Annexe A: New/Revised Course Content in OBTL+ Format

Course Overview

The sections shown on this interface are based on the templates UG OBTL+ or PG OBTL+
If you are revising/duplicating an existing course and do not see the pre-filled contents you expect in the subsequent sections e.g. Course Aims, Intended Learning Outcomes etc. please refer to Data Transformation Status for more information.

Expected Implementation in Academic Year	AY2024-2025
Semester/Trimester/Others (specify approx. Start/End date)	Semester 2
Course Author * Faculty proposing/revising the course	Professor Tim White
Course Author Email	tjwhite@ntu.edu.sg
Course Title	Crystal Chemistry of Nanomaterials
Course Code	MS6010
Academic Units	3
Contact Hours	39
Research Experience Components	

Course Requisites (if applicable)

Pre-requisites	
Co-requisites	
Pre-requisite to	
Mutually exclusive to	
Replacement course to	
Remarks (if any)	

Course Aims

This practical course provides you with the tools to design nanomaterials and validate their crystal chemistry and morphology. The emphasis is on learning to access key databases and training in scientific software packages for visualisation and quantitative extraction of crystallographic information. In Module 1, the 'Patterns in Crystal Lattices' are space symmetry is introduced to enable you to read Crystallographic Information Files (CIF) from the Crystallography Open Database. With this data crystal structures can be visualised and powder X-ray diffraction patterns calculated. In Module 2, the 'Chemistry of Crystal Structures' provides strategies to design stable compounds with acceptable bond valence sums, characterise materials through crystal structure refinement, and find the dimensions of nanocrystals through least squares refinement of experimental diffraction data. In Module 3, the 'Character of Crystal Assemblages' will equip you to conduct quantitative phase analysis of polyphase nanocrystal assemblages and consistent with energy dispersive X-ray spectroscopic chemical analysis. You will master four software packages – ATOMS (crystal structure visualisation), VESTA (bond valence summation), HIGHSCORE (quantitative phase analysis) and DSTA-II (chemical microanalysis) – that collectively provide a platform for discovering and certifying the properties of nanomaterials. This practical course will prepare you for placement with companies engaged in materials development, employment in government agencies conducting environmental and chemical audits, or continue higher postgraduate studies.

Course's Intended Learning Outcomes (ILOs)

Upon the successful completion of this course, you (student) would be able to:

ILO 1	Understand the principles of crystal chemical design through the integration of space symmetry and solid state chemistry
ILO 2	Refine crystal structures from powder X-ray diffraction patterns using the Rietveld method and validate the crystallographic output
ILO 3	Conduct quantitative phase analysis of nanomaterial assemblages to monitor the progression of synthesis, recognise amorphous content and check mass balance
ILO 4	Master the ATOMS, VESTA, HIGHSCORE and DSTA-II software packages for the design and characterisation of nanomaterials

Course Content

This course is organised in three Modules that take students from the principles to the practice of nanomaterials design and property validation.

1. **Module 1 Patterns in Crystal Lattices**: Introduction to the rules of space symmetry, literacy in Crystallographic Information Files, Visualisation of crystal structures with ATOMS, and simulation of powder X-ray diffraction patterns using HighScore
2. **Module 2 Chemistry of Crystal Structures**: Application of Rietveld analysis to refine crystal structures using HighScore and testing the validity of crystal chemistry using bond valence summation as implemented in VESTA
3. **Module 3 Character of Crystal Assemblages**: Quantitative phase analysis of nanomaterials assemblages containing crystalline and amorphous components with HighScore and integration with chemical microanalyses interpreted using DSTA-II

Reading and References (if applicable)

Module 1 Patterns in Crystal Lattices

1. Point Groups, Space Groups, Crystals, Molecules - R Mirman World Scientific ISBN 978-981-3105-36-2
2. Crystal Chemistry and Crystal Structures - RJD Tilley, Wiley ISBN 978-0470018217

Module 2 Chemistry of Crystal Structures

1. Crystal Chemistry: From Basics To Tools For Materials Creation - G Ferey, World Scientific, ISBN 978-9813144194
2. Rietveld Refinement: Practical Powder Diffraction Pattern Analysis using TOPAS - RE Dinnebier, A Leineweber and JSO Evans De Gruyter STEM ISBN 978-3110456219

Module 3 Character of Crystal Assemblages

1. The Rietveld Method - RA Young IUCR ISBN 9780198559122
2. Fundamentals of Energy Dispersive X-Ray Analysis - JC Russ Butterworths-Heinemann, ISBN 978-0408110310

