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SCHOOL OF MATERIALS SCIENCE AND ENGINEERING

A thesis submitted to the Nanyang Technological University in partial fulfilment of the requirement for the degree of Master of Science in Materials Science and Engineering

**20xx (year of submission of final thesis)**

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I have reviewed the content and presentation style of this thesis and declare it is free of plagiarism and of sufficient grammatical clarity to be examined. To the best of my knowledge, the research and writing are those of the candidate except as acknowledged in the Author Attribution Statement. I confirm that the investigations were conducted in accord with the ethics policies and integrity standards of Nanyang Technological University and that the research data are presented honestly and without prejudice.



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Chapter 4 is published as D.T. Murphy, S. Schmid, J.R. Hester, P.E.R. Blanchard, and W. Miiller. Coordination site disorder in spinel-type LiMnTiO4. *Inorganic Chemistry* **54**, 4636-4643 (2015). DOI: 10.1021/ic502747p.

The contributions of the co-authors are as follows:

* A/Prof Schmid provided the initial project direction and edited the manuscript drafts.
* I prepared the manuscript drafts. The manuscript was revised by Dr Hester and Dr. Blanchard.
* I co-designed the study with A/Prof Siegbert Schmid and performed all the laboratory work at the School of Materials Science and Engineering and the Singapore Synchrotron Light Source. I also analyzed the data.
* All microscopy, including sample preparation, was conducted by me in the Facility for Analysis, Characterization, Testing and Simulation.
* Dr James Hester assisted in the collection of the neutron powder diffraction data.
* Dr Peter Blanchard assisted in the interpretation of the X-ray absorption spectroscopy data and carried out the spectral interpretation.
* Dr Wojciech Miiller assisted in the collection and provide guidance in the interpretation of the magnetic measurement data.

Chapter 5 is published as H. V Doan, B. Yao, Y. Fang, A. Sartbaeva, U. Hintermair, V. P Ting, Controlled Formation of Hierarchical Metal-Organic Frameworks using CO2 Expanded Solvent Systems. In press, *ACS Sustainable Chemistry & Engineering* (2017). DOI: 10.1021/acssuschemeng.7b01429.

The contributions of the co-authors are as follows:

* Prof Ting suggested the materials area and edited the manuscript drafts.
* I wrote the drafts of the manuscript. The manuscript was revised together with Dr. Sartbaeva and Dr. Yao.
* I performed all the materials synthesis, collected X-ray diffraction patterns and visible light spectra, carried transmission electron microscopy, and conducted data evaluation.
* Dr. Y. Fang conducted the Rietveld analysis of the powder X-ray diffraction data and single crystal structure determinations.
* Dr U. Hintermair conducted the molecular dynamics simulations.
* Ms. A. Sartbaeva prepared the samples for electron microscopy.



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The abstract should summarize the aims, scope, major findings and conclusion of the thesis. It will normally be no more than 2 pages in length.

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Always include one additional line spacing between paragraphs.

Do not use “I”, “we”, “our”, etc. in your thesis (except in ‘Acknowledgements’).

Lay Summary (Times New Roman, Size 14)

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Do not use “I”, “we”, “our”, etc. in your thesis (except in ‘Acknowledgements’).

Abstracts and summaries in materials science and engineering usually make extensive use of language and terminology inaccessible to the general public and other professionals. Consequently, the impact of research outcomes can be lost and societal benefits poorly understood.

The Lay Summary provides the opportunity to express your scientific and technical conclusions in terms a non-specialist can understand. This skill is essential when engaging the public, recruiting students or employees, and applying for project funding. This section, composed in straightforward language with accessible vocabulary, should convey to the reader the purpose for conducting the research, the impact on the community, environment and/or economy, and the novelty of your outcomes.

The Lay Summary will normally be no more than 2 pages in length.

