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Local structure around the Co, Ni and Cu dopants in the calcium orthovanadates as seen by X-ray absorption

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Calcium orthovanadate $Ca_3(VO_4)_2$ crystallizes in R3c space group with structure similar to that of mineral whitlockite. In the pure crystals some part of Ca cations can be replaced by transition metals (TM), of valences from +1 to +4, without a change of structure. In such case, the corresponding structural modification consists in a partial or full replacement of Ca cations at one (case of substitutionally ordered compound) or more of Ca sites (disordered compound case) by the substituting ion. The resulting novel materials have promising properties that can be utilized in optoelectronic applications, among others can be used for white light-emitting diodes.

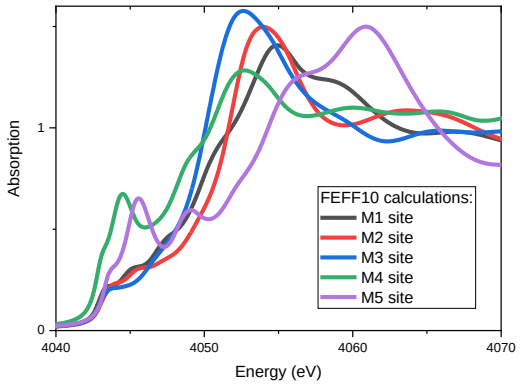

Figure 1. The Ca atoms located in 5 inequivalent crystallographic positions (M1-M5) at the Ca K-edge

The Ca cations are located in 5 inequivalent crystallographic positions (M1-M5). The X-ray absorption technique, by probing the local neighbourhood around specific element, is a perfect tool to determine whether one of the sites is preferred. Fig. 1 presents the FEFF10 simulations of the XANES spectra for all the sites in case of the pure crystal showing the clear differences between each position.

The presented research is focused on the orthovanades crystals: $Ca_{10.5-x}TM_x(VO_4)_7$ doped with TM = Co, Ni or Cu where x ranges nominally from 0.50 to 0.72 %. The XANES and EXAFS measurements were performed at the ASTRA beamline (SOLARIS) in a fluorescence mode.

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