Planned Schedule

Week or Session	Topics or Themes	ILO	Readings	Delivery Mode	Activities
1	Objectives and Methodology; Periodic Plane Symmetry; Periodic Space Symmetry	1, 4	ATOMS Training Videos (Visualisation) CIF Training Videos (Database Extraction) HIGHSCORE Training Videos (CIF upload and Simulation)	Online	Software Installation & testing
2	ATOMS, HIGHSCORE, VESTA, DSTA	1, 4	ATOMS Training Videos (Visualisation) CIF Training Videos (Database Extraction) HIGHSCORE Training Videos (CIF upload and Simulation)	Online	Software Installation & testing
3	Crystal Lattice versus Crystal Structure; Crystal Structure Databases and Visualisation; Powder X-ray Diffraction Pattern Calculation	1, 4	ATOMS Training Videos (Visualisation) CIF Training Videos (Database Extraction) HIGHSCORE Training Videos (CIF upload and Simulation)	Online	Train with Practice Data
4	Study & Practice	1, 4	ATOMS Training Videos (Visualisation) CIF Training Videos (Database Extraction) HIGHSCORE Training Videos (CIF upload and Simulation)	Online	CA1: Visualisation & Simulation (20%)
5	Position, Intensity and Width of Diffraction Peaks; Pauling's Rules for the Size and Charge of Ions; Methodology for Refining Crystal Structures	1, 2, 4	HIGHSCORE Training Videos (Crystal Structure Refinement) VESTA Training Videos (Bond Valence Summation)	Online	Train with Practice Data

Week or Session	Topics or Themes	ILO	Readings	Delivery Mode	Activities
6	Phase Changes and the Unit Cell Trends; Chemical Analysis by X-ray diffraction	1, 2, 4	HIGHSCORE Training Videos (Crystal Structure Refinement) VESTA Training Videos (Bond Valence Summation)	Online	Train with Practice Data
7	Chemical Validation using Bond Valence Sums	1, 2, 4	HIGHSCORE Training Videos (Crystal Structure Refinement) VESTA Training Videos (Bond Valence Summation)	Online	Train with Practice Data
8	Study & Practice	1, 2, 4	HIGHSCORE Training Videos (Crystal Structure Refinement) VESTA Training Videos (Bond Valence Summation)	Online	CA2: Refinement & Validation (30%)
9	Quantitative Phase Analysis; Correlation of XRD Patterns with Backscattered Electron Images	1, 2, 3, 4	HIGHSCORE Training Videos (Quantitative Phase Analysis) DSTA-II (EDS Simulation and Analysis	Online	Train with Practice Data
10	Measuring Non-diffracting Content; Correlation of XRD patterns and Secondary Electron Images	1, 2, 3, 4	HIGHSCORE Training Videos (Quantitative Phase Analysis) DSTA-II (EDS Simulation and Analysis	Online	Train with Practice Data
11	Phase Changes and Functional Property Inflections; Hierarchy for Nanomaterials Characterisation	1, 2, 3, 4	HIGHSCORE Training Videos (Quantitative Phase Analysis) DSTA-II (EDS Simulation and Analysis	Online	Train with Practice Data
12	Study & Practice	1, 2, 3, 4	HIGHSCORE Training Videos (Quantitative Phase Analysis) DSTA-II (EDS Simulation and Analysis	Online	CA3: Quantitative Analysis (50%)

Learning and Teaching Approach

Approach	How does this approach support you in achieving the learning outcomes?
On-line lectures	On-line lectures hosted by the Adaptive Teaching and Learning Applications System (ATLAS) are coupled with dynamic learning trees, in- video formative assessments and closed captioning will accelerate learning and allow self-checking of understanding at your own pace.
Software training videos	Comprehensive software training videos will guide you through the installation and use of the scientific programs ATOMS, HIGHSCORE, VESTA and DSTA-II that established tools for crystal chemical design and characterisation of nanomaterials. Ahead of the add-drop period period face-to-face sessions will be available to assist with software installation.
Authentic data analysis	As a practice based course, you will be trained to access open source databases and exposed to quantitative analysis of real laboratory data sets. Practice data sets will allow to refine your skills.
On-line assessment	Three continuous assessments will be conducted on-line through the semester. The complexity and weight of CA1 (20%), CA2 (30%) and CA (50%) increases gradually so you can master the software incrementally without jeopardizing your grade.

