxides (LDH) are a broad group of widely studied materials. The layered character of these materials and their high flexibility for accommodating different metals and anions make them technologically interesting in a range of areas including catalysis, photocatalysis, gas sorption and separation, medicine, pigments, thermal barriers, polymer fillers, and fire retardants. The general formula for an LDH compound is [M1−xIIMxIII(OH)2][An−]x/n·mH2O, where MII is a divalent metal cation which can be substituted by an MIII trivalent cation, and An− is a charge compensating anion located between positively charged layers. Here we present a comprehensive study on possible structural disorder in LDH. We show how X-ray powder diffraction (XRPD) can be used to reveal important features of the LDH crystal structure such as stacking faults, random interlayer shifts, anion−molecule orientation, crystal water content, distribution of interlayer distances, and also LDH slab thickness. All calculations were performed using the Discus package, which gives a better flexibility in defining stacking fault sequences, simulating and refining XRPD patterns, relative to other commonly used programs such as DIFFaX, DIFFaX+, and FAULTS. Finally, we show how the modelling can be applied to two LDH samples: Ni0.67Cr0.33(OH)2(CO3)0.16·mH2O (3D structure) and Mg0.67Al0.33(OH)2(NO3)0.33 (2D layered structure). The presented examples show how XRPD can be successfully used for both highly crystalline and very disordered materials. In summary, we present a novel way of modelling the structure function, F(Q), to provide a source of structural information for poorly crystalline and 2D flake-type samples of LDH.

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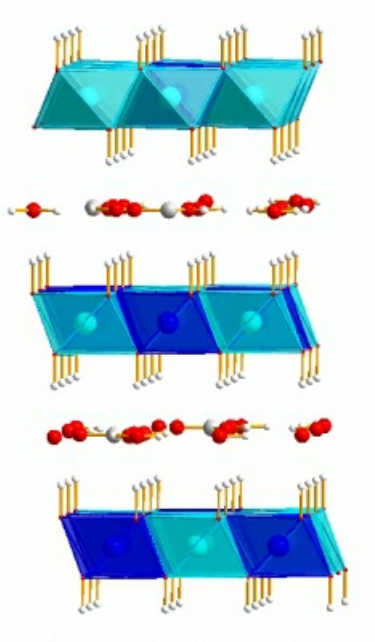

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