Acknowledgements (Times New Roman, Size 14)

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**The use of personal pronouns such as ‘I, we, he, she, they, me, us and them…' are quite acceptable in the Acknowledgements, but should be completely avoided elsewhere in the thesis. The Acknowledgements are the only place where your own voice is acceptable.**

Acknowledgements afford the opportunity to thank those who provided support (financial, technical, and emotional) that enabled the research. Appreciation should be expressed concisely while avoiding strongly emotive statements.

The usual hierarchy of Acknowledgements is as follows:

1. Funders including scholarship source, travel grants, research grants, large equipment access grants, conference support and so on without which the research would have been impossible.
2. Supervisor/Co-supervisor/Mentor
3. Other faculty in MSE
4. Technical and support staff in MSE
5. Faculty from other Schools and Universities
6. Other institutions, organizations or companies
7. Group Members
8. Family and Friends

Typical statements include:

This dissertation would not have been possible without funding from the Funding Agency A, and the travel grant from Funder B etc.

Special thanks are conveyed to my research project supervisor Professor Xxxx for her continual guidance and support and to my mentor Dr. Yyyyy for his incisive recommendations concerning the scope of the research.

This thesis greatly benefited from the input of Mr. Aaaaa and Ms. Bbbb who patiently reviewed many drafts and improved the quality of the English expression.

Key data were collected at laboratory HHHHH by the staff scientist at the National facility KKKK.

I am most grateful to Dr. Nnnnn and Ms. Mmmm, and all the technicians of the Zzzz facility, who were wonderful hosts and persevered in training me to use instrument Ddddd and credibly interpret the results.

I was fortunate for the generosity of Prof Jjjjj from University Wwww who graciously shared his unpublished data for comparison with my own studies.

This work relied heavily on the computer code/database developed by Dr. Sssss who helped me install this software on our supercomputer cluster.

**Table of Contents (Times New Roman, Size 14)**

**Paragraph Settings:**

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**Table 1.2** xxxxxxx.

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ANSTO Australian Nuclear Science and Technology Organization

ATR Attenuated Total Reflectance

BEI Backscatter Electron Images

BSE Backscattered Electron

BVS Bond Valence Sum

EDS Energy Dispersive X-ray Spectroscopy

EPMA Electron Probe Microanalysis

FTIR Fourier Transform Infrared Spectroscopy

HRTEM High Resolution Transmission Electron Microscopy

PXRD Powder X-ray Diffraction

SAED Selected Area Electron Diffraction

SEM Scanning Electron Microscopy

SEI Secondary Electron Images

TEM Transmission Electron Microscopy

XRD X-ray Diffraction

Z Atomic Number

**Chapter 1 (Times New Roman, Size 16)**

**Introduction (Times New Roman, Size 16)**

*Every chapter should begin with a short abstract describing the purpose and content. (Only the main text in the short chapter abstract should be typed in Times New Roman, Italics, Size 14, line spacing 1.5 lines). Chapter abstracts should not exceed one paragraph and fit on one page.*

*Chapter must start on odd numbered page on the right.*

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**It is strongly recommended that all hidden characters are activated in MS Word while composing the thesis to ensure correct word spacings, numbers of line spacings between paragraphs/headers, and placement of breaks (page breaks, section breaks (continuous), section breaks (odd pages), section breaks (even pages)).**

**1.1 Hypothesis/Problem Statement**

Main text typed in Times New Roman, Size 12. Insert one additional line spacing after headers, sub headers, and between paragraphs. Do not use “I”, “we”, “our”, etc. in your thesis (except in ‘Acknowledgements’).

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The chapter should begin with a problem statement that contextualizes the thesis. It provides a rationale for the research and outlines the goals and scope.

For a **scientific thesis,** a hypothesis must be presented.

For an **engineering/technological theses,** a performance/design target is required.

**1.2 Objectives and Scope**

**1.3 Dissertation Overview**

The thesis addresses …….

*Chapter 1* provides a rationale for the research and outlines the goals and scope.