Assessment Structure

Assessment Components (includes both continuous and summative assessment)

No.	Component	ILO	Related PLO or Accreditation	Weightage	Team/Individual	Rubrics	Level of Understanding
1	Continuous Assessment (CA): Test/Quiz(CA1: Visualisation & Simulation)	1,4	Crystal Database Discovery	20	Individual	Holistic	Relational
2	Continuous Assessment (CA): Test/Quiz(CA2: Refinement & Validation)	1,2,4	Crystal Structure Refinement	30	Individual	Holistic	Relational
3	Continuous Assessment (CA): Test/Quiz(CA3: Quantitative Analysis)	1,2,3,4	Crystal Chemical Analysis	50	Individual	Holistic	Relational

Description of Assessment Components (if applicable)

All software packages must be installed and tested during the add-drop period. This scientific software requires a Windows computer and is incompatible with Apple Mac operating systems. Students are responsible for accessing the required computer hardware to undertake this course.

During the Continuous Assessment the software will be deployed and assessed as follows:

1. CA1 (Module 1, 20% of grade): ATOMS, HIGHSCORE
2. CA2 (Module 2, 30% of grade): VESTA, HIGHSCORE
3. CA3 (Module 3, 50% of grade): DSTA-II, ATOMS, VESTA, HIGHSCORE

For all CAs students will be given materials science case studies to interrogate using the software packages and involve: (i) extracting crystallographic information files from databases; (ii) preparing computer visualisations of crystal structures; (iii) simulating powder X-ray diffraction patterns; (iv) analysing crystal structures using bond valence summing; (v) conducting crystal structure refinement of experimental data; (vi) quantifying mixed phase materials assemblages; (vi) correlating microchemical analyses with crystallographic properties.

The CAs become progressively more integrative of techniques and depth of interpretation. Students will populate a rubric template with the answers (tables, structure drawings, graphs etc.) derived from the software and upload to ATLAS.

Formative Feedback

More than 50 short Competency Videos that explore case studies to provide students with practice.

Practice data sets and exercises that model the style of questions used in CA1, CA2 and CA3 will allow you to gain experience in the using the software. All CAs will measure your ability to use the software to analyse the crystal chemistry of materials.

NTU Graduate Attributes/Competency Mapping

This course intends to develop the following graduate attributes and competencies (maximum 5 most relevant)

Attributes/Competency	Level
Digital Fluency	Advanced
Problem Solving	Advanced
Sense Making	Advanced
Information Literacy	Advanced
Critical Thinking	Advanced

Course Policy

Policy (Academic Integrity)

Good academic work depends on honesty and ethical behaviour. The quality of your work as a student relies on adhering to the principles of academic integrity and to the NTU Honour Code, a set of values shared by the whole university community. Truth, Trust and Justice are at the core of NTU's shared values. As a student, it is important that you recognize your responsibilities in understanding and applying the principles of academic integrity in all the work you do at NTU. Not knowing what is involved in maintaining academic integrity does not excuse academic dishonesty. You need to actively equip yourself with strategies to avoid all forms of academic dishonesty, including plagiarism, academic fraud, collusion and cheating. If you are uncertain of the definitions of any of these terms, you should go to the academic integrity website for more information. On the use of technological tools (such as Generative AI tools), different courses / assignments have different intended learning outcomes. Students should refer to the specific assignment instructions on their use and requirements and/or consult your instructors on how you can use these tools to help your learning. Consult your instructor(s) if you need any clarification about the requirements of academic integrity in the course.

Policy (General)

You are expected to complete all assigned readings, activities, assignments, attend all classes punctually and complete all scheduled assignments by due dates. You are expected to take responsibility to follow up with assignments and course related announcements. You are expected to participate in all project critiques, class discussions and activities.

Policy (Absenteeism)

In-class activities make up a significant portion of your course grade. Absence from class without a valid reason will affect your participation grade. Valid reasons include falling sick supported by a medical certificate and participation in NTU's approved activities supported by an excuse letter from the relevant bodies. There will be no make-up opportunities for in-class activities.

Policy (Others, if applicable)

This graduate course requires a high level of self-discipline and continuous effort to succeed. You are encouraged to form study groups with your peers and access the many sources of on-line information related to the course content. As the emphasis is on understanding, rather than memorisation, all CAs are open-book and you can use whatever resources will enable you achieve a high grade.

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