

# Revisiting structural, magnetic and electronic properties of CaCoSi<sub>n</sub>O<sub>2n+2</sub> series.

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In a public space<sup>1</sup> there are several reports of materials with general stoichiometry CaCoSi<sub>n</sub>O<sub>2n+2</sub>. For n=2 it is a known pyroxene CaCoSi<sub>2</sub>O<sub>6</sub><sup>2,3</sup>. However, not much is known about materials with n=3 and n=4, which seem to be analogous to known pigments CaCuSi<sub>n</sub>O<sub>2n+2</sub>.

In this study several attempts were carried out to synthesize those phantom materials and it was found that they do not exist as a single phase. A quantitative XRD analysis revealed that their stoichiometry is correct but the formula should be written as CaCoSi<sub>2</sub>O<sub>6</sub> + (n-2)SiO<sub>2</sub>. 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. The apparent influence of the excess of SiO<sub>2</sub> on magnetic properties of this "series" can be understood in terms of presence of secondary phases like Ca<sub>2</sub>CoSi<sub>2</sub>O<sub>7</sub>, which form when the starting materials are not homogenized properly. Addition of surplus SiO<sub>2</sub> suppresses their formation leaving clear signature from CaCoSi<sub>2</sub>O<sub>6</sub>, which also can be synthesized from stoichiometric mixture using proper techniques.

## References:

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