Soft X-ray Absorption and IR reflectivity study of selected materials from $CaCoSi_nO_{2n+2}$ series

Poster

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Wide energy spectrum available at synchrotron radiation sources opens up great possibilities of studying material properties 'at one's fingertips'. For example, X-Ray absorption spectroscopy (XAS) is a powerful tool for studying site specific contribution to the electronic density of states at and above electronovolt levels. In turn, Infrared reflectivity allows to study lattice vibration of the order of milielectronovolts.

In this study we have used both techniques to characterize electronic and vibrational properties of $CaCoSi_2O_6$ pyroxene[1, 2] and several of its potential derivatives $CaCoSi_nO_{2n+2}$.

A quantitative XRD analysis of synthesized samples revealed that despite earlier reports[3] there are no other materials than n = 2. Similar qualitative conclusions were drawn from investigation of magnetic (DC magnetometry) and electronic properties including XPS and Si K edge XANES. Additionally, ab initio DFT calculations were carried out to get insight into electronic structure of the base system and compare them to XAFS results[4].

The influence of the excess of SiO_2 was investigated using Si K XANES. Further study concentrated on n = 2 material and the IR study revealed possible lowering of local symmetry evidenced by splitting of vibrational modes.

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