

## Defence announcement

**Public Defence on 23 May 2024**

# “The structure of A-site ordered double perovskites on the example of $\text{CaMnTi}_2\text{O}_6$ ”

<b>Title of the doctoral thesis</b>	Structural Principles of A-site ordered double perovskites: ferroelectric $\text{CaMnTi}_2\text{O}_6$ as a model system
<b>Content of the doctoral thesis</b>	<p>Perovskite oxide ceramics are one of the most versatile classes of crystalline materials. They are vastly researched and yet there is much more to explore. The tunability of perovskites makes them favorable because it allows one to tailor the material to very specific needs and therefore optimize efficiency. Amongst the most interesting properties that perovskites and perovskite-related materials can show are ferromagnetism, piezo-, ferro- and pyroelectricity, multiferroicity, electric conductivity, and superconductivity as well as thermal and optical features.</p> <p>Influencing and experimentally analyzing the crystal structure of a material is a key aspect of inorganic solid-state chemistry and materials science. Computational methods on the other hand can be used to predict the structures before synthesis or help understand the results of the analysis of already synthesized materials. Combining both techniques, experimental and computational chemistry, becomes more and more common nowadays and enhances the scientific value of the research.</p> <p>In this thesis, a computational approach to formation and structure prediction in A-site ordered double perovskites is presented. Furthermore, the structure of <math>\text{Ca}_{2-x}\text{Mn}_x\text{Ti}_2\text{O}_6</math> is experimentally studied and the change with <math>x</math> studied as it might be an alternative to current lead containing, harmful ferroelectrics.</p>
<b>Field of the doctoral thesis</b>	Inorganic Materials Chemistry
<b>Doctoral candidate and contact information</b>	M.Sc. (Tech.) Elisabeth Albrecht <a href="mailto:ekalbrecht@outlook.com">ekalbrecht@outlook.com</a>
<b>Public defence date and time</b>	23 May 2024 at 12 o'clock (in Finnish time)
<b>Remote defence</b>	<a href="https://aalto.zoom.us/j/63910435542">https://aalto.zoom.us/j/63910435542</a>
<b>Place of public defence</b>	Aalto University School of Chemical Engineering, Lecture hall Ke2 (Komppa-Sali), Kemistintie 1, (main door at Biologinkuja) Espoo
<b>Opponent(s)</b>	Professor emeritus Markku Leskelä, University of Helsinki
<b>Custos</b>	Professor Antti Karttunen, Aalto University School of Chemical Engineering
<b>Link to electronic thesis</b>	<a href="https://aaltodoc.aalto.fi/handle/123456789/51">https://aaltodoc.aalto.fi/handle/123456789/51</a>
<b>Keywords</b>	A-site ordered double perovskites, Computational Chemistry, Perovskite structure, High pressure synthesis, Single crystals, Ferroelectricity