Revised Course Code and Title	**MS734M: Crystal Chemistry of Materials (2AUs)**
Course Coordinator	Timothy White
Details of Course	**Rationale for introducing this course** The ability to design, manipulate and validate the crystal chemistry of materials is fundamental to materials science. 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 defect described. The role of nonstoichiometry in controlling functional materials properties will be illustrated for galvanic cells, sensors, catalysts and environmental remediation.
	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: • Find crystal structure databases accessible and be able to interpret Crystallographic Information Files (CIFs); • Understand orderly variations in atomic and ionic radii and exploit these systematics to design materials; • Know the characteristics and crystal chemical diversity of simple crystal structure families; • Predict the changes in crystal structures when perturbed by changes in temperature, pressure and chemistry; • Recognize the types of nonstoichiometric adaptations and the mechanism for incorporating these in crystal structures; • Critically read authentic texts describing nonstoichiometric functional materials.
	Course Syllabus (Refer to Page 2 and 3) MODULE 1: PRINCIPLES AND ADAPTATION MODULE 2: VARIATION AND NONSTOICHIOMETRY
Assessment	Components are assessed Individually 2 x Continuous Assessment — *50%* 1 x Essay — *50%* Total: 100 %
To be offered with effect from (state Academic Year and Semester)	Semester 1, academic year 2016-2017
Any Duplication of Course	NIL
Cross Listing (if applicable)	*N/A*

<table>
<tr><td>Prerequisites (if applicable)</td><td colspan="2">NIL</td></tr>
<tr><td>Preclusions (if applicable)</td><td colspan="2">NIL</td></tr>
<tr><td>Mode of Teaching & Learning
(Lectures, regular tests, Q&A, problem-based learning)</td><td colspan="2">Lectures, expert interviews, MCQ, tutorials, authentic texts, peer discussion</td></tr>
<tr><td>Basic Reading List
• Compulsory Reading - NIL
• Supplementary Reading</td><td colspan="2">1. Crystals and Crystal Structures (2006) by Richard J. D. Tilley
2. Foundations of Crystallography with Computer Applications (2014) by Maureen M. Julian
3. Inorganic Structural Chemistry (1993) by Ulrich Müller</td></tr>
<tr><td>Maximum Class Size</td><td colspan="2">30</td></tr>
<tr><td>Hours of Contact/Academic Units</td><td colspan="2">26 hours/ 2 AUs</td></tr>
<tr><td rowspan="2">Workload Per Week
(The workload for a 3-AU course must add up to 39 hours of contact hours)</td><td>Lecture hours per week
Tutorial hours per week</td><td>2 hours</td></tr>
<tr><td>Total hours</td><td>26 hours</td></tr>
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Course Syllabus
The following topics will be covered:

MODULE 1: PRINCIPLES AND ADAPTATION

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 and the 230 Space Groups
The symmetry operations found in space symmetry are described and 230 space groups reviewed. Enantiomers will illustrate the role of symmetry in atomic positioning.

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

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

5: Atomic and Ionic Radii
Systematic changes in atomic and ionic radii as a function of atomic number, valence and co-ordination.

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

7: Crystal Structure Families
The use of crystal structure families to simplify and systematize hundreds of crystal structures will be taught.

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

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

Module 2: Variation and Nonstoichiometry

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

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

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

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

14: 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.

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

16: 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.

17: Nonstoichiometric Functional Materials
Mechanisms by which nonstoichiometry functionalizes galvanic cells, sensors, catalysts and environmental remediation will be explained

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