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

Course Overview

Expected Implementation in Academic Year (New format)	AY2026-2027
Semester/Trimester/Others (specify approx. Start/End date)	Semester 1
Course Author * Faculty proposing/revising the course	Prof Tim White
Course Author Email	tjwhite@ntu.edu.sg
Course Title	Introduction to Crystal Chemistry
Course Code	MS6030
Academic Units	3
Contact Hours	39
Research Experience Components	

Course Requisites (if applicable)

Pre-requisites	
Co-requisites	
Pre-requisite to	
Mutually exclusive to	MS7340 Crystal Chemistry of Materials
Replacement course to	
Remarks (if any)	Coursework students who have previously completed MS7340 Crystal Chemistry of Materials will not be allowed to read MS6030 Introduction to Crystal Chemistry.

Course Aims

This course will provide you with resources and tools to critically link crystal chemistry with performance and functionality, and subsequently tailor materials with optimal properties. By the end of this course the students will:

1. Intuit the periodicity and symmetry elements of periodic structures.
2. Access crystal structure databases and be able to interpret Crystallographic Information Files.
3. Understand systematic variations in ionic radii and exploit these to design new materials.
4. Learn the characteristics and crystal chemical diversity of common crystal structural families.
5. Predict the changes in crystals when perturbed by temperature, pressure and chemistry.
6. Recognize nonstoichiometric adaptations and their incorporation in crystal structures.
7. Appreciate the difference between displacive and reconstructive phase transformations.
8. Develop idealised structures as a starting point for quantitative investigation of relaxation.
9. Construct and visualise physical models of crystal structures using precision polyhedra.
10. Critically read and evaluate the crystal chemical content of research papers

Course's Intended Learning Outcomes (ILOs)

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

ILO 1	Access the International Tables of Crystallography and the Bilbao Crystallographic Server
ILO 2	Extract and interpret Crystallographic Information Files (CIF) found in crystal structure databases
ILO 3	Exploit CIF for the visualisation of crystal structures and extraction of crystal chemical information
ILO 4	Develop competence in using ATOMS software to design and check idealised crystal structures
ILO 5	Predict the behaviour of structures during systematic changes in chemistry through quantitative assessment of bond lengths and bond valence sums
ILO 6	Construct physical models of idealised crystal structures as a baseline for crystallographic relaxation
ILO 7	Use Pauling's Rules of Crystal Design to validate the behaviour of structures when perturbed by temperature and pressure
ILO 8	Describe phase transformations as displace or reconstructive and appreciate the physical/chemical drivers of the transformation
ILO 9	Recognize the polyhedral topology of common crystal structures and the variants that arise from chemical ordering
ILO 10	Link symmetry with chemistry quantitatively to probe the reliability of journal articles and crystal structure and recognize errors

Course Content

This course is organised in three Modules that take students from the principles to the practice of crystal chemistry for materials science and engineering.

1. **Module 1 Foundations in Crystallography:** Introduction to the rules of space symmetry, literacy in Crystallographic Information Files, Visualisation of crystal structures with ATOMS, and 2D nets and 3D polyhedral representations of crystal structures
2. **Module 2 Practice of Crystal Chemistry:** Know the characteristics and crystal chemical diversity of simple crystal structure families and predict perturbations driven by changes in temperature, pressure and chemistry. Recognize the types of nonstoichiometric adaptations and the mechanism for incorporating these in crystal structures. Undertake critical reading and interpretation of journal articles.
3. **Module 3 Application of Crystal Chemistry:** A practical component is included where students are provided with precision polyhedra to construct a physical model of a crystal structure that will reinforce an appreciation of 3D visualizations generated from crystallographic information.

Reading and References (if applicable)

General Text: Crystal Chemistry and Crystal Structures RJD Tilley, 2006, Wiley ISBN 978-0470018217

Note: The above listing comprises the foundational references for the course and up-to-date relevant references/scientific articles will be provided each semester.

Planned Schedule

Week or Session	Topics or Themes	ILO	Delivery Mode	Activities	Readings
1	The Plane and Space Groups; Wyckoff Symbols	1	Online	Study Lectures 1-6; Attempt practice CA1	No reading
2	Platonic solids and polyhedral representations; Crystallographic Information Files	2, 3, 4	Online	Study Lectures 7-13; Attempt practice CA1	No reading
3	Continuous Assessment 1 (CA1): Individual Invigilated Assessment (Module 1) Study & Practice	1, 2, 3, 4	In-person	Continuous Assessment 1 (CA1): Individual Invigilated Assessment (Module 1) (20%)	No reading
4	Symmetry-driven solid composition	5, 7, 8, 9	Online	Study Lectures 14-26; Attempt practice CA2	No reading
5	Non-stoichiometry with ions of fixed and variable valence	5, 7, 8, 9	Online	Study Lectures 14-26; Attempt practice CA2	No reading
6	Pauling's Rules for structure building	5, 7, 8, 9	Online	Study Lectures 14-26; Attempt practice CA2	No reading
7	Continuous Assessment 2 (CA2): Individual Invigilated Assessment (Module 2) Study & Practice	5, 7, 8, 9	In-person	Continuous Assessment 2 (CA2): Individual Invigilated Assessment (Module 2) (20%)	No Reading
8	Analysis of phase transition and functionality	1,2,3, 4, 5, 6, 7, 8, 9, 10	Online	Read prescribed journal articles	Prescribed journal articles
9	Verification and extension of published data	1,2,3, 4, 5, 6, 7, 8, 9, 10	Online	Plan and construct physical model using ATOMS	Prescribed journal articles

