Annex A

REVISED COURSE CONTENT

Existing Course Code and Title	MS734M Crystal Chemistry of Materials
	Summary of course content This course will equip students with the tools needed to understand crystals (their types, descriptions, properties, applications) in a rigorous fashion, without becoming a crystallographer. The content begins with the basics and is designed for students entering the field. The approach is to learn the principles and systematics of crystal chemistry that greatly simplifies the analysis of inorganic compounds, functional materials and minerals. To do this, databases and software will be introduced to allow the critical interpretation of experiments. Students will be led through the process of preparing to attend a research seminar, evaluating its content, and finally preparing a critique. The term paper provides an opportunity for students to demonstrate their skills through the scaffolded exploration of a published article. 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. By the end of this course, students will be prepared to interrogate the solid state in a crystal chemical sense and have the implements and resources to find answers to their questions.
	Rationale for introducing this course The ability to design, manipulate and validate the crystal chemistry of crystalline solids is central to materials science and engineering. This course will provide students with the strategies and tools to rationally tailor functional materials. Formal descriptions of plane and space symmetry will be introduced and the imposition of chemistry on these mathematical precepts explained. The compilation of key crystal structure families and the derivation of complex structures from simple prototypes will systematize the most common materials encountered. Responses of crystals to pressure, temperature and chemical composition are explored. Mechanisms for introducing nonstoichiometry are classified and common extended defects described. The role of nonstoichiometry in controlling functional materials properties will be illustrated. Integration of crystallographic databases, diffraction simulation, 3D visualization and physical model construction provide students with a unified skill set not offered elsewhere in NTU.

	Aims and objectives The aim of this course is to provide students with the tools to critically link crystal chemistry with performance and functionality, and subsequently tailor materials with optimal properties. At the end of this course the students will: 1. Find crystal structure databases accessible and be able to interpret Crystallographic Information Files (CIFs); 2. Understand orderly variations in atomic and ionic radii and exploit these systematics to design materials; 3. Know the characteristics and crystal chemical diversity of simple crystal structure families; 4. Predict the changes in crystal structures when perturbed by changes in temperature, pressure and chemistry; 5. Recognize the types of nonstoichiometric adaptations and the mechanism for incorporating these in crystal structures; 6. Critically read authentic texts and attend research seminars describing nonstoichiometric functional materials.
	Syllabus **MODULE 1: PRINCIPLES OF CRYSTAL CHEMISTRY** *FOUNDATIONS AND REPRESENTATIONS* 1. What is Crystal Chemistry? 2. Space Symmetry and the 230 Space Groups 3. Symmetry and the Wyckoff Symbols 4. Atomic and Ionic Radii 5. Platonic solids and polyhedral 6. Crystallographic Information Files **MODULE 2: APPLICATION OF CRYSTAL CHEMISTRY** *VARIATIONS AND NON-STOICHIOMETRY* 7. The Composition of Solids 8. Crystal Chemical Equations and Formula 9. Nonstoichiometry: Ions of Fixed Valence 10. Nonstoichiometry: Ions of Variable Valence 11. Pauling's Rules for Structure Building 12. Extraction of CIF from Crystallographic Databases **MODULE 3: PRACTICE OF CRYSTAL CHEMISTRY** *PERTURBATIONS AND ADAPTATION* 13. 2-Dimensional Nonstoichiometric Structures 14. 3-Dimensional Nonstoichiometric Structures 15. Framework Structure Adaptation 16. Interpretation of Scientific Papers on Crystal Chemical Driven Tailoring of Materials Functionalisation 17. Analysis of materials research seminars 18. 3D Visualization of Crystal Structures **MODULE 4: APPRECIATION OF CRYSTAL CHEMISTRY** *VISUALIZATION AND ANALYSIS* 19. Building Physical Models of Crystal Structures 20. Exploration of connectivity and topological variations

	21. Limitations of Experimental Observations in Crystal Chemistry 22. Design of Crystal Chemical Experiments 23. Crystallographic Transformations and Alternate Representations 24. Inadequacy of 230 Space Groups in Incommensurate and Modulated Crystal; Structures.
Assessment Please specify if components are individually assessed or group assessed	*Continuous Assessment 1 (MCQ) - Foundational Understanding* — *Individual* — *5%* *Continuous Assessment 2 (MCQ) - Application of Software* — *Individual* — *10%* *Essay (Instructor + Peer Marked) - Critique of Research Seminar* — *Individual* — *20%* *Term Essay (Instructor + Peer Marked) - Analysis of Published Article* — *Individual* — *40%* *Practical Class (Instructor + Peer Marked) - Polyhedral Model Construction* — *Individual* — *25%* Total: 100 %
Hours of Contact/Academic Units	*52 hours / 4 AU*
Proposed Date of Offer	*Semester 1, AY2021-22*
Instructor and Co-instructor (if any)	Tim White Christian Kloc
Class size	25-50
Any duplication of course	No

Course Syllabus
The following topics will be covered:

MODULE 1: PRINCIPLES OF CRYSTAL CHEMISTRY

1: What is Crystal Chemistry?
Introduces plane symmetry as a mathematical concept and the 17 plane groups. The non-equivalence of a crystal lattice and a crystal structure is explored.