The hypothesis/problem statement will takes the general form:

*“This thesis tests the hypothesis that when material(s) A/algorithm(s) B etc. are subjected to a ‘perturbation’/’adjustment’ in a particular fashion they will respond to deliver a certain functionality/property.”* (For science focused theses).

or

*“This thesis describes and validates the design/fabrication/invention of a device/material/method that delivers quantitatively superior performance/outcomes in the domain/market/product sector.”* (For engineering focused theses).

This statement will be preceded by a justification/explanation for the choice a suitable thesis topic. The key point is that the thesis does not deliver a right or wrong answer, but ‘tests’ and idea and faithfully describes the outcomes of the ‘test’.

*Chapter 2* reviews the literature concerning …….. This chapter must demonstrate your awareness of historical and contemporary literature. It will also guide the reader to the gaps in knowledge that your thesis is addressing.

*Chapter 3* discusses the principles underlying the synthesis/characterization/modeling techniques employed and the methods of data analysis, including errors. An explanation of why particular methods are appropriate is required. This is an important chapter that demonstrates your understanding of the techniques and approach used. **This chapter will normally be 20 – 30 pages**.

*Chapter 4* elaborates the first major set of results.

*Chapter 5* elaborates the second major set of results.

*Chapter 6* elaborates the third major set of results.

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*Chapter X* draws together the threads of your thesis. Reconnaissance studies that did not warrant a complete chapter can be included. The extent to which the hypothesis was proven/disproven, or the design target is met/not met is essential and must be adequately addressed. This must be more than a summary of results. It must demonstrate that you have reflected deeply on the implications of your research. The opportunities and strategies for future work are required. The chapter must end with a statement explaining how your outcomes were reflected in the original hypothesis. **This chapter will typically be 10 – 15 pages.**

**1.4 Findings and Outcomes/Originality**

This research led to several novel outcomes by:

1. Establishing a …..

2. Correlating ……

3. etc.

**References**

[1] B. L. Sawhney, C. R. Frink. *Water, Air, and Soil Pollution*. **1991**, 57-58, 289-296.

[2] L. C. Tan, V. Choa, and J. H. Tay. *Environ. Monitor. & Assess*. **1997**, 44, 275-28

**Chapter 2 (Times New Roman, Size 16)**

**Literature Review (Times New Roman, Size 16)**

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**2.1 Main Section Heading**

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This chapter must demonstrate your awareness of historical and contemporary literature. It will also guide the reader to the gaps in knowledge that your thesis is addressing.

**2.1.1 Second Order Heading**

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| **0.5** | 9.75(6) | 0.45(3) | 0.42(3) | 5.12(9) | 1.65(5) | 23.95(4) | 1.63 |
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| 9.78(7) | 0.46(2) | 0.43(2) | 5.11(9) | 1.26(4) | 24.13(6) | 1.63 |

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**References**

[1] B. L. Sawhney, C. R. Frink. *Water, Air, and Soil Pollution*. **1991**, 57-58, 289-296.

[2] L. C. Tan, V. Choa, and J. H. Tay. *Environ. Monitor. & Assess*. **1997**, 44, 275-284.

**Chapter 3 (Times New Roman, Size 16)**

**Experimental Methodology (Times New Roman, Size 16)**

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**Chapter 4\* (Times New Roman, Size 16)**

**First Results Chapter (Times New Roman, Size 16)**

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**4.1 Introduction**

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**References**

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[2] L. C. Tan, V. Choa, and J. H. Tay. *Environ. Monitor. & Assess*. **1997**, 44, 275-284.

**Chapter X (Times New Roman, Size 16)**

**Implications/Impact/Outstanding Questions (Times New Roman, Size 16)**

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**APPENDIX (Times New Roman, Size 16)**

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| **2.5** | 9.73(7) | 2.45(3) | 2.55(5) | 1.00(9) | 1.33(3) | 24.12(9) | 1.62 |
| **3.0** | 9.88(6) | 2.96(6) | 3.04(5) | - | 1.65(9) | 24.27(9) | 1.65 |

\* Footnotes to tables. (Times New Roman, Size 11)

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