Week or Session	Topics or Themes	ILO	Delivery Mode	Activities	Readings
10	Compilation of data analysis	1,2,3, 4, 5, 6, 7, 8, 9, 10	Online	Submission of Individual Assignment 1 (A1) (Module 3) (30%) – Crystal Structure Design, Computed Visualisation and Physical Model Construction	Prescribed journal articles
11	Submit Assignment 1 Term Paper	1,2,3, 4, 5, 6, 7, 8, 9, 10	Online	Conduct quantitative critique of journal articles	Prescribed journal articles
12	Develop idealised structure	1,2,3, 4, 5, 6, 7, 8, 9, 10	Online	Conduct quantitative re-evaluation of data in published article.	Prescribed journal articles
13	Submit Assignment 2 Physical model construction and visualisation	1,2,3, 4, 5, 6, 7, 8, 9, 10	Online	Submission of Individual Assignment 2 (A2) (Modules 1, 2 & 3) (30%) – Critique of Scientific Paper	Prescribed journal articles

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 and demonstration videos	Comprehensive software training videos will guide you through the installation and use of the scientific programs ATOMS. Demonstration videos on the practice of building physical crystal structure models.
Authentic texts analysis	As a practice-based course, you will be trained to access open-source databases and learn to critique and recognize errors in published data.
On-line assessment	Two continuous assessments will be conducted on-line before the mid-semester break. CA1 (20%) and CA2 (20%) will test foundational knowledge contained in Module 1 and Module 3 respectively.
Assignment Preparation	Two assignments will be prepared. Assignment 1 (30%) will describe the design and construction of an idealised crystal structure and Assignment 2 (30%) will critique a journal article. The assignments will be peer reviewed and moderated for consistent marking.

Assessment Structure

Assessment Components (includes both continuous and summative assessment)

No.	Component	ILO	Related PLO or Accreditation	Weightage	Description of Assessment Component	Team/Individual	Rubrics	Level of Understanding
1	Continuous Assessment (CA): Test/Quiz(Continuous Assessment 1 (CA1): Crystallography and Symmetry)	1, 2, 3, 4		20	Open book examination consisting of 10 questions, 1 hr duration. Testing understanding of point, plane and space symmetry, access of Bilbao Crystallographic Server and crystal structure visualisation.	Individual	Holistic	Relational
2	Continuous Assessment (CA): Test/Quiz(Continuous Assessment 2 (CA2): Crystal chemistry and phase transitions)	5, 7, 8, 9		20	Open book examination consisting of 10 questions, 1 hr duration. Testing concepts in stoichiometry and nonstoichiometry in crystal systems, connectivity polyhedra, integration chemical composition and symmetry.	Individual	Holistic	Relational

No.	Component	ILO	Related PLO or Accreditation	Weightage	Description of Assessment Component	Team/Individual	Rubrics	Level of Understanding
3	Continuous Assessment (CA): Report/Case study(Assignment 1: Crystal structure design and construction)	1,2, 3, 4, 5, 6, 7, 8, 9, 10		30	Individual assignment to interpret crystal chemical scientific article with paragraphs written that describe (1) developing idealised structure model, (2) extracting crystal chemical data (bond valence sums, bond lengths, topology etc), (3) building physical polyhedral model, and(4) linking structural adaptation to functional properties. The Assignment will be peer reviewed (2 students) and moderated.	Individual	Holistic	Extended Abstract

No.	Component	ILO	Related PLO or Accreditation	Weightage	Description of Assessment Component	Team/Individual	Rubrics	Level of Understanding
4	Continuous Assessment (CA): Report/Case study(Assignment 2: Critique of journal article)	1,2, 3, 4, 5, 6, 7, 8, 9, 10		30	Individual assignment to interpret crystal chemical scientific article with paragraphs written that describe (1) general characteristics of structural family, (2) phase transformations in response perturbations (temperature pressure, chemistry), (3) reliability of published article, (4) analysis and suggestions of future investigations of crystal chemical system. The Assignment will be peer reviewed (2 students) and moderated.	Individual	Holistic	Extended Abstract

Description of Assessment Components (if applicable)

The ATOMS software package must be mastered to visualise crystal structures.

Formative Feedback

In-video questions will be embedded in every lecture for self-assessment of your understanding of crystal chemical principles. Answers with explanations are also provided.

Discussion of student questions posted in the Teams Group will provide deeper explanation of challenging aspects of the course.

Practice exercises that model the style of questions used in CA1 and CA2 will allow you to gain confidence in understanding materials.

Sample Assignments (A1 and A2) will be provided to demonstrate the level of competence expected.

NTU Graduate Attributes/Competency Mapping

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

Attributes/Competency	Level
Adaptability	Advanced
Communication	Advanced
Creative Thinking	Advanced
Curiosity	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 and complete all scheduled assignments by due dates. You are expected to take responsibility to follow up with assignments and course related announcements.

Policy (Absenteeism)

Non-participation in CA1 and CA2 will severely impact your grade. With the exception of students holding a valid Medical Certificate make-up tests will not be entertained under any circumstances.

Peer review of Assignment 1 (A1) and Assignment 2 (A2) is an important learning opportunity and is compulsory. Failure to compete peer review will lead to zero marks.

Policy (Others, if applicable)

This graduate course requires a high level of 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.

Technical Skills To Be Developed

All skills to be developed for this course:

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