2: Space Symmetry
The symmetry operations found in space symmetry are described and 230 space groups reviewed. The Bilbao Crystallographic Server will be introduced.

3: Symmetry and the Wyckoff Symbols
Coupling of symmetry and chemical composition will be established and Wyckoff position multiplicity introduced.

4: 3D Bravais Lattices
Formal relationship between Bravis lattices and space symmetry

5: Platonic Solids
Use of Platonic solid shapes and symmetry together with other polyhedra as simplifications for recognizing crystallographic tesselations

6: Crystallographic Information Files
The format of Crystallographic Information Files (CIFs) and access to crystal structure databases introduced. The Bilbao Crystallographic Server to interpret CIF will be taught.

7: Representation of Planes and Directions
Definition of Miller indices and recognition of crystallographic projections.

MODULE 2: APPLICATION OF CRYSTAL CHEMISTRY

8: Structural Modification
Commonly occurring structural modifications – allotrophism, polytypism, polymorphism, polysomatism – will be described and illustrated.

9: Structure Responses to External Perturbation
Prediction of crystal structure responses to heating/cooling and pressure.

10: Structure Responses to Internal Perturbation
Prediction of crystal structure responses to compositional changes.

11: Pauling's Rules for Structure Building
Linus Pauling's rules for connecting cation-centered polyhedra provide a means for predicting structures. The concept of partial bond valence is introduced.

12: Crystal Chemical Equations and Formula
Students will learn how to write crystal chemical equations and prepare crystal chemical formula.

13: Nonstoichiometry: Ions of Fixed Valence
Mechanisms of incorporating ions of fixed valence in oxides, nitrides and fluorides.

14: Nonstoichiometry: Ions of Variable Valence
Mechanisms of incorporating and controlling the valence of ions in oxides, nitrides and fluorides.

MODULE 3: PRACTICE OF CRYSTAL CHEMISTRY

15: **Interpretation of Authentic Texts on Nonstoichiometric Functional Materials**
Students will development skills to critically read contemporary journal articles describing functional materials.

16: Evaluation of Research Seminars
Students will be guided in the art of listening to and interpreting research seminars delivered by faculty through analysis of the seminar's design, content selection and data interpretation.

17: Crystal Structure Families
The use of crystal structure families to simplify and systematize hundreds of crystal structures will be taught in the context of complex materials systems.

18: The Composition of Solids
Interpretation of phase diagrams and the appearance of nonstoichiometric compounds.

19: Two Dimensional Nonstoichiometric Structures
Mimetic twinning and crystallographic shear as key mechanisms for incorporating non-stoichiometry are described.

20: Three Dimensional Nonstoichiometric Structures
Classical block structures are shown early examples of extended defects for accommodating nonstoichiometry, as are contemporary modulated structures that exist in 4- and 5- dimensions.

21: Nonstoichiometric Functional Materials
Mechanisms by which nonstoichiometry functionalizes galvanic cells, sensors, catalysts etc. will be explained

MODULE 4: APPRECIATION OF CRYSTAL CHEMISTRY

21: 3D Visualization of Crystal Structures
Use ATOMS to create polyhedral representations of complex structures for comparison of analogues, polytypes and polymorphs.

22: Crystal Structure Databases
Practice in selecting and extracting CIF from the Crystallography Open Database and American Mineralogist Structure Database

23: Quality checking of Published Crystal Data
Learn the process of examining bond lengths and bond angles to recognize errors in published CIF and false assignment of symmetry

24: Construction of Precision Plastic Polyhedral Models
Integrate 3D visualisation with physical models to fully appreciate connectivity and topological variations in polyhedral connectivity, adaptation and nonstoichiometry.

25: Geometric Transformations
Transformations between crystal settings including change of origin, centred versus non-centred unit cells, non-standard space group settings and use of the International Tables of Crystallography.

26: Linkage between Structure and Diffraction
Use of ATOMS to calculate X-ray and neutron diffraction patterns, qualitatively evaluate sensitivity to variations in crystallographic parameters, and guide experimental for crystal structure solutions.

27: Modulated Structures
Introduction to incommensurate, Vernier and modulated structures where the 230 space group and inadequate.

28: Phase Contrast Atomic Resolution Microscopy to Recognize Crystal Chemical Adaptation
Integrate 3D visualisation, CIF and ATOMS to use JEMS to simulate atomic resolution images and for the design and interpretation of phase contrast images.